

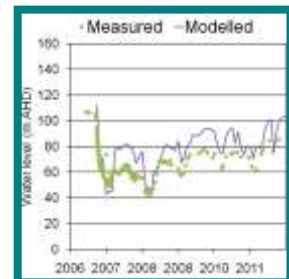
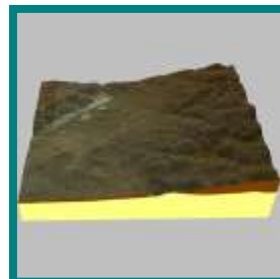


Australian Government
National Water Commission

Australian groundwater modelling guidelines

**Sinclair Knight Merz and
National Centre for Groundwater Research
and Training**

Waterlines Report Series No. 82, June 2012



Waterlines

A SERIES OF WORKS COMMISSIONED BY THE
NATIONAL WATER COMMISSION ON KEY WATER ISSUES

Waterlines

This paper is part of a series of works commissioned by the National Water Commission on key water issues. This work has been undertaken by Sinclair Knight Merz and the National Centre for Groundwater Research and Training on behalf of the National Water Commission.

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Abbreviations and acronyms

1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
4D	four-dimensional
A	cell or element size
ADE	advection dispersion equation
asl	above mean sea level
ΔH	the range of measured heads across the model domain
Δt_c	critical time step
h	head or modelled head
h calc	head calculated by a groundwater model
h _f	freshwater head
h _i	saline head
h obs	head measured in an observation well
g	acceleration due to gravity
GIS	geographic information system
GUI	graphical user interface
J(u)	objective function
m	metres
MAP	maximum a posteriori
MSR	mean sum of residuals
NCGRT	National Centre for Groundwater Research and Training
NRETAS	(the Department of) Natural Resources, Environment, the Arts and Sport
ρ_i	saline density
ρ_f	freshwater density
R	recharge

RMS	root mean squared error
SKM	Sinclair Knight Merz
SMSR	scaled mean sum of residuals
SRMS	scaled root mean squared error
Sy	specific yield
T	transmissivity
TDS	total dissolved solids
TVD	total variation diminishing
Wi	weights between 0 and 1
WLSE	weighted least squares estimation
z	elevation of a node
zhi	measurements of head

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Executive summary

The objective of the *Australian groundwater modelling guidelines* is to promote a consistent and sound approach to the development of groundwater flow and solute transport models in Australia. It builds on existing guidelines (Murray–Darling Basin Commission 2001) that have been adopted throughout Australia in recent years. While it is acknowledged that the term groundwater modelling refers to a variety of methods, the guidelines focus on computer-based numerical simulation models. The guidelines should be seen as a point of reference and not as a rigid standard. They seek to provide direction on the scope and approaches common to modelling projects. The continual evolution of modelling techniques through adaptation and innovation is not only acknowledged, but encouraged. It is recognised there are other approaches to modelling not covered in these guidelines and that such approaches may well be appropriate and justified in certain circumstances.

The guidelines promote an approach to model development that is underpinned by a progression through a series of interdependent stages with frequent feedback loops to earlier stages. Figure ES-1 illustrates the process.

In the **planning** stage the modellers and key stakeholders should agree on various aspects of the model and the process leading to its development. The process should document the agreed modelling objectives and the model's intended use in contributing to or providing certain outcomes required by the larger project. The model confidence-level classification should be addressed at this stage. The classification is a benchmark that illustrates the level of confidence in the model predictions and generally reflects the level of data available to support model development, the calibration process and the manner in which the predictions are formulated.

Conceptualisation involves identifying and describing the processes that control or influence the movement and storage of groundwater and solutes in the hydrogeological system. The conceptualisation should consider the physical processes and resulting heads and flows of groundwater. In this regard it provides information on how the project is expected to impact on the groundwater and the surface water bodies that depend on groundwater. The conceptual model must explain (qualitatively and quantitatively) all observed groundwater behaviour in the region. The guidelines encourage regular reassessment of the conceptual model at all stages of the project, with refinements made as other stages of the process suggest that these may be appropriate or necessary. In many cases the conceptual model may not be unique (i.e. different conceptual models can explain all observations) and it is encouraged to propose and maintain alternative conceptualisations for as long as possible through the modelling project. In some cases this may lead to the development and use of alternative numerical models.

The **design and construction** stage involves a series of decisions on how to best implement the conceptualisation in a mathematical and numerical modelling environment. The decisions required at this stage include selection of a numerical method and modelling software, selection of an appropriate model dimension, definition of a model domain and the spatial and temporal discretisations to be used in the model. The guidelines encourage modellers to take a pragmatic approach to these issues and to explore simple modelling options where these may be appropriate. For example, they encourage the consideration of two-dimensional (2D) rather than 3D models and consideration of steady state rather than transient models where these simpler approaches may be adequate to address the modelling objectives.

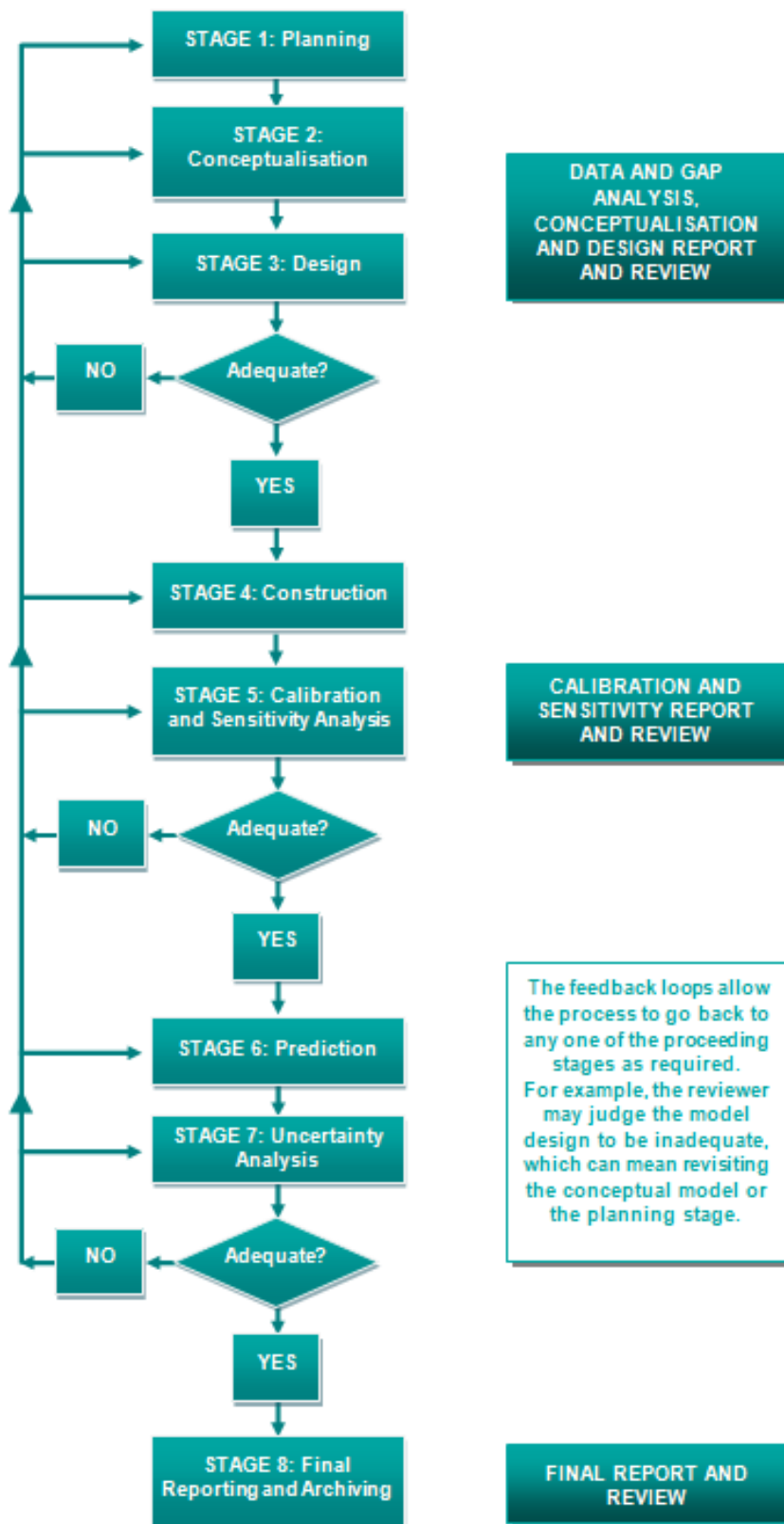


Figure ES 1: Groundwater modelling process (modified after MDBC 2001 and Yan et al. 2010)

Model calibration involves an iterative process to estimate parameters describing hydrogeological properties and boundary conditions so that the model's results closely match historical observations. The guidelines encourage the use of as many different datasets as possible for calibration. Calibration can be achieved through a manual trial-and-error process or through an automated parameter-fitting procedure. The challenge is to find parameter values that allow a model to fit historical measurements, while preparing a model for use in predictions. A balance is needed between simplicity and complexity.

Predictive scenarios are designed to answer the questions posed in the modelling objectives. They are run with various levels of applied stresses that represent anticipated changes from the implementation of the project. The guidelines provide advice on how the climatic, pumping and drainage stresses might be implemented in the predictive scenarios. The guidelines encourage the acknowledgement of uncertainty and suggest methods to formulate predictions in which uncertainties are minimised.

Because models simplify reality, their outputs are **uncertain**. Model outputs presented to decision-makers should include estimates of the goodness or uncertainty of the results. Linear methods for calculating uncertainty are less computationally intensive than non-linear methods. For many decisions, linear methods are sufficient to convey expectations of uncertainty. Presentation of uncertainty results, regardless of the methods used, should include a visual depiction that the model prediction is more than a single result or set of results, and a presentation of uncertainty that most directly addresses the decision of interest.

Model reporting encompasses documentation and communication of different stages of the model through a written technical document. The report should describe the model, all data collected and information created through the modelling process. The report should be accompanied by an archive of all the model files and all supporting data so the results presented in the report can, if necessary, be reproduced and the model used in future studies.

The guidelines suggest that the **model review** process should be undertaken in a staged approach, with separate reviews taking place after each reporting milestone (i.e. after conceptualisation and design, after calibration and sensitivity, and at completion). Three levels of review are suggested: a model appraisal by a non-technical audience to evaluate model results; a peer review by experienced hydrogeologists and modellers for an in-depth review of the model and results; and a post-audit, a critical re-examination of the model when new data is available or the model objectives change. Examples of review checklists are provided for model appraisal and model review.

The guidelines include a detailed description of **solute transport modelling** where the solute of interest is non-reactive, and for problems relating only to groundwater flow and storage. These investigations involve additional difficulties and complexities and require special considerations. The guidelines promote a staged approach to model development with a step-wise increase of model complexity. They recommend the use of approximate calculations, analytical models and particle-tracking estimates before the development of a comprehensive numerical solute transport model.

Modelling of **surface water–groundwater interaction** requires knowledge of groundwater modelling, and an understanding of the exchange processes that occur between surface water and groundwater. These interactions can sometimes be adequately represented using boundary conditions in a groundwater-flow model while in others it is necessary to link or couple surface hydrological models with groundwater models, so that exchange of water and solutes can be computed between both models. In these type of mathematical representations, issues of scale, spatial and temporal discretisations, and head and flow variability are very important. The lag between groundwater abstraction and impacts on river baseflow can be tens of years, while event-based variations in surface water flows are of the order of minutes to weeks in duration.

1 Introduction

In this chapter:

- Overview
- Structure of the guidelines
- Need for and use of the guidelines
- What are the groundwater models?
- Fundamentals of groundwater
- The modelling process.

1.1 Overview

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 (refer section 1.5.5 and Chapter 7).

These guidelines are intended as a reference document for groundwater modellers, project proponents (and model reviewers), regulators, community stakeholders and model software developers who may be involved in the process of developing a model and/or modelling studies.

The guidelines provide the non-specialist modeller with a view of the scope of the model development process (e.g. when reviews and reports are required) and highlight key guiding principles relating to the modelling process. For the specialist groundwater modeller, the guidelines provide best-practice guidance on topics such as conceptualisation, model design, calibration and uncertainty analysis to create greater consistency in approaches. Importantly, they seek to provide a common terminology that can be adopted by all stakeholders typically involved in modelling projects.

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.

1.2 Structure of the guidelines

The structure of the guidelines reflects the modelling process proposed in section 1.6 (evident through comparison with the process diagram in Figure 1-2).

Chapter 2 contains an overview of the planning process and highlights the importance of gaining early agreement on modelling objectives and intended uses of the model. Chapter 3 describes the process of creating one or more conceptual models that describe the key groundwater-related processes and architecture of the groundwater system. Chapter 4 provides an overview of the model design and construction process. The calibration and sensitivity analysis process is described in Chapter 5, with an outline of the performance measures that can be used to judge the quality calibration. A series of approaches to model predictions is provided in Chapter 6. Chapter 7 contains an overview of concepts and approaches to the analysis of predictive uncertainty (with more introductory material in this Introduction). The importance of effective presentation of model results during reporting is highlighted in Chapter 8, and Chapter 9 contains a recommended approach to model review.

The guidelines include two focus topics that are important applications of groundwater models:

- the modelling of conservative solutes in the saturated zone (Chapter 10 Focus topic: Solute transport)
- the modelling of the interaction between surface water and groundwater bodies (Chapter 11 Focus topic: Surface water–groundwater interaction).

As both of these focus areas involve stages of development that are similar to and interdependent with the development of groundwater flow models, these sections should be read in conjunction with other chapters of the guidelines that refer specifically to the individual stages of the modelling process.

Throughout the guidelines key statements or paragraphs (of particular importance or interest) are presented in boxes for added emphasis. Each chapter also highlights:

- a set of numbered **guiding principles** for the associated stage in the modelling process (provided as a list at the start of each chapter and in individual highlight boxes within relevant sections of the chapter—see example below)

Guiding Principle 2.1: The modelling objectives

- **examples** of concepts or principles (numbered consecutively within each chapter and provided in plain text boxes—see example below)

Example 2.1: Typical model exclusions

- numbered **information boxes** containing caution notes or useful additional information—see example below

Box 1A: **CAUTION** regarding model extent

An annotated bibliography of other modelling guidelines and standards is provided in Appendix A.

1.3 Need for and use of the guidelines

The development of a groundwater model is a complex process and not free of subjective choices. During the past decade the Australian groundwater modelling community has benefitted from the *Groundwater flow modelling guidelines* developed for the Murray–Darling Basin Commission (MDBC) in 2001 (MDBC 2001). However, the evolution of new approaches to modelling processes since the publication of the 2001 guidelines, and the use of models in Australia extending beyond the Murray–Darling Basin, instigated the National Water Commission to initiate the development of these new guidelines that incorporate contemporary knowledge and approaches for environments and applications encountered nationally.

Box 1A: Role of the guidelines

These guidelines are a point of reference for best practice for all those involved in the development, application and review of groundwater models, and those who use the outputs from models. It is anticipated that the guidelines will be adopted by regulatory bodies, modellers, reviewers and proponents of groundwater models as a nationally consistent guide to groundwater modelling.

The guidelines are not intended to prescribe a particular approach to modelling. Groundwater modelling is an active field of research and developments are driven by the need for better process descriptions, newly encountered management issues and expanding computing capabilities. The content represents a reasonably comprehensive summary of what is considered good practice in groundwater modelling, based on historic and current literature and the experience of a variety of practitioners involved in the development of the guidelines.

The guidelines recognise there are other approaches to modelling that can also be considered as best practice but may not be covered by these guidelines. It is acknowledged that these other approaches will be appropriate and justified in certain circumstances. The continual evolution of modelling techniques through adaptation and innovation is not only acknowledged but encouraged.

The guidelines should be reviewed and updated regularly (about every five years) to take account of the changing questions being asked of modelling, the development in software and shifts in modelling approaches.

Box 1B: Limitation

These guidelines are not regulation or law, as they have not received endorsement from any jurisdiction. They should not be considered as de facto standards, as they are likely to evolve with modelling requirements and the sophistication of modelling approaches (modified after MDBC 2001).

1.4 What are groundwater models?

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. The guidelines do not aim to provide guidance on physical models, although some aspects may be applicable.

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.

The authors of the guidelines considered whether it was feasible to provide a comprehensive list of model codes and software packages. The principal benefit associated with frequent reference to model codes in the document is that the different attributes of individual codes can be discussed and guidance provided on the relative strengths and weaknesses of particular modelling products. The difficulty with references to codes in guidelines is that software changes frequently (every year) and features that appear in one version may not be available in another. It is also difficult to create a comprehensive list without a rigorous review of available software packages.

The guidelines include limited reference to specific software packages. The evaluation of specific software packages is therefore beyond the scope of these guidelines.

1.5 Fundamentals of groundwater and modelling

1.5.1 Groundwater flow

Groundwater is water that occurs in pores and fractures in soil and rock below the watertable. Formally, the watertable (sometimes referred to as the phreatic surface) is defined as the level at which the water pressure equals the atmospheric pressure. In a less formal sense, the watertable can be thought of as a surface at the boundary between the saturated and the unsaturated zone. In the saturated zone, the pores and fractures are filled with water only, whereas in the unsaturated zone, the pores are filled with both water and air. The water in the unsaturated zone is often referred to as soil water.

By measuring water levels in the subsurface, the direction of groundwater flow can be determined. The term water level requires careful definition. The water level in a well or borehole that is installed (i.e. it has a screen, or open interval) across or just below the watertable will indicate the position of the watertable. However, a well or borehole that is installed at a depth below the watertable is likely to indicate a different level than the watertable. This water level is called the **hydraulic or piezometric head** (or simply head) and is the most fundamental quantity in the analysis of groundwater flow. The hydraulic head expresses the energy (potential energy) of the groundwater per unit weight and thereby influences the direction of groundwater flow: flow occurs from regions of high hydraulic head to areas of low hydraulic head. This concept applies in most (if not all) hydrogeologic situations, but the determination of flow direction becomes more complicated when there are significant spatial differences in groundwater density (e.g. due to variable temperature and or salinity of the water).

Broadly speaking, the subsurface is subdivided into hydrostratigraphic units that have similar properties from the point of view of storage and transmission of groundwater. Units that store significant amounts of water and transmit this water relatively easily are called aquifers. Units that offer a high resistance to flow are called aquitards, or confining layers.

Aquifers are broadly categorised as being either confined or unconfined. Confined aquifers are bounded at the top by an aquitard. The water level in a well that penetrates a confined aquifer will rise to a level that is higher than the top of the aquifer (Figure 1-1). If the hydraulic head is so high that the water level rises above the elevation of the land surface, the aquifer is said to be artesian. By measuring the hydraulic head in multiple wells within a confined aquifer and contouring the measured water-level elevations, an approximate piezometric surface is obtained.

Unconfined or phreatic aquifers are usually found near the ground surface. An aquifer in which the watertable is located is called a watertable (or phreatic) aquifer. If there is no vertical flow, the watertable and the hydraulic heads in a phreatic aquifer coincide. If there is infiltration, the watertable will be higher than the hydraulic head that is measured in the deeper parts of the aquifer. If there is upward flow, for example, near a discharge feature such as a river, the watertable will be lower than the hydraulic head in the deeper parts of the aquifer.

Transient groundwater models (models that simulate changes in heads and flows over time) need to be able to calculate changes in groundwater storage. Confined and unconfined aquifers differ fundamentally in the way they release water from storage. In unconfined aquifers water enters and leaves storage as the watertable rises and falls in the pore spaces. When the water level drops, pores desaturate, and when the water level rises, air-filled pores become saturated. Comparatively, in confined aquifers the pores are all filled with water at all times. This means that changes in stored water volume can occur primarily by compression (or expansion) of water and the aquifer matrix (consolidated and unconsolidated rock). The relative contributions to changes in storage provided by the compressibility of the groundwater and the aquifer matrix vary with geological setting. Deformation of water and matrix also occurs in unconfined aquifers, but the associated changes in volume are much smaller than those brought about by draining and filling pore space that occurs as the watertable elevation changes.

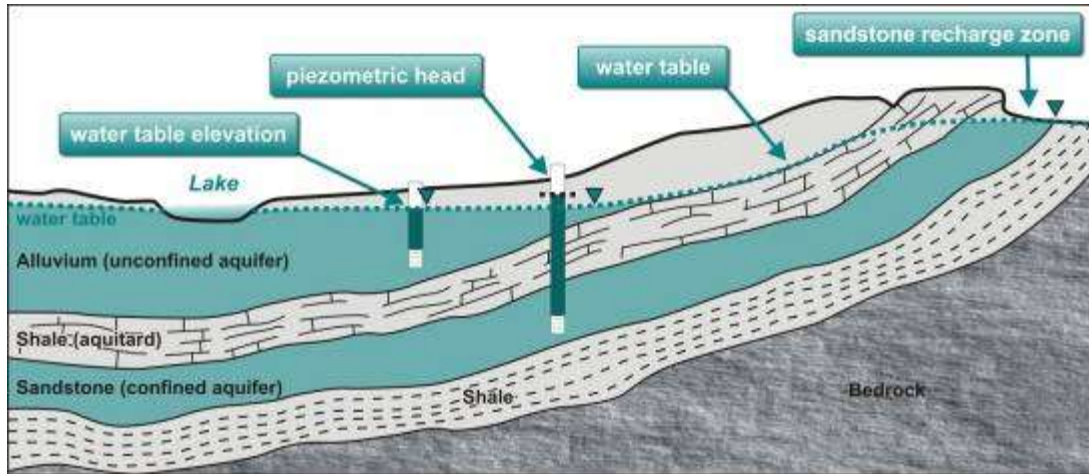


Figure 1-1: A schematic cross-section showing a groundwater system with unconfined and confined aquifers, and connectivity between a surface water body (a lake) and the shallow groundwater

Note that the confined aquifer is unconfined in the recharge area. (Figure modified after a version provided by NTEC Environmental Technology)

Groundwater can be connected with surface water bodies such as lakes and rivers or the ocean. Similar to flow within an aquifer, the flow between surface and groundwater bodies occurs from areas of high head to those of low head. Along the length of a river there may be areas where the river loses water to the groundwater system and where it gains water from the groundwater system. Other processes affecting groundwater systems include recharge from rainfall infiltration, evapotranspiration, pumping of groundwater from wells, atmospheric pressure variations and tidal oscillations. In groundwater modelling, these and similar processes are referred to as **stresses**.

Groundwater models require that the water storage and transmission properties of the subsurface are expressed in quantitative terms. The storage properties are:

- **Porosity:** The total porosity expresses the volume of pores as a fraction (or percentage) of the total aquifer volume. It measures the maximum amount of water that can be stored in a hydrostratigraphic unit.
- **Specific yield:** The specific yield expresses the volume of water that is released per unit of watertable drop per unit surface area. Specific yield is less than the porosity, as some water is retained by the aquifer matrix against the force of gravity. Specific yield is only applicable in an unconfined aquifer.
- **Storativity:** The storativity (or storage coefficient) of a hydrostratigraphic unit expresses the volume of water that is released per unit of hydraulic head drop per unit surface area due to the compressibility of water and the deformation of the aquifer matrix. In unconfined aquifers water is gained to and released from storage through the filling and draining of the aquifer pores and the storativity is referred to as the specific yield. The numerical values of the specific yield generally are several orders of magnitude larger than those of the storativity in confined aquifers.
- **Specific storage** is the storativity divided by the saturated thickness of a hydrostratigraphic unit.

The term **hydraulic conductivity** is a measure of the ease with which water can be transmitted through a geological material. In nature, there can be very strong variations of the hydraulic conductivity in space (this is called **heterogeneity**). Hydraulic conductivity can be different in one direction than in another (this is called **anisotropy**). Related transmission properties are:

- **Transmissivity:** This is the product of the hydraulic conductivity and aquifer thickness.
- **(Vertical) hydraulic resistance:** This is the resistance against flow experienced by water moving vertically through or between hydrostratigraphic units. It is mostly used in the description of vertical flow between aquifers, through aquitards. Hydraulic resistance increases with aquitard thickness and decreases with aquitard hydraulic conductivity. The inverse of hydraulic resistance is the hydraulic conductance.

1.5.2 Solute transport

Solutes in groundwater are generally transported by flow. This process is termed advection (or sometimes, convection). Besides being carried by groundwater flow, solutes move from regions of high solute concentration to regions of low solute concentration in a process known as diffusion. Even if there is no groundwater flow, solutes are transported through a groundwater system if spatial concentration differences exist.

The quantitative expressions of groundwater flow and solute transport processes are, for all practical purposes, ‘macroscopic’ descriptions. That is, they describe the overall direction and rate of movement of a parcel of groundwater and the solutes contained therein, but they do not resolve the complex flow paths at the microscopic scale. The spreading of solutes that occurs due to microscopic flow variations is called dispersion. Dispersion also occurs due to the spatial variability of the hydraulic properties of the subsurface. The hydraulic conductivity representation in models is an approximation of the ‘true’ hydraulic conductivity distribution and thus the model does not directly capture all of the solute spreading that occurs in reality. Dispersion and diffusion cause solute spreading both parallel and perpendicular to the flow direction.

Solute concentrations can also change as a result of interaction with other solutes, with aquifer material through degradation or decay, and through mass transfer between the four commonly described phases (dissolved, vapour, sorbed (solid) and liquid (separate)).

Groundwater flow can be affected where significant spatial variation in solute concentration and/or temperature causes significant groundwater density variations. Examples include coastal aquifers or deep aquifers containing waters of elevated temperature like those in the Great Artesian Basin. In some instances, groundwater flow can be driven purely by density differences, such as underneath salt lakes where strong evaporation at the surface results in an unstable density stratification.

1.5.3 Common simplifications

In nature, groundwater flow patterns are complex, and continuously change with time, but for the purposes of modelling, simplifications are required.

One important consideration in the description of flow processes relates to the temporal variability of the flow. A system is said to be in a steady state when the flow processes are (at least to a good approximation) constant with time. The inflows to and the outflows from the system are equal and, as a result, there is no change in storage within the aquifer. This also means that the heads and watertable elevation do not change with time. When the inflows term and outflows term differ, the total amount of water in the system under consideration changes, the heads and watertable elevation are changing with time and the system is described as being in an unsteady, or transient, state.

Simplifying assumptions regarding the direction of flow in aquifers and aquitards are often made to reduce the complexity for the purposes of mathematical analysis of the flow problem (both for steady state and unsteady state systems). One of these is that the flow in the aquifer is strictly horizontal, and that flow in aquitards is vertical. These assumptions are based on the observation that horizontal head gradients in aquifers are usually much greater than vertical gradients, and that the flow through aquitards tends to be along the shortest possible flow path. The use of this simplifying assumption has led to a method known as the quasi 3D approach in groundwater modelling. It is suited for the description of regional flow when the hydraulic conductivities of aquifers and aquitards differ by a factor of 100 or more. It must be used with caution for local scale problems, or where the thickness of the aquifer is substantial and resolution of the vertical flow and vertical hydraulic gradients is required. Alternative modelling methods that allow vertical flow in aquifers through the use of multiple aquifer model layers and the explicit representation of the aquitards are also commonly used and can be considered as a fully 3D approach.

1.5.4 Flow and solute transport modelling

The fundamental relationships governing groundwater flow and solute transport are based on the principle of mass conservation: for an elementary control volume, the change in storage of water or solute mass within the volume equals the difference between the mass inflow and outflow. This principle can be expressed in mathematical terms and combined with the empirical laws that govern the flow of water and solutes in the form of differential equations. The resulting differential equations can be solved in two ways:

- **Using techniques of calculus.** The resulting analytical models are an exact solution of the governing differential equation. Many simplifying assumptions are needed to obtain an analytical solution. For example, the decline in groundwater level can be determined at a given distance from a single, fully penetrating well pumping at a constant rate in a homogeneous aquifer of constant thickness. Analytical models exist for a wide range of hydrogeological problems. Natural systems incorporate complexities that, depending on the scale of the study, may violate the simplifying assumptions of analytical models. Examples include spatial variation of hydraulic or transport properties, complex geometry associated with rivers or coastlines, spatial and temporal recharge and evapotranspiration variability.
- **Using numerical techniques.** In numerical models, space and time are subdivided into discrete intervals and the governing differential equations are replaced by piecewise approximations. Heads and solute concentrations are calculated at a number of discrete points (nodes) within the model domain at specified times. Numerical models are used when spatial heterogeneity and/or temporal detail are required to adequately describe the processes and features of a hydrogeological system.

In both cases, conditions at the model boundaries, and for time-dependent problems at the start of the simulation, need to be defined to solve the differential equations. This is done by specifying boundary conditions for heads and/or fluxes and initial conditions for heads (and/or solute concentrations). The combination of the governing equations, the boundary and initial conditions, and the definition of hydrogeological parameters required to solve the groundwater flow and solute transport equations is what is referred to as the mathematical model.

Analytical models are usually solved quickly, but require more simplifying assumptions about the groundwater system. Numerical models enable more detailed representation of groundwater systems, but typically take longer to construct and solve. Analytic element models are a category of models that superimpose analytic expressions for a number of hydrologic features, and thus provide increased flexibility compared to analytical solutions of single features. However, they are still not as versatile as numerical models. Analytical and numerical models can each be beneficial, depending on the objectives of a particular project.

Most of the information included in these guidelines relates to numerical groundwater models. There are two primary reasons for this emphasis:

- First, the use of numerical modelling in the groundwater industry has been expanding more rapidly than the use of analytical techniques. This has largely been brought about by increased computational power, solution techniques for the non-linear partial differential equations, and the development of user-friendly modelling software.
- Second, the level of system complexity that can be considered in a numerical model exceeds that of analytical and analytic element models. Therefore, more detailed discussion is required to adequately cover numerical models.

1.5.5 Uncertainty associated with model predictions

Model predictions are uncertain because models are built on information constraints and because the capacity to capture real-world complexity in a model is limited.

In many cases results from models are presented in a way that suggests there is one right answer provided by the model, such as the presentation of a single set of head contours or hydrographs for a particular prediction. However, it is more useful (and correct) to show that all model predictions contain uncertainty and that, given the available data, there is a distribution or range of plausible outputs that should be considered for each model prediction.

Open and clear reporting of uncertainty provides the decision-maker with the capacity to place model outputs in the context of risk to the overall project objectives.

Uncertainty can be handled in different ways. A manager may accept the level of prediction uncertainty that is estimated and make decisions that reflect an acceptable level of risk stemming from that uncertainty. It may be possible to reduce the level of uncertainty by gathering more data or taking a different modelling approach.

Example 1A: Handling uncertainty

Uncertainty is commonly handled in everyday life such as with concepts of probability used in weather forecasts. Another common approach to handling uncertainty is an engineering safety factor. For example, the parameter hydraulic conductivity is intrinsically variable and has some scale dependence in the natural world. Therefore, exact predictions of how much a pump will discharge is uncertain. Yet a decision on what size pipe is needed to convey the pump's discharge is decided in the context of well-defined thresholds that are set by manufacturing standards. Therefore, in cases where the capacity of a standard pipe may be exceeded, the intrinsic uncertainty of the pump discharge can be handled by incurring slightly larger costs with use of a larger pipe diameter. Such a safety factor approach will likely be more effective and cost-efficient than detailed characterisation of the sediments around the well screen and sophisticated uncertainty analyses. However, if the goal of the analysis is to protect a public water supply, effective and cost-efficient hydraulic capture of a contaminant plume using pumping wells requires a more detailed uncertainty analysis to ensure that the system functions as intended and the public protected.

A discussion of concepts and approaches for estimation of uncertainty associated with model predictions is provided in Chapter 7. While the description of uncertainty analysis is presented in these guidelines as a single chapter, the models most suited for decision-making are those that address the underlying sources of uncertainty, and the effect of model simplifications on uncertainty, throughout the entire modelling process.

Potential sources of uncertainty can be assessed during conceptualisation once the modelling objectives, predictions and intended use(s) of the model have been agreed. The complexity in the groundwater system is characterised during conceptualisation, and decisions are made on how to simplify the representation of the system prior to model design and construction. Different sources of uncertainty are explored further during parameterisation and calibration. Parameter distributions (and other model inputs) are characterised at this stage, possibly for multiple conceptual models and designs.

Once the predictive modelling stage is reached the modelling team will have a view of how the potential sources of uncertainty will influence the predictions. This view can be supported by qualitative or quantitative assessments of uncertainty, as described in Chapter 7.

The level of effort applied to uncertainty analysis is a decision that is a function of the risk being managed. A limited analysis, such as an heuristic assessment with relative rankings of prediction uncertainty, or through use of the confidence-level classification, as described in section 2.5, may be sufficient where consequences are judged to be lower. More detailed and robust analysis (e.g. those based on statistical theory) is advisable where consequences of decisions informed by model predictions are greater. Because uncertainty is an integral part of any model, it is recommended to consider early in the modelling project the level of effort required for uncertainty analysis, the presentation of results and the resources required.

1.6 The 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 1-2) 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.

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. The guidelines recognise that in some cases model calibration is not necessary, for example, when using a model to test a conceptual model.

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** (refer section 1.5) 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.

While the reviewer has primary responsibility for judging whether or not a stage of modelling work has been completed to an 'adequate' standard (and move to the next stage), there is a need to involve the modelling team and model owner in this discussion.

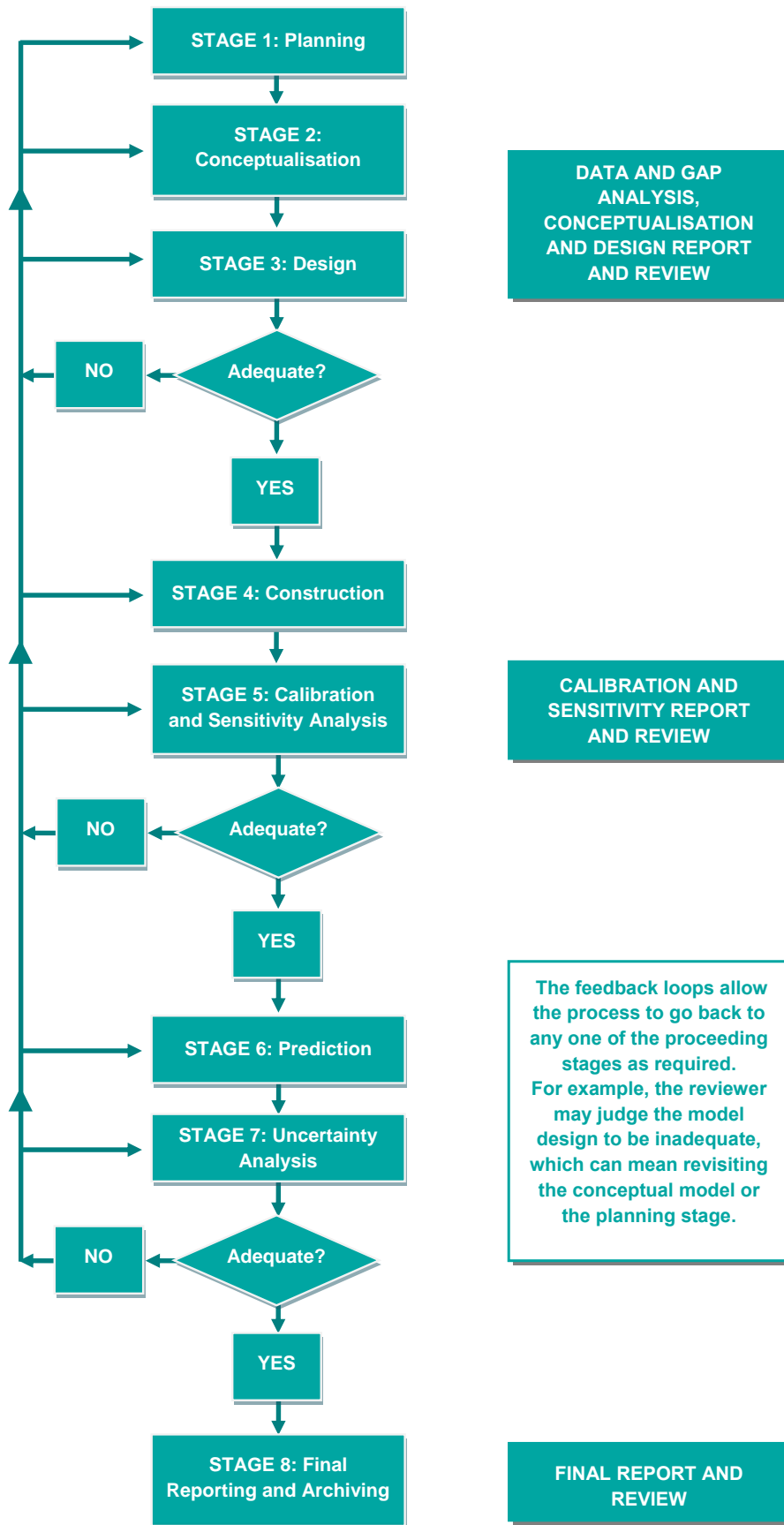


Figure 1-2: Groundwater modelling process (modified after MDBC 2001 and Yan et al. 2010)

2 Planning

In this chapter:

- Introduction
- Intended use of the model
- Defining modelling objectives
- Initial consideration of investigation scale
- Model confidence-level classification
- Defining exclusions
- Review and update
- Model ownership.

Guiding principles for planning a groundwater model

Guiding Principle 2.1: Modelling objectives should be prepared early in a modelling project as a statement of how the model can specifically contribute to the successful completion or progress of the overall project.

Guiding Principle 2.2: The modelling objectives should be used regularly throughout the modelling process as a guide to how the model should be conceptualised, designed, calibrated and used for prediction and uncertainty analysis.

Guiding Principle 2.3: A target model confidence-level classification should be agreed and documented at an early stage of the project to help clarify expectations. The classification can be estimated from a semi-quantitative assessment of the available data on which the model is based (both for conceptualisation and calibration), the manner in which the model is calibrated and how the predictions are formulated.

Guiding Principle 2.4: The initial assessment of the confidence-level classification should be revisited at later stages of the project as many of the issues that influence the classification will not be known at the model planning stage.

2.1 Introduction

This chapter outlines the key issues that need consideration at the planning stage of a project such as how the model will be used, the modelling objectives and the type of model to be developed (e.g. simple analytical or numerical; flow only or flow and solute transport). In general terms, the planning process seeks to determine what is achievable and what is required.

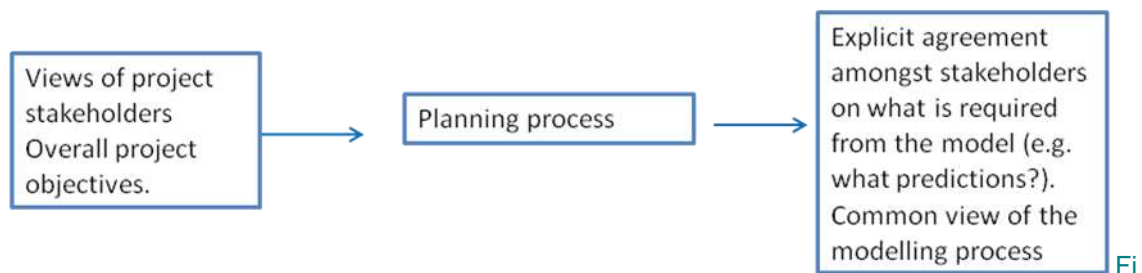


Figure 2-1: The planning process

Planning seeks alignment of expectations of the modelling team, the model owner and other key stakeholders. It provides the basis for a subsequent judgement on whether the model products that are created (e.g. conceptualisation, calibrated model, predictions) are fit for purpose. To this end, the concept of a model confidence level classification is introduced, which provides a means of ranking the relative confidence with which a model can be used in predictive mode. At the planning stage it is recommended that agreement be made on a target confidence level classification (refer to section 2.5) based on the objectives and requirements of the project as well as on the available knowledge base and data from which the model can be developed.

2.2 Intended use of the model

It is never possible for one model to answer all questions on groundwater behaviour. For example, a model designed to simulate regional-scale groundwater flow cannot be expected to predict local-scale groundwater processes (e.g. groundwater interaction with one stream meander loop). Similarly, a local-scale model of impacts of pumping at a single well cannot be extrapolated to predict the drawdown due to development of an extensive borefield in a heterogeneous aquifer. In the planning stage, at the outset of a modelling project it is necessary to clearly understand the intended use of the model so that it can be designed, constructed and calibrated to meet the particular requirements of the problem at hand.

The modelling team must consider how the model will be used. The discussion of the intended use of the model must include not only the final products sought but also confirmation of the specific modelling features that will be used to provide the desired outcomes, as this will affect how the model will be designed and calibrated. It may also consider the manner in which the required outcomes will be obtained from model results, including additional data processing that may be needed to convert the model predictions into a form that can illustrate the particular behaviour of interest.

Example 2.1: How the intended use of the model influences model calibration and data requirements

If a model is required to predict the future impacts of groundwater extraction on river base flow with a high level of confidence, the calibration should include a comparison of calculated groundwater fluxes into the river with measured or estimated fluxes (e.g. as inferred from base-flow analysis).

In some cases the intended model uses may change as a project progresses or after it has been completed. For example, a groundwater flow model may initially be developed to investigate regional water resource management issues. It may subsequently be used as the basis for a solute transport model to investigate water quality issues.

In describing the intended model uses it is appropriate to also provide or consider the justification for developing a model as opposed to choosing alternative options to address the question at hand. In this regard it may be necessary to consider the cost and risk of applying alternative methods.

At this time it is also worth reviewing the historical and geographical context within which the model is to be developed. A thorough review and reference to previous or planned models of the area or neighbouring areas is appropriate.

2.3 Defining modelling objectives

Guiding Principle 2.1: Modelling objectives should be prepared early in a modelling project as a statement of how the model will specifically contribute to the successful completion or progress of the overall project.

Guiding Principle 2.2: The modelling objectives should be used regularly throughout the modelling process as a guide to how the model should be conceptualised, designed, calibrated and used for prediction and uncertainty analysis.

The modelling objectives:

- establish the context and framework within which the model development is being undertaken
- guide how the model will be designed, calibrated and run
- provide criteria for assessing whether the model is fit for purpose and whether it has yielded the answers to the questions it was designed to address.

In general, a groundwater model will be developed to assist with or provide input to a larger project (e.g. an underground construction project, a groundwater resource assessment or a mining feasibility study). Models are developed to provide specific information required by the broader project and will usually represent one aspect of the overall work program undertaken for a particular project.

Often the objectives will involve the quantitative assessment of the response of heads, flows or solute concentrations to future stresses on the aquifer system. However, in some cases the objective may not be to quantify a future response. Rather it may be to gain insight into the processes that are important under certain conditions, to identify knowledge gaps and inform where additional effort should be focused to gather further information.

2.4 Initial consideration of investigation scale

It is necessary to initially define the spatial and temporal scales considered to be important within the overall project scope. The spatial scale depends on the extent of the groundwater system of interest, the location of potential receptors (e.g. a groundwater dependent ecosystem) or the extent of anticipated impacts. The timescale of interest may relate to planning or development time frames, system response time frames (including system recovery such as water-level rebound after mine closure) or impacts on water resources by decadal-scale changes in recharge. Further and more detailed consideration of model scale and extent occurs during the conceptualisation stage (refer Chapter 3) and is confirmed in the design stage of the project (refer Chapter 4).

2.5 Model confidence level classification

Guiding Principle 2.3: A target model confidence level classification should be agreed and documented at an early stage of the project to help clarify expectations. The classification can be estimated from a semi-quantitative assessment of the available data on which the model is based (both for conceptualisation and calibration), the manner in which the model is calibrated and how the predictions are formulated.

Guiding Principle 2.4: The initial assessment of the confidence level classification should be revisited at later stages of the project, as many of the issues that influence the classification will not be known at the model planning stage.

Because of the diverse backgrounds and make-up of the key stakeholders in a typical modelling project, it is necessary to define in non-technical terms a benchmark or yardstick by which the reliability or confidence of the required model predictions can be assessed. The guidelines recommend adoption of confidence level classification terminology.

The degree of confidence with which a model's predictions can be used is a critical consideration in the development of any groundwater model. The confidence level classification of a model is often constrained by the available data and the time and budget allocated for the work. While model owners and other stakeholders may be keen to develop a high-confidence model, this may not be practicable due to these constraints. The modeller should provide advice (based on experience) on realistic expectations of what level of confidence can be achieved.

Agreement and documentation of a target confidence level classification allow the model owner, modellers, reviewers and other key stakeholders to have realistic and agreed expectations for the model. It is particularly important for a model reviewer to be aware of the agreed target model confidence level classification so that it is possible to assess whether or not the model has met this target.

In most circumstances a confidence level classification is assigned to a model as a whole. In some cases it is also necessary to assign confidence-level classifications to individual model predictions as the classification may vary depending on how each prediction is configured (e.g. the level of stress and the model time frame in comparison to those used in calibration).

Factors that should be considered in establishing the model confidence-level classification (Class 1, Class 2 or Class 3 in order of increasing confidence) are presented in Table 2-1. Many of these factors are unknown at the time of model planning and, as such, the guidelines recommend reassessing the model confidence-level classification regularly throughout the course of a modelling project. The level of confidence typically depends on:

- the **available data** (and the accuracy of that data) for the conceptualisation, design and construction. Consideration should be given to the spatial and temporal coverage of the available datasets and whether or not these are sufficient to fully characterise the aquifer and the historic groundwater behaviour that may be useful in model calibration
- the **calibration procedures** that are undertaken during model development. Factors of importance include the types and quality of data that is incorporated in the calibration, the level of fidelity with which the model is able to reproduce observations, and the currency of calibration, that is, whether it can be demonstrated that the model is able to adequately represent present-day groundwater conditions. This is important if the model predictions are to be run from the present day forward

- the **consistency between the calibration and predictive analysis**. Models of high confidence level classification (Class 3 models) should be used in prediction in a manner that is consistent with their calibration. For example, a model that is calibrated in steady state only will likely produce transient predictions of low confidence. Conversely, when a transient calibration is undertaken, the model may be expected to have a high level of confidence when the time frame of the predictive model is of less or similar to that of the calibration model
- the **level of stresses** applied in predictive models. When a predictive model includes stresses that are well outside the range of stresses included in calibration, the reliability of the predictions will be low and the model confidence level classification will also be low.

Table 2-1 provides a set of quantifiable indicators from which to assess whether the desired confidence-level classification has been achieved (i.e. fit for purpose).

In many cases a Class 1 model is developed where there is insufficient data to support conceptualisation and calibration when, in fact, the project is of sufficient importance that a Class 2 or 3 model is desired. In these situations the Class 1 model is often used to provide an initial assessment of the problem and it is subsequently refined and improved to higher classes as additional data is gathered (often from a monitoring campaign that illustrates groundwater response to a development).

In some circumstances Class 1 or Class 2 confidence-level classification will provide sufficient rigour and accuracy for a particular modelling objective, irrespective of the available data and level of calibration. In such cases documentation of an agreement to target a Class 1 or 2 confidence level classification is important as the model can be considered fit for purpose, even when it is rated as having a relatively low confidence associated with its predictions. At this point it is worth noting that there is a strong correlation between the model confidence-level classification and the level of resources (modelling effort and budget) required to meet the target classification. Accordingly, it is expected that lower target-level classifications may be attractive where available modelling time and budgets are limited.

The model confidence-level classification provides a useful indication of the type of modelling applications for which a particular model should be used. Table 2-1 includes advice on the appropriate uses for the three classes of model. A Class 1 model, for example, has relatively low confidence associated with any predictions and is therefore best suited for managing low-value resources (i.e. few groundwater users with few or low-value groundwater dependent ecosystems) for assessing impacts of low-risk developments or when the modelling objectives are relatively modest. The Class 1 model may also be appropriate for providing insight into processes of importance in particular settings and conditions. Class 2 and 3 models are suitable for assessing higher risk developments in higher-value aquifers.

It is not expected that any individual model will have all the defining characteristics of Class 1, 2 or 3 models. The characteristics described in Table 2-1 are typical features that may have a bearing on the confidence with which a model can be used. A model can fall into different classes for the various characteristics and criteria included in Table 2-1.

It is up to the modelling team and key stakeholders to agree on which of these criteria are most relevant for the model and project at hand, and to agree on an overall confidence-level classification that reflects the particular requirements and features of that model. In general, it should be acknowledged that if a model has any of the characteristics or indicators of a Class 1 model it should not be ranked as a Class 3 model, irrespective of all other considerations. It may also be appropriate to provide classifications for each of the three broad sectors included in Table 2-1 (i.e. data, calibration and prediction) based on all characteristics and criteria for that sector. An overall model classification can be chosen that reflects the importance of the individual criteria and characteristics with regard to the model and project objectives. If a model falls into a Class 1 classification for either the data, calibration or prediction sectors, it should be given a Class 1 model, irrespective of all other ratings.

When considering the confidence level classification there is a class of model commonly referred to as a 'generic model' that is worthy of special consideration. These models are developed primarily to understand flow processes and not to provide quantitative outcomes for any particular aquifer or physical location. They can be considered to provide a high level of confidence as their accuracy is only limited by the ability of the governing equations to replicate the physical processes of interest. While they provide high confidence when applied in a general, non-specific sense, if the results are applied to or assumed to represent a specific site the confidence level will automatically decrease. This is because the simplifying assumptions (e.g. the aquifer geometry) implemented in the generic model are highly unlikely to be exactly applicable to the real physical setting.

Example 2.2: Generic groundwater flow model

Consider a groundwater flow model developed to calculate the relationship between groundwater extraction location and the associated impact on base flow in a nearby river. The model may be developed by a regulator in order to help define rules that constrain the location of groundwater extraction in relation to a river to help minimise impacts on river flow. It is intended that the results will be applied to all rivers and aquifers in the jurisdiction. The model is required to assess the phenomena generally within a wide spectrum of aquifer conditions and geometries, and is classed as a 'generic model'.

A target confidence-level classification for the model should be defined at the outset, as subsequent project stages, such as the conceptualisation (refer Chapter 3), design (refer Chapter 4), calibration (refer Chapter 5) and predictive scenario development (refer Chapter 6), are influenced by the confidence-level classification. As the model development progresses, the model confidence-level classification should be reassessed to determine whether the targeted classification has or can be achieved and, if necessary, whether the target classification can be revised. At the completion of the modelling project, it is expected that the model reviewer will assess whether the final model meets the key criteria that define the stated level of confidence classification.

Table 2-1: Model confidence level classification—characteristics and indicators

<i>Confidence level classification</i>	<i>Data</i>	<i>Calibration</i>	<i>Prediction</i>	<i>Key indicator</i>	<i>Examples of specific uses</i>
Class 3	<ul style="list-style-type: none"> • Spatial and temporal distribution of groundwater head observations adequately define groundwater behaviour, especially in areas of greatest interest and where outcomes are to be reported. • Spatial distribution of bore logs and associated stratigraphic interpretations clearly define aquifer geometry. • Reliable metered groundwater extraction and injection data is available. • Rainfall and evaporation data is available. • Aquifer-testing data to define key parameters. • Streamflow and stage measurements are available with reliable baseflow estimates at a number of points. • Reliable land-use and soil-mapping data available. • Reliable irrigation application data (where relevant) is available. • Good quality and adequate spatial coverage of digital elevation model to define ground surface elevation. 	<ul style="list-style-type: none"> • Adequate validation* is demonstrated. • Scaled RMS error (refer Chapter 5) or other calibration statistics are acceptable. • Long-term trends are adequately replicated where these are important. • Seasonal fluctuations are adequately replicated where these are important. • Transient calibration is current, i.e. uses recent data. • Model is calibrated to heads and fluxes. • Observations of the key modelling outcomes dataset is used in calibration. 	<ul style="list-style-type: none"> • Length of predictive model is not excessive compared to length of calibration period. • Temporal discretisation used in the predictive model is consistent with the transient calibration. • Level and type of stresses included in the predictive model are within the range of those used in the transient calibration. • Model validation* suggests calibration is appropriate for locations and/or times outside the calibration model. • Steady-state predictions used when the model is calibrated in steady-state only. 	<ul style="list-style-type: none"> • Key calibration statistics are acceptable and meet agreed targets. • Model predictive time frame is less than 3 times the duration of transient calibration. • Stresses are not more than 2 times greater than those included in calibration. • Temporal discretisation in predictive model is the same as that used in calibration. • Mass balance closure error is less than 0.5% of total. • Model parameters consistent with conceptualisation. • Appropriate computational methods used with appropriate spatial discretisation to model the problem. • The model has been reviewed and deemed fit for purpose by an experienced, independent hydrogeologist with modelling experience. 	<ul style="list-style-type: none"> • Suitable for predicting groundwater responses to arbitrary changes in applied stress or hydrological conditions anywhere within the model domain. • Provide information for sustainable yield assessments for high-value regional aquifer systems. • Evaluation and management of potentially high-risk impacts. • Can be used to design complex mine-dewatering schemes, salt-interception schemes or water-allocation plans. • Simulating the interaction between groundwater and surface water bodies to a level of reliability required for dynamic linkage to surface water models. • Assessment of complex, large-scale solute transport processes.
Class 2 <i>Cont'd overleaf</i>	<ul style="list-style-type: none"> • Groundwater head observations and bore logs are available but may not provide adequate coverage throughout the model domain. 	<ul style="list-style-type: none"> • Validation* is either not undertaken or is not demonstrated for the full model domain. • Calibration statistics are generally reasonable but may suggest significant errors in parts of the 	<ul style="list-style-type: none"> • Transient calibration over a short time frame compared to that of prediction. • Temporal discretisation used in the predictive model is different from that used in transient 	<ul style="list-style-type: none"> • Key calibration statistics suggest poor calibration in parts of the model domain. • Model predictive time frame is between 3 and 10 times the duration of transient calibration. • Stresses are between 2 and 5 times greater than those 	<ul style="list-style-type: none"> • Prediction of impacts of proposed developments in medium value aquifers. • Evaluation and management of medium risk impacts.

<i>Confidence level classification</i>	<i>Data</i>	<i>Calibration</i>	<i>Prediction</i>	<i>Key indicator</i>	<i>Examples of specific uses</i>
Class 2 Cont'd	<ul style="list-style-type: none"> Metered groundwater-extraction data may be available but spatial and temporal coverage may not be extensive. Streamflow data and baseflow estimates available at a few points. Reliable irrigation-application data available in part of the area or for part of the model duration. 	<ul style="list-style-type: none"> model domain(s). Long-term trends not replicated in all parts of the model domain. Transient calibration to historic data but not extending to the present day. Seasonal fluctuations not adequately replicated in all parts of the model domain. Observations of the key modelling outcome data set are not used in calibration. 	<ul style="list-style-type: none"> calibration. Level and type of stresses included in the predictive model are outside the range of those used in the transient calibration. Validation* suggests relatively poor match to observations when calibration data is extended in time and/or space. 	<ul style="list-style-type: none"> included in calibration. Temporal discretisation in predictive model is not the same as that used in calibration. Mass balance closure error is less than 1% of total. Not all model parameters consistent with conceptualisation. Spatial refinement too coarse in key parts of the model domain. The model has been reviewed and deemed fit for purpose by an independent hydrogeologist. 	<ul style="list-style-type: none"> Providing estimates of dewatering requirements for mines and excavations and the associated impacts. Designing groundwater management schemes such as managed aquifer recharge, salinity management schemes and infiltration basins. Estimating distance of travel of contamination through particle-tracking methods. Defining water source protection zones.
Class 1	<ul style="list-style-type: none"> Few or poorly distributed existing wells from which to obtain reliable groundwater and geological information. Observations and measurements unavailable or sparsely distributed in areas of greatest interest. No available records of metered groundwater extraction or injection. Climate data only available from relatively remote locations. Little or no useful data on land-use, soils or river flows and stage elevations. 	<ul style="list-style-type: none"> No calibration is possible. Calibration illustrates unacceptable levels of error especially in key areas. Calibration is based on an inadequate distribution of data. Calibration only to datasets other than that required for prediction. 	<ul style="list-style-type: none"> Predictive model time frame far exceeds that of calibration. Temporal discretisation is different to that of calibration. Transient predictions are made when calibration is in steady state only. Model validation* suggests unacceptable errors when calibration dataset is extended in time and/or space. 	<ul style="list-style-type: none"> Model is uncalibrated or key calibration statistics do not meet agreed targets. Model predictive time frame is more than 10 times longer than transient calibration period. Stresses in predictions are more than 5 times higher than those in calibration. Stress period or calculation interval is different from that used in calibration. Transient predictions made but calibration in steady state only. Cumulative mass-balance closure error exceeds 1% or exceeds 5% at any given calculation time. Model parameters outside the range expected by the conceptualisation with no further justification. Unsuitable spatial or temporal discretisation. The model has not been reviewed. 	<ul style="list-style-type: none"> Design observation bore array for pumping tests. Predicting long-term impacts of proposed developments in low-value aquifers. Estimating impacts of low-risk developments. Understanding groundwater flow processes under various hypothetical conditions. Provide first-pass estimates of extraction volumes and rates required for mine dewatering. Developing coarse relationships between groundwater extraction locations and rates and associated impacts. As a starting point on which to develop higher class models as more data is collected and used.

(*Refer Chapter 5 for discussion around validation as part of the calibration process.)

Example 2.3: Project objectives and modelling objectives related to intended use and confidence level classification

Water resource management model

Project objective: To determine the maximum sustainable extraction from an aquifer.

Intended use: Model outcomes will assist resource managers determine appropriate volumetric extraction rates.

Modelling objective: To provide quantitative estimates of drawdown, loss of baseflow and reduction in water availability to groundwater dependent ecosystems for various levels of groundwater extraction and future climate assumptions.

Target confidence level: Class 3, in keeping with the availability of extensive groundwater data within the area of interest.

Mine-dewatering model

Project objective: To design a dewatering scheme for a planned mine.

Intended use: To estimate the drawdown caused by an array of dewatering wells.

Modelling objective: To determine optimum groundwater pumping (including the rate, the number of bores and their location) required to dewater an open-pit mine.

Target confidence level: Class 1—2 level of confidence due to a lack of useful time series data that can be used for calibration. The level of confidence is expected to increase once mining starts and model validation can be undertaken.

Tunnel construction and operation

Project objective: To assess the environmental impacts of tunnel construction and operation.

Intended use: Predict drawdown and associated loss of baseflow arising from inflows to the tunnel.

Modelling objective: To provide quantitative estimates of the groundwater inflows and associated drawdown during the construction and operation of a new tunnel.

Target confidence level: Class 2, as the available data only allows for a steady state calibration.

2.6 Defining exclusions

In this section the term ‘modelling exclusions’ refers to specific elements of the model that, for any reason, should not be used to generate or report predictive outcomes. In the course of the modelling process, it may be found that specific features or areas of the model have a particularly low level of confidence. This may arise, for example, when the particular application or model area has insufficient reliable data on which to base calibration, when the model code may be unsuitable for a particular application or when the model was not developed for that purpose and hence outcomes are likely to be unreliable. In such cases, it should be noted that certain model outputs are likely to be particularly uncertain and hence should not be relied upon. The modellers should provide an explicit statement of exclusions to help avoid inappropriate model use in the current project, or any future projects that make use of the model.

Although model exclusions may first be identified at the initial planning stage, they will also be defined and confirmed during the course of model development and calibration. Often the modelling exclusions will be accumulated and reported at the completion of the project within a modelling limitations section of the final modelling report. Chapter 8 provides more details on reporting.

Example 2.4: Typical model exclusions

Basement layers. Depressurisation of an aquifer in response to pumping can trigger the release of water from underlying strata into the pumped aquifer. These underlying layers can be explicitly considered in the model to simulate this process. However, often there is no data available in these strata that can be used for calibration purposes. Hence, little or no confidence must be placed on the specific responses predicted in this part of the model.

Aquitards. Aquitards present in a model domain are often represented in a groundwater model as a single model layer with appropriately chosen parameters to reflect their poor transmission characteristics. This configuration does not adequately resolve the vertical hydraulic head distribution across the aquitard. In this case it may not be appropriate to report the predicted groundwater responses in the aquitard (refer to section 4.4.4).

2.7 Review and update

In many modelling projects the conceptualisation, calibration and predictive analysis will be updated and revised as more information becomes available and as modelling results illustrate the need for such revisions. It may be necessary to revise expectations of the confidence levels associated with the model outputs. This may be required if, for example, model calibration is more difficult than expected and the final calibrated model is less constrained than originally envisaged. Conversely, an upgrade in model confidence-level classification is also possible when additional data is obtained that leads to an improvement in the calibration of model parameters.

In some cases the modelling objectives themselves will need to be revised or updated. This is rarely required if the overall project objectives remain unchanged, but may be appropriate if the model is required to address additional issues that may arise during the course of the project or when an existing model is applied in a new project.

2.8 Model ownership

The planning stage is an appropriate time for the modeller and model owner to agree on a number of issues about the future ownership and ongoing maintenance of the model. An agreement on intellectual property is a key aspect that should be understood by both parties at the outset. The discussion should extend to agreement on how the model will be archived, including the data-file formats, the physical location of where model files will be stored, long-term custodianship and third-party access to the model. More information on model archiving can be found in section 8.6.

3 Conceptualisation

In this chapter:

- Introduction
- The principle of simplicity
- Conceptualisation of current and future states
- Alternative conceptual models
- Data collection, analysis and data checking
- Developing the conceptual model
- Checking the conceptual model
- 3D visualisation
- Conceptualisation as an ongoing process
- Reporting and review.

Guiding principles for conceptualisation

Guiding Principle 3.1: The level of detail within the conceptual model should be chosen, based on the modelling objectives, the availability of quality data, knowledge of the groundwater system of interest, and its complexity.

Guiding Principle 3.2: Alternative conceptual models should be considered to explore the significance of the uncertainty associated with different views of how the system operates.

Guiding Principle 3.3: The conceptual model should be developed based on observation, measurement and interpretation wherever possible. Quality-assured data should be used to improve confidence in the conceptual model.

Guiding Principle 3.4: 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.

Guiding Principle 3.5: There should be an ongoing process of refinement and feedback between conceptualisation, model design and model calibration to allow revisions and refinements to the conceptual model over time.

3.1 Introduction

Conceptualisation is a process that provides the basis for model design and communicates how the system works to a wide range of audiences. The conceptual model should be developed collaboratively across relevant disciplines and project stakeholders.

A conceptual (hydrogeological) model is a descriptive representation of a groundwater system that incorporates an interpretation of the geological and hydrological conditions (Anderson and Woessner 1992). It consolidates the current understanding of the key processes of the groundwater system, including the influence of stresses, and assists in the understanding of possible future changes.

This chapter outlines the process of developing a conceptual model as a prelude to designing and constructing a model of the groundwater system, which broadly involves using all existing information to create an understanding of how the system operates (Figure 3-1).

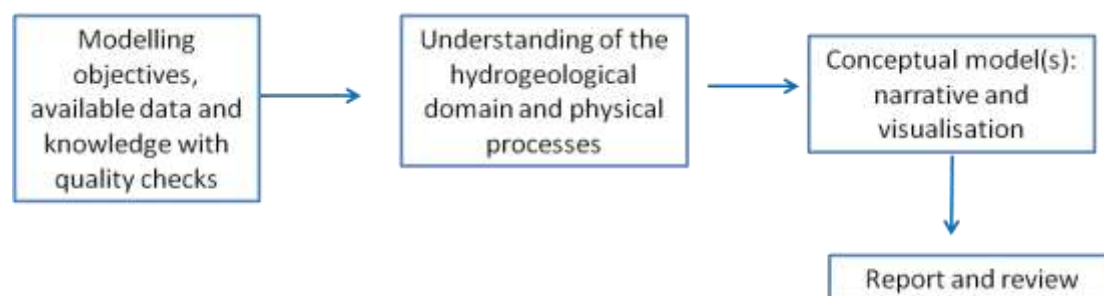


Figure 3-1: Creating a conceptual model

The development of the most appropriate conceptual model is required to ensure that the model activity achieves its objectives. The conceptual model development process may need to include people with a range of skills (modelling, hydrogeology, climate, environmental systems etc.), and represents a key point in the modelling process where a decision to proceed past the conceptual stage is required. It may be the case that it is not possible to proceed in the current format given the state of knowledge of the groundwater system. Some project re-scoping and redesign may also need to occur, irrespective of a decision to proceed.

The following sections provide a series of suggestions about the issues that can arise during the conceptualisation process. Conceptualisation has the potential to embed structural problems in a model from the outset if poor decisions are made—problems that cannot be removed through later parameter optimisation during the calibration stage. If a model is conceptually poor, no amount of calibration can fix it. This is the primary reason for paying strict attention to the conceptualisation process and why it is fundamental to the entire modelling process that the conceptualisation is as close to ‘correct’ as possible, recognising that it is difficult to understand what ‘correct’ looks like (refers Box 3B on conceptual surprise). The guidance below provides some suggestions to enable the project to iterate towards this ‘correct’ conceptual model.

3.2 The principle of simplicity

Guiding Principle 3.1: The level of detail within the conceptual model should be chosen, based on the modelling objectives, the availability of quality data, knowledge of the groundwater system of interest, and its complexity.

When developing conceptual models, there is always a trade-off between realism, generality and precision; it is not possible to maximise all three simultaneously (Levins 1966). The conceptualisation process involves simplifying a groundwater system, which is inherently complex, in order to simulate the system’s key behaviour. This is the principle of simplicity. Levins’s original ideas were developed for population biology models and there are suggestions that they may not equally apply to the more deterministic sciences. This issue is not relevant to this discussion; rather it is the general principle of having to trade off to some degree in the conceptualisation process or, in a more general manner, to be aware that trade-offs may be required. This has been more generally popularised as ‘less is more’ and provides a good philosophy for hydrogeological conceptualisations.

There is no perfect way to simplify a system within a conceptualisation. The only issue is whether the model suffices for the task it is expected to address. Which aspects of the groundwater system should be considered in simplification, and to what level of detail, is dictated by:

- the objectives of the study for which the model is being developed and the target confidence level classification of the model (refer Chapter 2). The objectives influence the lateral and vertical extent of the model domain, what processes will be modelled (e.g. flow, solute transport) and on what timescale they will be investigated. The confidence level classification provides context to the level of detail or complexity that is warranted.
- the amount and quality of the data available on the groundwater system of interest.

Over-simplification or under-simplification of the groundwater system is a common pitfall in the conceptualisation process; typically the consequences of which can be reflected later in terms of poor model performance.

3.3 Conceptualisation of current and future states

Conceptualisation is based on what is known about the system and its responses both under historic stresses and in its current condition. The conceptualisation must be strongly linked to the modelling objectives by providing a view of the possible range of impacts that may occur over the time frame of interest.

For example, the conceptual model could provide a view of current groundwater flow conditions in an area with horticulture, but also describe future changes such as the development of a watertable mound due to increased recharge as a result of irrigation. This future view of the system is a prerequisite for the model design stage (Chapter 2) when questions about the length of model time frame and extent of the model domain are addressed.

3.4 Alternative conceptual models

Guiding Principle 3.2: Alternative conceptual models should be considered to explore the significance of the uncertainty associated with different views of how the system operates.

In some cases uncertainty about the hydrostratigraphy or aquifer heterogeneity, or the influence of key processes (e.g. river–aquifer interactions), may present the need to test more than one conceptual model so that the effect of conceptual (or structural) uncertainty on model outputs can be tested. Multiple conceptual models should be developed where a single conceptual model cannot be identified based on the available data. These should be reviewed during the conceptualisation process and reported accordingly. Depending on the intended model use and the modelling objectives, this may lead to different mathematical models. However, it may not always be possible to generate multiple conceptualisations, or the data may not support the full range of possible interpretations that might be plausible. Often the uncertainty in the conceptualisation translates into the set of model parameters finally settled upon, and hence propagates through calibration and to model predictions.

Ye et al. (2010) provide a discussion of how alternative conceptual models can be evaluated to give insight into conceptual uncertainty. Their work assessed the contributions of conceptual model differences and parametric changes to overall levels of uncertainty and concluded that model uncertainty (i.e. the uncertainty due to differing conceptualisations) contributed at significantly larger levels when compared to that contributed by parametric uncertainty. Interestingly, for their particular suite of conceptual model differences, they found that uncertainty in geological interpretations had a more significant effect on model uncertainty than changes in recharge estimates.

Refsgaard et al. (2012) provide a discussion of strategies for dealing with geological uncertainty on groundwater flow modelling. This paper recognises the contribution that geological structures and aquifer properties makes to model uncertainty. It provides methods for dealing with this issue and discusses the merits of creating alternative conceptual models.

3.5 Data collection, analysis and data checking

Guiding Principle 3.3: The conceptual model should be developed based on observation, measurement and interpretation wherever possible. Quality-assured data should be used to improve confidence in the conceptual model.

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 (refer Chapter 7)
- 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.

Establishing relationships between various datasets is often an important step in the data analysis stage of a conceptualisation. 'Cause-and-effect' (or 'stress response' relationship) assessments can be particularly useful in confirming various features of the conceptualisation.

Example 3.1: A ‘cause-and-effect’ assessment

A comparison of river stage or flow hydrographs with hydrographs of hydraulic heads measured in nearby observation wells can establish whether heads in the aquifer respond to river flow events, and hence if the river and the aquifer are hydraulically connected.

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.

Example 3.2: Data accuracy

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.

3.6 Developing the conceptual model

3.6.1 Overview

In the first instance it is important that an appropriate scale for the conceptual model is decided upon so that a boundary can be placed around the data collection and interpretation activities. The definition of the **hydrogeological domain** (or the conceptual domain) provides the architecture of the conceptual model and aquifer properties, which leads to consideration of the **physical processes** operating within the domain, such as recharge or surface water–groundwater interaction (refer Chapter 11).

3.6.2 The hydrogeological domain

Guiding Principle 3.4: 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 (Chapter 4 provides further advice on design of a model domain and grid).

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 **timescale** (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 (refer Chapter 10)
- 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, drillhole 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 (refer Chapter 7).

Hydraulic properties that should be characterised include hydraulic conductivity (or transmissivity), specific storage (or storativity) and specific yield (section 1.5.1). Parameters pertaining to solute transport specifically are discussed in section 10.4.8.

There are a number of key questions to be answered when compiling information on aquifer and aquitard properties:

- *How heterogeneous are the properties?* In all groundwater systems there is a degree of spatial variation. It is necessary to determine whether the given property should be represented as homogeneous, divided into areas that themselves are homogeneous or distributed as a continuous variable across the model area. It is also important to consider how information is extrapolated or interpolated in the development of a continuous distribution across the conceptual domain. In some cases, the distribution is estimated using contouring software and this can introduce errors into the distribution. When applying automatic contouring methods, resultant distributions should be independently verified as fit for purpose.
- *Is hydraulic conductivity isotropic?* That is, does it have the same magnitude/impact on flow or solute movement in all directions? Again, unless there is access to detailed data, this characteristic is difficult to quantify, and is usually decided by making certain assumptions. These assumptions need to be noted for later model review (refer chapters 8 and 9). Knowledge of the rock formation process and geological history is helpful in understanding the potential for anisotropy.
- *In the case of the unsaturated zone, how do the aquifer properties change with the degree of saturation?* Does the process exhibit hysteresis (i.e. are the parameters dependent on the saturation history of the media)?
- *How are the parameter values quantified?* Estimates of the aquifer properties should ideally be derived from in situ aquifer tests, analysis of drill core material and/or geophysical measurements. In the absence of such information, values used in previous studies or suggested by the literature based on known geology are used and a justification should be provided in the report as to whether these are acceptable. It is preferable in that case to use conservative values, but this depends on the objectives of a particular study. The range of values considered can be reassessed later during a sensitivity analysis (refer section 5.5).
- *At what scale are the parameter values quantified?* Measurements of properties occur at a wide range of scales, and this introduces the need to upscale some of these measurements to apply to the common scale of a conceptual model. This must be considered when combining information to parameterise the model. It must be remembered that all measurements are of value during the conceptualisation process (and at later stages of the modelling process), but they apply to different scales. For instance, consider the scale of permeameter tests, slug tests, aquifer tests, geologic mapping and basin-wide water budget studies. These different scales must be considered when combining information from many sources and over different timescales and periods to define the structure and parameters of the conceptual model.

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 (refer Chapter 11). 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. A more thorough discussion of the specific considerations for modelling surface water-groundwater interactions is provided in Chapter 11.

3.6.3 Physical processes

The processes affecting groundwater flow and/or transport of solutes (refer Chapter 10 for considerations specific to solute transport modelling) 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 (refer Chapter 8).

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 (refer to section on 'stresses' above).

3.7 Checking the conceptual model

There are different approaches to overcome errors/reduce uncertainty in the conceptualisation so that it is adequate to fulfil the modelling objectives with all the available data and resources. Some suggestions include:

- developing preliminary water balances to help with 'sanity checking' of later model results (refer Box 3A for more detail on using water balances)
- experimenting numerically with a variety of conceptual models to compare how well they reproduce reality and choose a preferred conceptualisation accordingly
- discussing the development of the conceptual model with peers and stakeholders.

Box 3A: The water balance

A critical element of the conceptual model is the water balance. That is, answering questions about where water comes from and where it goes can allow the model to be built in a logical manner. A water balance informs the design of a numerical model and the choice of appropriate boundary conditions. A well-constrained conceptual water balance can also aid calibration of a numerical model, providing better confidence in its predictive ability than if it were to be calibrated against hydraulic head data only.

A water balance equation can be used to describe the flow of water into and out of a system. A general formulation of the equation is:

$$\text{Input} = \text{Output} + \Delta\text{Storage}$$

In the case where the system is in steady state the $\Delta\text{Storage}$ term will be equal to zero.

In the context of the conceptualisation of the groundwater processes, 'inputs' are the various sources of recharge and 'outputs' are the various sources of groundwater discharge. The quantification of these components within the constraints of the water balance equation adds a degree of rigour to the conceptualisation.

The water balance can be estimated as a prelude to generating more-detailed knowledge of the system. A semi-quantitative analysis of the water balance provides a useful discipline to, first, define all processes operating in a catchment and second, assess the magnitude of their contribution to the overall hydrologic system. A water balance approach is, by its nature, highly simplified and usually spatially aggregated. An approach to undertaking a semi-quantitative analysis is to define all recharge and discharge processes operating (usually supported by some form of review of the knowledge available for the area of interest), provide estimates of the likely volumes or fluxes involved at an annual scale, and sum these into a water balance. This process will almost certainly be iterative, with successive analysis aimed at closing the error in the water balance.

The water balance equation can (and should) be written at the level of detail as is required, and can relate to the complete flow system or link various components of the flow system. In the end, however, the water balance quantification is a first approximation as it usually involves major assumptions and attempts to approximate complex processes.

The semi-quantitative water balance, or at least the individual components of it, can be useful in constraining the calibrated model at a later stage. Independently derived data such as this, even at a gross scale, can provide confidence during later model evaluation.

A water balance approach at this stage will also highlight where volumetric flow or solute flux rate data is most lacking and/or uncertain and provide useful insight into components that would benefit from increased data collection (for instance, installation of meters on groundwater extraction bores) within the time frame of the model project.

3.8 3D visualisation

Understanding and communicating concepts and results can be enhanced by data visualisation. Three-dimensional analysis of the data (as in interpolation of stratigraphy and water level data for visualisation purposes) can be a component of a hydrogeological conceptualisation in areas where a complex model is required or the groundwater system is itself complex. There are a number of packages available to assist development of both data and visualisation products, including software that interfaces directly with groundwater model codes and allows data input to the model to be automated. In addition, these interfaces allow visualisation of model outputs.

Other packages exist that are more related to data management and visualisation, without being linked to a groundwater model directly. These packages allow data to be interpreted as a hydrogeological conceptual model, with output explicitly forming 3D understandings of the groundwater system. These visualisation outputs are not numerical models, but conceptual models in their own right and are useful tools in communicating with key stakeholders.

Areas where such a visualisation approach can be of benefit are where there are simple geological models that allow complex or voluminous data to be managed in an efficient manner and understandings portrayed much more simply to non-technical audiences. Such an approach will allow better control over model layers and their geometry through the use of features such as automated contouring. However, visualisation packages can be highly automated and control is required by the operator to ensure that package output still makes sense within the context of the conceptualisation and is consistent with the data available.

There are currently no guidelines for the use of these types of tools/packages. The decision of whether to use such visualisation software and which package to use is best left to individual projects. It should be understood that where visualisation approaches are not linked to numerical models, the outputs are not a quantitative description of the hydrogeological system and therefore have no informative value on the water balance.

Data visualisation packages should be used both as an adjunct to hydrogeological conceptualisation and process understanding, and as an aid to data management and organisation. The use of such packages will depend on the overall objectives and available budget. Data visualisation should not be used as a surrogate for a groundwater model, especially if a numerical simulation is required.

3.9 Conceptualisation as an ongoing process

Guiding Principle 3.5: There should be an ongoing process of refinement and feedback between conceptualisation, model design and model calibration such that revisions and refinements to the conceptual model can be made over time.

The model design stage starts once a conceptual model has been reviewed and found appropriate for the problem at hand. The development of the conceptual model is not necessarily a linear process. Preliminary model simulations can be conducted to test elements of the conceptualisation and highlight additional data that may be required.

In this way the conceptualisation process follows an iterative approach based on the interplay between the mathematical model and the conceptual model (Figure 1-2).

As a general rule the conceptual model should be updated, based on insights obtained during the subsequent stages of the modelling process or when additional data becomes available. Difficulties producing a satisfactory calibration might point to mistakes in the data analysis, which lead to the wrong estimation of parameter ranges, misrepresentation of a specific process or lack of detail in the hydrostratigraphy. Lack of calibration may also point to fundamental errors in the original data, for instance, errors in the topographic elevations or in surveyed observation bore data.

The conceptualisation process is never truly finished and will only be deemed adequate for the purposes of the study when the project has provided satisfactory (validated) answers to the defined problem.

Box 3B: Conceptual surprise

Bredehoeft (2005) coined the term '**the conceptual model problem**' in a study of the adequacy of model conceptualisation.

Within the context of these guidelines, this is referred to as **conceptual surprise**. Conceptual surprise occurs when a review of a model many years after its completion shows that the model simulation was in error because the conceptual model is not considered valid. For example, the information available at the time of developing the conceptual model might be found invalid, or there might be new information that invalidates the conceptual model. In about 30% of cases that Bredehoeft reported, the conceptual model changed significantly enough that the original simulation was invalid.

Bredehoeft concluded that this was a common occurrence and it represented irreducible uncertainty inherent in models. That is, the correct conceptualisation was unknowable and therefore, regardless of the effort expended, would never be able to be made valid. He further concluded that there was no ready remedy to conceptual surprise other than to collect as much data as feasible, using all applicable methods, and for the conceptualisation process to be open to the fact that there are alternate conceptualisations and that the model can change dramatically.

To mitigate for conceptual surprise, there should be alternative conceptual models (refer section 3.4). In an ideal world, as many models as possible should be carried through to the model design. Obviously, there are cost implications to this approach and the chosen approach needs to optimise the available budget with the level of certainty required from the eventual model process.

3.10 Reporting and review

An interim report describing the conceptualisation (and design, which is described in Chapter 4) should be produced for review prior to proceeding to model construction. All steps and assumptions will need to be clearly and thoroughly exposed to render the information accessible to all stakeholders (refer Chapter 8).

The use of maps, diagrams and graphs is particularly helpful to describe the conceptual model. The compilation of information may involve plan views and cross-sections, which will facilitate the understanding of the conceptualisation process by visualising the groundwater system.

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.

The conceptual model should undergo both peer review (for technical soundness), as well as review by project stakeholders so that alternative views of the conceptualisation can be tested against the preferred option and to determine whether it is fit for purpose.

4 Design and construction

In this chapter:

- Introduction
- Numerical method
- Software
- Model domain
- Boundary conditions
- Initial conditions
- Model construction.

Guiding principles for model design and construction

Guiding Principle 4.1: The size, discretisation and the dimensionality of the model domain should be chosen to reflect the modelling objectives, conceptual model and target confidence-level classification.

Guiding Principle 4.2: Spatial discretisation of the model domain should be chosen so that it will not lead to excessive model run times that may prevent or hamper the successful development of the model within the available project time frame.

Guiding Principle 4.3: The model grid should provide sufficient refinement to be able to adequately represent the problem geometry, including the layout of proposed developments and the processes of importance.

Guiding Principle 4.4: If temporal variation (including periodic fluctuations or long-term trends) is important in either the groundwater stresses to be modelled or the model results being sought, transient simulations are required. Otherwise steady state predictions should be considered.

Guiding Principle 4.5: 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.

Guiding Principle 4.6: A model should be constructed according to the design, and documented as built. It is reasonable and sometimes essential for the design and construction to change as more is learned about the system and the way it can be represented.

4.1 Introduction

The design stage involves describing how the modeller intends to represent the conceptual model in a quantitative (mathematics-based) framework. Construction is the implementation of that approach in that a model is created through the use of appropriate software (model code and graphical user interface (GUI)).

This chapter provides a description of the design and construction process (summarised in Figure 4-1) with a focus on selection of a suitable software platform in which to construct and run the model as well as deciding on model dimensionality, the model size, the way it is discretised spatially and temporally, the type and location of boundary conditions, and parameterisation of the model.

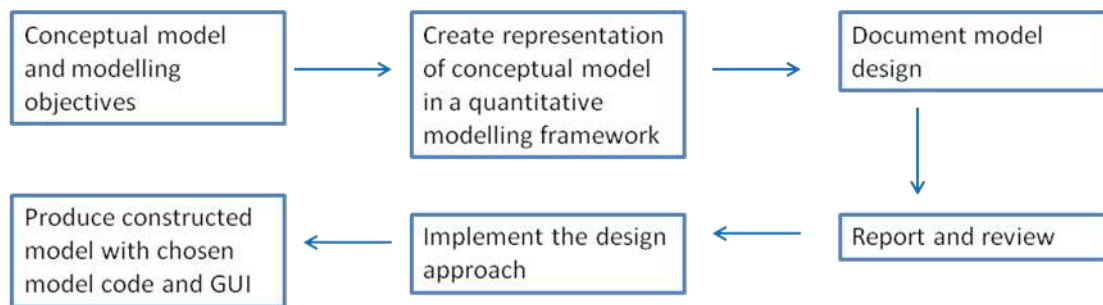


Figure 4-1: Creating a groundwater model

The way the model is designed and constructed has a direct effect on whether a successful calibration can be achieved and whether subsequent predictions will be fit for purpose. Failure to represent key aspects of the conceptualisation may reduce the level of confidence in model outputs.

Although much of this chapter has been written to address the design and construction of a numerical simulation model, most of the issues are equally applicable to analytical and analytic element models.

4.2 Numerical method

Once agreement has been reached among all the parties involved in the project about the conceptual model, the type of numerical method to be used needs to be decided upon. This step involves formulating the physical problem represented by the conceptual model in mathematical terms. For most practical purposes the mathematical formulation is an implicit step in the sense that the modeller will choose an existing analytical solution or numerical model code that will be used to solve the groundwater flow problem. The assumptions in the analytical solution or numerical formulation of the equations that describe groundwater flow (or solute transport) must hold for the groundwater system that is being studied. For example:

- The calculation of hydrogeologic properties from aquifer tests involves the application of a groundwater flow model. Commonly, analytical solutions of groundwater flow to a pumping well are used to fit the calculated drawdown to the observed drawdown during pumping. It was noted in Chapter 1 that numerous simplifying assumptions are made to derive analytical solutions, for example, that the aquifer is of infinite extent. If the pumped bore was located close to an impermeable barrier (e.g. a major fault that displaces the aquifer), this assumption is not valid and the adopted model type is inappropriate. A more complex model is needed (e.g. one that includes image theory to represent boundary effects).
- The groundwater flow equations are simplified considerably by assuming that the density of groundwater is constant. In deep aquifer systems with significant temperature variations, or in coastal aquifers with significant variation in groundwater salinity, this assumption does not hold, and a model is required that is based on a problem formulation that includes the effects of non-constant groundwater density.

To a large degree, the choice of numerical method to be adopted for a particular modelling problem depends on the conceptual model (i.e. given the complexity of the system, are all simplifications contained in the model justified?) and on the modelling objectives and the required confidence level classification (i.e. what features of the system must be resolved).

There are different mathematical approaches to setting up and solving the flow and solute transport differential equations. The two methods that are most commonly encountered are the finite difference and the finite element methods. From a practical point of view, the principal difference between these two techniques lies in the shape of the model cells or elements that discretise the model domain.

An example of a finite element mesh developed in the FEFLOW model code is shown in Figure 4-2. The mesh consists of a network of nodes that form the vertices of triangular elements¹. Figure 4-2 illustrates that the triangular elements can be arranged in a manner that provide a relatively dense array of fine elements in areas of interest while maintaining relatively coarse elements in areas where less detail is required. In multiple-layered models a number of slices with identical node locations are stacked onto one another.

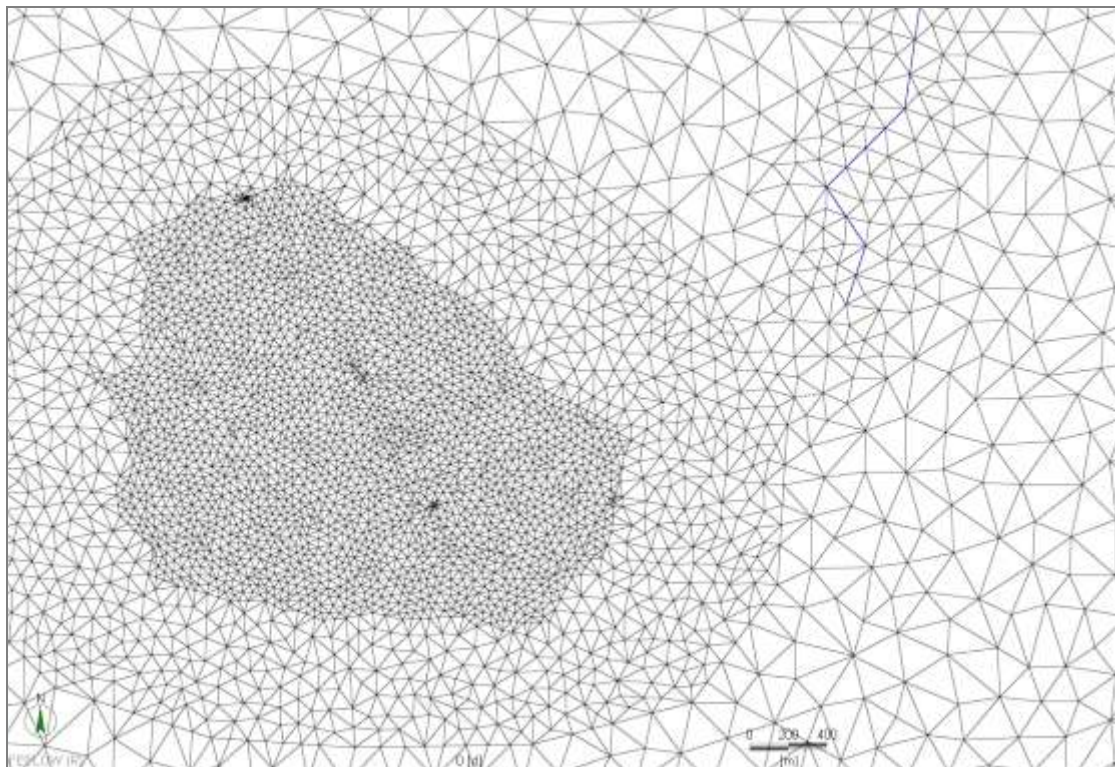


Figure 4-2: Typical finite element mesh

Note: This model was developed for a mine dewatering investigation and the mesh has been heavily refined in the area of the planned mine pit to provide a denser distribution of nodes and elements in the area of particular interest. Additional refinement is also provided in the vicinity of a stream that drains the valley.

An example of a finite difference groundwater model grid with rectangular model cells is illustrated in Figure 4-3.

One of the drawbacks of a finite difference grid is that the refinement also extends into regions where less detail would suffice, thereby generating redundant computational burden. This is not necessarily a limitation of finite differences, but it is a limitation of the ‘regular’ finite difference method that requires a simple, symmetric matrix structure to solve with linear solvers. Recently, model codes have become available that implement local (or telescopic) grid refinement or allow for unstructured finite difference grids and it is anticipated that these will soon become more widely available through the commonly used commercial GUIs.

¹ While the example shows a finite element mesh of triangular elements the use of other shapes such as quadrilaterals is also possible in many codes.

Where grids are refined locally, the increase in node spacing or grid size between adjacent elements should be kept within limits to avoid numerical difficulties with large contrasts in cell size. As a rule of thumb, a factor of 1.5 should be maintained as the maximum ratio of the volumes of neighbouring cells. In finite element grids, the number of neighbouring nodes for any given node should be controlled. The most regularly-shaped triangular elements (and the most stable numerical solutions) are obtained when each node (that is not on the model boundary) has six neighbouring nodes. Where the nodal spacing increases, more connections are acceptable.

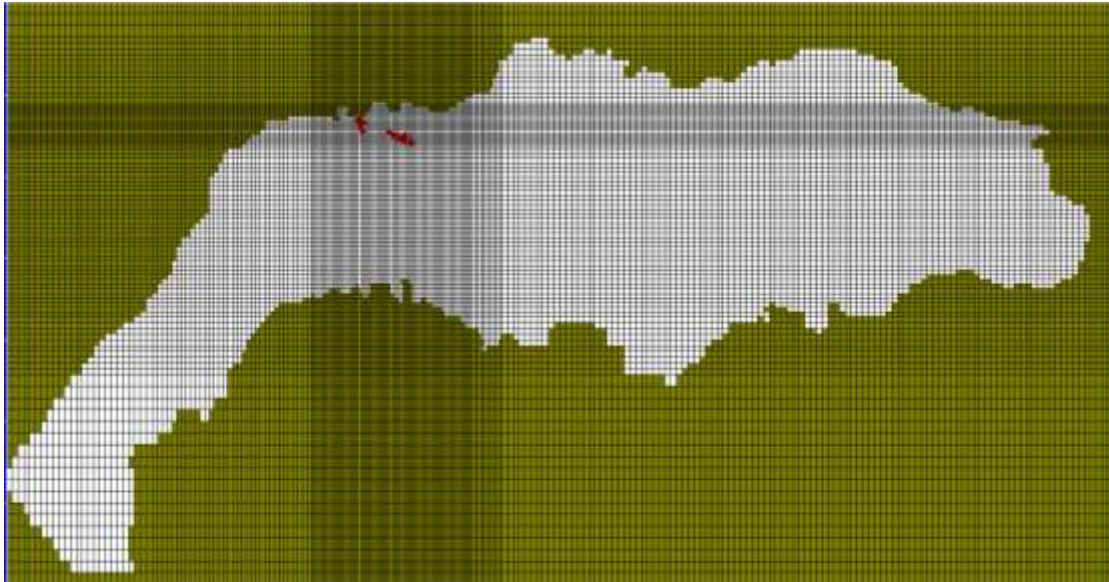


Figure 4-3: Typical regular finite difference mesh

Note: This model was developed for assessing the impacts of a groundwater extraction borefield (bores shown as red spots). Grid refinement is provided around the borefield and groundwater discharge sites in the northwest of the model domain. Mustard coloured cells are inactive.

For completeness it is also necessary to mention the *finite volume* method. Although less commonly used in groundwater modelling, one advantage of the finite volume method is that it allows for unstructured meshes.

4.3 Software

The following definitions are useful when describing software:

- **Model code:** An executable program or a spreadsheet that implements a method or a sequence of methods and produces outputs.
- **Model:** An assemblage of parameter values, boundary conditions and initial conditions defined in a model code for the purpose of making site-specific calculations.
- **Graphical user interface:** A software package that facilitates the construction of a model through the definition of inputs and allows results to be extracted and visualised.
- **Parameter:** A value that is fundamental to a method and that must be assigned as an input to a model.

An important step in the modelling process is a formal software selection process in which all possible options are considered. This step has often been short-circuited in the past. In many cases modellers have immediately adopted MODFLOW, developed by the US Geological Survey (USGS) (Harbaugh et al. 2000), with little thought given to the alternatives. However, in recent years a number of sophisticated and powerful modelling software has become available in easily used commercial software packages that are becoming increasingly popular.

As discussed in section 1.4, the evaluation of specific software packages (computer codes) is beyond the scope of these guidelines—although frequent reference to model codes would allow different attributes of individual codes to be highlighted.

An important reason for not naming specific software is that the range of available software changes every year. Software available in 2012 is different from that available in 2002, and will almost certainly be superseded by 2022. This is mainly because:

- Most commercial software is updated annually, with major revisions or releases every 3-5 years. MODFLOW was first released in 1984, and was subsequently revised or rewritten in 1988, 1996, 2000 and 2005. MODFLOW-96, MODFLOW-2000 and MODFLOW-2005 are all still in use in Australia, although the USGS already considers the first two of these to be legacy versions. Reference to any software by name should include the version number.
- During the period when any version is actively supported by software developers, there are often minor revisions or bug fixes. Minor revisions affect the functionality of the software, and it is the responsibility of the modeller to track and install these revisions.
- MODFLOW presents a particular challenge because its modular nature allows third parties to develop modules, called packages, that can be called from MODFLOW. These packages are also released and revised at irregular intervals.

Some software is widely used, but this does not mean that it is more appropriate or accurate than software designed for specific purposes and used by appropriately trained professionals, for example, in universities and research institutions.

Producing an exhaustive list of all available software codes is therefore problematic and not included in these guidelines. A selection of commonly used software packages is presented below and those interested in obtaining more information about them and other modelling codes and GUIs should search the internet.

4.3.1 Types of 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.

4.3.2 Examples of modelling software

Table 4-1 lists some examples of modelling software commonly used in Australia.

Table 4-1: Modelling software commonly used in Australia.

<i>Name of software</i>	<i>Type of software</i>	<i>Description</i>
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.
MODFLOW-SURFACT	Simulation of saturated and unsaturated flow, solute transport	Commercial software developed to overcome specific limitations in open source versions of MODFLOW and MT3D. Available in an extended form called MODHMS, which includes 2D diffusive wave simulation of overland flow and 1D simulation of 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.
HydroGeoSphere	Simulation of saturated and unsaturated flow, transport of mass and heat	Commercial software based on a control volume finite element method. Includes solution of 2D overland flow and 1D flow in river and stream networks. Also includes discrete fracture networks.
SEEP/W, CTRAN/W	Simulation of saturated flow and solute transport	Commercial software based on the finite element method in 2D vertical section, being part of GeoStudio suite, used mainly by geotechnical engineers for slope stability analysis.
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.
TOUGH2	Simulation of multi-phase, transport of mass and heat	Open source software based on an integral finite difference method. Used extensively throughout the geothermal energy industry.
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.
RT3D	Simulation of multi-species reactive transport in groundwater	Open source software that can be coupled with MODFLOW to compute coupled flow and transport.
PHT3D	Simulation of multi-species reactive transport in groundwater	Open source software that can be coupled with MODFLOW to compute coupled flow and transport. Includes MT3DMS and PHREEQC.
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.

<i>Name of software</i>	<i>Type of software</i>	<i>Description</i>
ZONEBUDGET	Mass balance calculations for parts of a MODFLOW model domain	Open source software commonly distributed with MODFLOW GUIs.
MODPATH	Particle tracking code used with MODFLOW	Open-source software commonly distributed with MODFLOW GUIs.
MIKE 11	River modelling, with integrated GUI	Commercial software that solves kinematic wave and diffusive wave approximations as well as the full Saint Venant equations for flow in networks of rivers and streams.
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.
MapInfo	GIS	Commercial software to manage spatial data.
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.
Leapfrog Hydro	Management of hydrogeological data	Commercial software aimed at development of 3D geological and hydrogeological conceptual models.
UCODE	Parameter estimation and uncertainty analysis	Open-source software designed to allow parameter estimation for any model.
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.

<i>Name of software</i>	<i>Type of software</i>	<i>Description</i>
FORTRAN, C, C++, C#, Python, MATLAB, Scilab	Programming and scripting languages	A wide range of commercial and open source software Can be used to develop new modelling software, extending existing modelling software, analysing data, preparing model data sets and analysing and plotting model results.

4.3.3 Software selection criteria

While most of the basic functions of each GUI and code are similar, they all have their individual strengths and weaknesses. The final choice depends on project-specific considerations that are related to the modelling objectives and the basic model functionality required to meet these objectives.

Table 4-2 lists criteria to guide the selection of a code or GUI.

Table 4-2: Issues to consider when selecting a model code and GUI

<i>Issue</i>	<i>Comment</i>
Dimension (1D, 2D or 3D)	Most simulation packages are designed for 2D areal or fully 3D models. 1D models are often developed to investigate unsaturated zone processes. 2D slice and 2D radial models provide economy of numerical effort and are useful for many modelling problems.
Saturated and/or variably saturated	Groundwater model codes usually model the saturated zone. Only a few include an unsaturated zone-modelling component. Often specialist modelling packages are used in addition to the groundwater model code to provide unsaturated zone assessments.
Solute transport capability	Solute transport models provide additional computation of solute concentration using advection estimated by the groundwater flow model. Reactive and passive transport options are possible with dispersion, diffusion, decay and adsorption options also available.
Density-dependent solute transport	Where concentrations have a significant impact on fluid density it is often necessary to consider density-dependent flow in the model.
Vertical flow processes	Some codes provide a quasi-3D modelling capability and if vertical flow is important it may be necessary to implement an alternative code that provides for a fully 3D approach.
Steady-state or transient mode	Most codes provide for both of these modelling options.
Ability to incorporate automated parameter estimation and uncertainty analysis	Many codes provide options to implement sophisticated inverse modelling routines that can be used to assist model calibration and undertake comprehensive uncertainty analysis.
Stochastic modelling	In many situations the model will be required to produce a range of modelling outcomes that reflects model uncertainty. Some codes and GUIs include options to implement automatic stochastic modelling routines that can be used to achieve such outcomes.
Fractured rock and inclusion of faults	Fractured rock aquifers are commonly modelled as equivalent porous media and this assumption is usually valid for large-scale groundwater flow models. Codes are available that provide a dual porosity formulation where each model cell is subdivided into a portion that represents the fractures through which water transmission mostly occurs and a portion representing the rock matrix where most of the water is stored in the aquifer. Discrete faults and/or fractures can be implemented explicitly in some porous media codes.
Heat transport and multiphase flow	Software codes are available that can simulate these conditions. Refer section 4.3.4 for more detail.
Numerical stability	Most numerical model codes produce numerical instability and modelling artefacts in certain situations. Code selection should address which available code is likely to avoid such problems for the particular modelling application.
Input and output options	GUIs have individual strengths and weaknesses in their utility to facilitate input and output processing.
Ease of modification of the source code	On some occasions it may be necessary or advantageous for the modeller to be able to alter the code for a specific problem.
Software support	Whether the software suppliers provide effective technical support to assist with modelling and software problems.
Computational efficiency	Solvers available in some codes are more efficient than others. Parallelised solvers can add great efficiencies, where available.
Familiarity with Code and GUI	Selecting a code and/or GUI that the modeller is familiar with can save time and money.
Model portability	Often model owners will require that the model be developed in a particular code or GUI so that the model can be used by third parties or by the owners themselves.
Cost	The cost criterion includes the cost of software licences and the cost associated with learning a new code or GUI.

<i>Issue</i>	<i>Comment</i>
Access to source codes	Some software packages are sold as a 'black box' that cannot be modified; others provide program interfaces or can be modified as required.
Benchmarking and industry acceptance	Codes that have been thoroughly tested and verified are usually preferred.

One particularly powerful category of software is formed by packages that solve any type of differential equation. These are sometimes referred to as multi-physics solvers, or generalised PDE (partial differential equation) solvers. These packages are useful when the mathematical model is not supported by available codes, or where code modification is impossible or too cumbersome. They allow the user to formulate the governing equations, boundary and initial conditions and model parameters. Usually the spatial and temporal discretisations are automated, although the user has at least some control over these. The versatility of these programs makes them very attractive alternatives to existing codes for specialised groundwater models.

4.3.4 Multiphase and non-isothermal models

In recent years there has been increased interest in flow-through porous media associated with new technologies that involve the extraction and disposal of fluids other than cold water. Some of these new areas of interest include:

- geothermal developments
- ground-source heat pumps
- coal seam gas developments
- carbon capture and storage (also referred to as geo-sequestration of CO₂)
- high-level nuclear waste disposal in deep geological formations
- the movement of volatile contaminants in groundwater.

In general, groundwater techniques are inherently unsuitable for dealing with many of these problems. The form of Darcy's Law (Hazel 1975) used throughout the groundwater industry and included in most groundwater model codes carries with it the basic underlying assumption that the fluid in the porous medium is water at typical ambient temperatures (i.e. between 10 and 20°C). While groundwater model codes can be easily modified to account for water at temperatures above ambient, for many modelling problems where temperature is important there will be temperature differences in the model domain that will lead to differences in water density and viscosity. These differences must be included in the equations that estimate water movement.

Hydraulic conductivity is a function not only of the intrinsic permeability of the porous medium but also the density and viscosity of the fluid(s) that fill(s) the pores. Given that water density and viscosity are both dependent on water temperature, modelling situations that involve water of variable temperature or of temperatures above 20°C will lead to serious complications for a groundwater model. Various groundwater model codes are able to model non-isothermal fluid movement through the use of solute transport algorithms as a surrogate for an explicit modelling of heat flow. The use of such model codes is recommended except where a modelling problem involves a strongly non-isothermal water environment; in this case, the use of a geothermal modelling code is recommended.

A further complication arises in those modelling environments that contain two-phase fluids, as commonly occur in oil and gas, high-temperature geothermal, and coal seam gas projects. The two-phase flow problem typically involves interacting phases where temperature and/or pressure changes that occur in the aquifer will lead to a change in phase or shift in phase saturation (i.e. liquid will change to gas and vice versa). When the pores contain two distinct fluid phases (e.g. steam and water, water and gas) the presence of one phase retards the movement of the other by limiting the pore space available for each of the phases to flow. Numerical model codes applied to such problems must take account of phase change and mobility retardation (using relative permeability functions). Most model codes commonly used in the groundwater industry are not suitable for modelling such problems.

Numerical model codes developed in the petroleum and geothermal industries have been designed to model two-phase fluid-flow problems and these codes should be considered for situations that involve the presence of two fluid phases in the aquifer.

Table 4-3 presents a summary of the recommended modelling platforms for various non-conventional groundwater modelling settings.

Table 4-3: Recommended model codes for non-conventional groundwater settings

<i>Problem type</i>	<i>Code by industry sector</i>	<i>Comment</i>
Low temperature geothermal (20–100° C)	Geothermal (e.g. TOUGH2) or groundwater (e.g. FEFLOW or MODFLOW SEAWAT)	Code must account for density and viscosity variability.
High temperature geothermal (100–375° C)	Geothermal	Heat-flow and two-phase capability required.
Ground source heat pumps	Geothermal or groundwater (e.g. MODFLOW or FEFLOW)	Usually involve relatively small variations in temperature.
Coal seam gas	Geothermal or petroleum (e.g. ECLIPSE)	Two-phase fluid problem in the coal seams.
Carbon capture and storage	Geothermal or petroleum	Two-phase fluid problem.
Groundwater movement around nuclear waste disposal sites	Geothermal or groundwater (FEFLOW or MODFLOW SEAWAT)	High thermal gradients are expected and code must account for density and viscosity variability.
Volatile Contaminants	Geothermal or petroleum	Two-phase fluid problem.

4.4 Model domain

4.4.1 Model dimension

Guiding Principle 4.1: The size, discretisation and the dimensionality of the model domain should be chosen to reflect the modelling objectives, conceptual model and target confidence level classification.

One of the first considerations in designing a groundwater model is to select the spatial dimensionality that can best represent the features of the environment being modelled.

Many groundwater models are formulated in 3D (or quasi-3D) with little thought given to the applicability of simpler two-dimensional representations of the problem. The model dimension should be chosen, based on the dimensions needed to describe the key processes controlling groundwater movement. Table 4-4 provides some examples of types of groundwater modelling applications and the appropriate model dimensionality.

Table 4-4: Examples of different model dimensions.

<i>Model dimension</i>	<i>Description</i>	<i>Range of application</i>	<i>Guidance</i>
One-dimensional (1D)	Radial flow	Predicting responses to pumping.	1D models generally provide a simplified groundwater flow domain and geometry. They are useful to assess groundwater behaviour where such simplifications can be justified or where complex calculations are not required.
	Horizontal flow models	Applications of Darcy's Law.	
			Solute movement along a single flow path (refer to Chapter 10).
Two-dimensional (2D)	Vertical slice or vertical section model	Where vertical flow is important.	These models are ideally suited to assess vertical flow processes and are commonly used to model density-dependent solute transport (refer Chapter 10). The chosen slice must be representative of a larger region of aquifer for the modelling outcomes to be of value (i.e. applicable to more than a unit thickness vertical slice of the aquifer). Not all aquifer geometries are suited to this type of model. Because flow to a pumping well is usually radial in direction, a 2D vertical slice of unit width does not provide an appropriate geometry with which to model the convergence or divergence of flow to or from pumping or injection wells. Accordingly, the implementation of groundwater extraction and injection must be approached with caution. It is recommended that such models be avoided if the flow to and from extraction and injection wells is an important feature of the model. In this case a 2D radial flow model (as described below) should be adopted.
		Density-dependent solute transport models for sea water intrusion.	
		Aquifer geometry that allows the definition of fluxes per unit length of aquifer.	
	Areal flow model	Where vertical flow is not important.	These models assume that the aquifer is a 2D planar feature where groundwater flow is predominantly in the horizontal plane. This assumption is usually valid for aquifers that have a horizontal extent that is much larger than the aquifer thickness, and have such a high vertical hydraulic conductivity that vertical head gradients within the aquifer are negligible.
	Radial flow	Flow to extraction and injection wells with negligible regional groundwater flow.	In this type of model the spatial domain is defined as a radial slice or wedge of defined angle with a source or sink at the centre. Such models are ideally suited to model flow towards or away from extraction or injection wells. The extraction or injection rate of the centrally located well must be consistent with the proportion of the full radial domain that is considered.
Three-dimensional (3D)		Where flows occurs in all directions.	3D groundwater flow models are needed to simulate groundwater movement in both the horizontal and vertical planes and are required when there are several overlying hydrogeological units where horizontal flow in individual units and flow between adjoining units are important. The definition and use of model layers and the associated interaction between layers is discussed in more detail in section 4.4.4.

4.4.2 Model extent

The area of interest for the overall project should be agreed and preferably mapped in the planning stage (refer Chapter 2) and the overall extent of the groundwater system (hydrogeological domain; refer section 3.6.2) of relevance to the project is defined in the subsequent conceptualisation stage. At the model design stage the model domain should be decided upon. An assessment must be made as to what part of the groundwater system is relevant and what part can be excluded given the characteristics of the system and the modelling objectives.

In general terms the model domain must cover the entire area of interest with, in most cases, a spatial buffer to ensure that the limits of the model domain are sufficiently remote to reduce the impact of the assumed boundary conditions on the model outcomes. Often it is not clear or obvious what size buffer is required. Simple analytical models can assist with determining the expected spatial extent of groundwater responses. Alternatively, a sensitivity analysis can be designed to test the impact of the model extent and the selected boundary conditions on model outputs.

Box 4A: CAUTION regarding model extent

It is usually inappropriate to formulate a model in which the boundaries are in close proximity to key areas of interest where model results will be reported or to locations of significant groundwater stress. The type of boundary condition applied at the edges of the model domain will influence groundwater behaviour at the model extents and this influence will propagate some distance into the model domain.

It is recommended to choose a larger model domain where there is any question of boundary condition unduly influencing modelling outcomes. In other words, it is better to err towards creating a larger model than necessary than to create a smaller model in which some of the key modelling outcomes are controlled by boundary conditions.

In some cases the model boundaries can be chosen to coincide with specific hydrological features that provide physical boundary conditions. For example, for a model of a shallow unconfined aquifer, a river may provide a suitable model domain boundary where an appropriate boundary condition is used to represent the river (refer to Chapter 11). Similarly, groundwater flow divides are also often selected as model domain boundaries where no-flow conditions are assumed. Some caution should be applied in this case because a groundwater flow divide can migrate as groundwater heads change in response to stresses applied during the prediction stage.

Box 4B: CAUTION regarding interacting model domains

Special care should be taken when two or more models share a common boundary or are close enough to interact with each other (i.e. the impact of stresses applied in one model domain is likely to propagate to the neighbouring or adjacent model domain). This situation may arise if a groundwater basin is divided into a number of subregions for management and modelling purposes. It should be recognised that a true synchronisation of head-dependent boundary conditions and predicted boundary fluxes is generally not possible. In other words, adjoining models are most likely to include different heads and/or fluxes at shared boundaries. The issue has been identified and quantified in the Southern Riverine Plain region of the Murray Basin in Victoria and New South Wales (Barnett et al. 2008).

It is recommended addressing the issue by creating larger models that include all interacting management regions. In some cases, this will result in excessively large model domains and a compromise may be required on model cell or element size to maintain reasonable model run times. This issue is discussed in more detail in section 4.4.3.

4.4.3 Spatial discretisation

Guiding Principle 4.2: Spatial discretisation of the model domain should be chosen so that it will not lead to excessive model run times that may prevent or hamper the successful development of the model within the available project time frame.

Guiding Principle 4.3: The model grid should provide sufficient refinement to be able to adequately represent the problem geometry, including the layout of proposed developments and the processes of importance.

Numerical models require the model domain to be subdivided (discretised) into a grid (or mesh) that defines the locations of the points (commonly referred to as nodes) at which heads or solute concentrations are calculated and the geometry of the cells (or elements) that controls the calculation of the volumetric or mass flow rates of water and solutes. The appropriate level of spatial discretisation depends on the size of the model domain, the modelling objectives and the desired level of accuracy. Moreover, the heterogeneity of the subsurface, the hydrologic boundary conditions and the available data dictate the resolution of the model grid if there is a need to explicitly represent these features in the model. Adopting a high-resolution discretisation will not only have implications for the time frame and budget for the project, but will also increase the model run time and memory requirements, especially for solute transport models.

Factors to consider in spatial discretisation include:

- **Adequate representation of the problem.** Fine discretisation is warranted, for example, when (i) the potentiometric surface is very steep (e.g. near pumping wells) or has an irregular shape; (ii) irregularly shaped surface water features are included in the model; (iii) highly heterogeneous aquifer properties are to be explicitly represented; or (iv) when the model domain has a shape that can only be resolved with a fine grid (e.g. a dewatering model of a mine excavation).
- **Model run time and memory requirements.** The time taken to run a numerical model simulation and its required computer memory depends to a large extent on the number of nodes at which calculations are made. Excessive model run times may hinder the modeller's ability to adequately calibrate the model within the time and budget constraints of the project. They may also preclude the application of comprehensive sensitivity and uncertainty analyses.
- **Model file sizes.** Large models with fine grids will generate large model input and output files that become difficult to process. As file sizes increase the time taken to manipulate and use the files also increases. In some cases model files become too large to open in some software packages.
- **Solute transport models.** A fine mesh is often required for solute transport models to achieve accurate numerical solutions (refer to Chapter 10) to the transport equations.

4.4.4 Model layer structure

In cases where a model is required to simulate vertical flow processes or to resolve vertical variations in heads or solute concentrations, the model domain must be discretised into a number of layers. Construction of model layers, especially dipping layers that pinch out or intersect the land surface or the base of a model domain can be difficult. Several approaches can be adopted with respect to selecting an appropriate model layer structure:

- If, during the conceptualisation stage, it is deemed appropriate to neglect vertical head gradients within aquifers and approximate the groundwater flow as being horizontal, a single model layer can be used to represent each aquifer. This assumption is usually appropriate in cases where an aquifer is relatively thin and there is no indication of head differences measured in nested bores. In this case the thickness of the model layer is designed to match the thickness of the aquifer it represents. Accordingly, layer thickness may be spatially variable. If multiple aquifers are being modelled, any aquitards in between them can be simulated (i) implicitly by specifying the hydraulic resistance (or conductance) between the nodes in adjoining layers or (ii) explicitly by representing the aquitard by a model layer. If the first approach is adopted, the hydraulic resistance incorporates the resistance against vertical flow through the aquitard as well as the aquifers.
- If vertical head variations within aquifers or aquitards are important (e.g. when these units are vertically extensive or when there are vertical head gradients observed in an aquifer unit), individual hydrostratigraphic units (aquifers as well as aquitards) can be subdivided into multiple model layers. The thickness of each model layer may be spatially variable, and will typically depend on the thickness of the hydrostratigraphic unit and the number of layers used to represent it. If an aquitard is represented by a single layer, the vertical propagation of head changes into and through the aquitard over time may not be simulated accurately. The solution is to subdivide the aquitard into several (three or more) model layers.
- In contrast to the previous approaches, models can be discretised vertically by using horizontal layers of constant thickness (although not all the model layers necessarily have the same thickness). In this type of model design the model layer boundaries do not necessarily coincide with the boundaries between the hydrostratigraphic units. The (vertical) variation of the hydrogeologic properties is accounted for by assigning to each model cell or node parameter values that are appropriately weighted according to the relative proportions of hydrostratigraphic units included in the layer.

Box 4C: CAUTION regarding vertical discretisation (layers).

In cases where it is important to model hydraulic gradients in the vertical direction within specific units (i.e. estimating the curvature of the hydraulic gradient with depth), it is necessary to subdivide individual hydrogeological units into a number of sub-layers. This issue is particularly relevant when considering how to model aquitards. If an aquitard is explicitly modelled as a single layer, groundwater responses are (sometimes erroneously) simulated to propagate instantaneously through the unit. In reality, groundwater responses travelling vertically will be retarded or delayed by an aquitard.

It is recommended that where a model is required to predict time lags of the propagation of responses in the vertical direction, thick aquitards should be subdivided into a number (at least three) of thinner layers.

4.4.5 Temporal discretisation

Guiding Principle 4.4: If temporal variation (including periodic fluctuations or long-term trends) is important in either the groundwater stresses to be modelled or the model results being sought, transient simulations are required. Otherwise, steady state predictions should be considered.

No temporal discretisation is needed for steady state models. They are constructed with time-averaged inputs and the model outputs illustrate the groundwater flow and piezometric heads that would arise when the system has equilibrated to all boundary conditions and defined stresses.

The steady state solution to a groundwater flow problem is not dependent on aquifer storage parameters (i.e. specific yield and specific storage). As a result, a steady state model calibration does not provide any constraint or information on these model parameters.

Transient models typically include time-varying inputs and the model calculates and saves output at various times throughout the duration of the model run. Transient models can predict time-varying groundwater responses and are therefore required when temporal trends and fluctuations in groundwater levels, and fluxes, are important. Aquifer storage parameters have a strong influence on transient model results. Water is calculated to be released from and enter into storage, as the model predicts groundwater levels to fall and rise respectively.

Box 4D: CAUTION regarding the interpretation of storage changes.

Care should be taken to ensure that the storage change that appears in the model's mass balance is correctly reported. When groundwater levels fall (e.g. in response to pumping) the storage change is reported on the 'water in' side of the mass balance. Conversely, when the piezometric heads in a model rise, the volume of water is included in the 'water out' side. This assignment of fluxes in the mass balance account is counterintuitive as, generally, we regard rising water levels as increasing the volume of water stored in the aquifer and vice versa. When reporting storage changes it is often useful to refer to terms such as storage depletion and replenishment rather than fluxes in or out of storage.

Many model codes and GUIs allow the user to easily alternate between steady state and transient model formulations. In this regard, the choice of temporal model domain is one that can easily change during the course of model development and use. One consideration in this choice is whether or not the available data is sufficient to allow a transient calibration where the model will be required to match historically measured time series data. If not, the model must be calibrated in steady state (if possible) and any subsequent attempt to use it to predict in transient mode would result in a low confidence-level classification being assigned to the model outcomes. On the other hand, it is not necessarily incongruous to calibrate a model in transient mode and then run predictive scenarios with high confidence in steady state mode.

The discretisation of the time domain (the time period being modelled) in transient models is determined by:

- **The frequency at which model stresses change.** To account for the temporal variability of stresses, the temporal domain is subdivided into stress periods. For example, regional water resource management models are often discretised into monthly stress periods. Typically, the modeller must aggregate or lump daily river-stage data and disaggregate annual groundwater extraction data (using an assumed monthly apportionment of the annual total) so that both datasets are represented as a sequence of monthly values.

- The rate of temporal changes of the hydraulic heads or solute concentration data.**
 To resolve these changes, and to obtain accurate numerical solutions, stress periods are subdivided into increments commonly termed 'time steps'. The number of time steps required for each stress period depends on the rate at which the changes occur. Switching on a pump, for example, may initially cause a rapid lowering of the head in an aquifer. This means that a fine time discretisation (many time steps) is needed to accurately resolve the head drop with time. As the rate of head decline slows down over time, the duration of the time steps can be allowed to increase. Often this is accomplished by defining a time-step increment that is greater than one that provides a geometric increase in time-step length from one time step to the next in any stress period. Some codes implement an automatic time-stepping approach in which the calculation interval is progressively modified according to the ease or speed with which a satisfactory numerical solution is attained. Other codes require the user to specify a time step or time-step increment between consecutive steps. Anderson and Woessner (1992) recommend a maximum or critical time step (Δt_c) as:

$$\Delta t_c = a^2 S / 4T \quad \text{Eqn 4.1}$$

Where:

- Δt_c = Critical time-step duration (T)
- S = Storage coefficient (-)
- a = Representative cell or element dimension (L)
- T = Transmissivity (L^2 / T)

It is recommended to use this equation to provide an initial estimate for the maximum time step and that if shorter model run times are desired, a trial-and-error approach be used to assess the suitability of longer time steps. The suitability of a particular time step can be judged by (i) whether numerical solution is attained and (ii) whether the mass balance closure error remains within reasonable limits.

- The frequency with which the model outputs are required.** At most the model is able to save results for every time step. Accordingly, the time-stepping scheme must provide a suitable temporal discretisation to capture or illustrate the scale of the temporal fluctuations or trends that are of interest.

Special considerations apply to the temporal discretisation of solute transport models (see Chapter 10).

4.5 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.

Box 4D: CAUTION regarding the use of time-varying boundary conditions.

Care should be exercised when using time-varying boundary conditions to constrain the model at the domain boundary where the time series heads or fluxes have been obtained from measurements in nearby groundwater observation bores. In this case, the model is predisposed to transient calibration by the choice of boundary condition. Perhaps more importantly, the boundary condition provides significant difficulties when formulating predictive model scenarios as appropriate time series data for the predictive time domain (the time period being modelled) is usually not available. Accordingly, it is recommended that such boundary conditions be replaced by time-constant boundary conditions, if possible.

4.6 Initial conditions

Guiding Principle 4.5: 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.

4.7 Model construction

Guiding Principle 4.6: A model should be constructed according to the design, and documented as built. It is reasonable, and sometimes essential, for the design and construction to change as more is learned about the system and the way it can be represented.

Model construction means implementing the model design, generally using commercial software, in such a way that simulations can be performed.

If the model is an analytical one, software may be needed to evaluate the closed-form solution. In this case, all parameters of the model need to be set up appropriately, ready for calculation of the analytical solutions.

For numerical models, construction usually involves setting up the model in a GUI, which acts as a front-end or pre-processor for the numerical algorithm itself. The steps involved depend on the type of model and on the modelling software chosen for the project. Most software packages provide the user with a number of tools for defining the extent of the model domain and the various types of parameters needed as model inputs. Most are able to read and manipulate files prepared using geographic information systems (GIS) to assist with the import of large and complex spatial data sets.

In general, model construction involves implementing the following features in a modelling code or GUI:

- Define model domain.
- Create a grid or mesh to provide spatial discretisation in each model layer.
- Create model layers.
- Define the distribution of model parameters to represent hydrogeological properties.
- Define model parameters to represent boundary conditions.
- Define initial conditions.
- Select time-stepping options, choose appropriate numerical solvers and set convergence criteria.

Parameterisation affects the way parameter values are assigned when a model is first set up, but is also very important during later stages of the modelling process. The parameterisation may need to be revised during model calibration for instance (refer section 5.2.3), when it becomes clear how much information historical data contains about model parameters, or during the predictive stage of modelling, if it becomes clear that predictions may require more spatial definition in aquifer properties.

Hydrogeological properties can be assigned in the following ways:

- as constant values for single or multiple model layers, representing homogeneous hydrostratigraphic units
- as constant values within multiple zones in each layer, for example, to distinguish between different hydrogeological materials that are present within the same layer
- at a small number of representative locations, with an interpolation algorithm to define how properties should be assigned in individual cells or elements (e.g. the *pilot point* method, where the representative locations are called pilot points and the interpolation algorithm is kriging)
- individually in all or many cells or elements.

In this list, the number of model parameters needed to represent spatial variations increases from one option to the next. Similar choices are possible for spatially varying parameters related to boundary conditions, for example, if riverbed conductance needs to be assigned along the length of a river. Model construction can be time-consuming and iterative. Regardless of how well a model is designed in advance, implementing the design in software can take longer than expected. Development of a grid or mesh to align with the shapes of boundaries, rivers or mine pits is not always straightforward. Construction of model layers, especially dipping layers that pinch out or intersect the land surface or the base of a model domain, can also be difficult.

Much of the initial effort relates to geometry. But it is the assignment of parameters that describe the spatial variation of aquifer properties and the spatial and temporal variations of boundary conditions that generally takes the most time. The choice of model parameters is known as parameterisation, and is discussed in the context of model calibration in 5.2.

During construction the modeller must select (from a number of alternatives available within the code or GUI) a mathematical solver. Often the solution method, or solver, chosen for a model may not initially provide convergence to the specified criteria. It is often beneficial to try a different solver, or relax the solver parameters to obtain numerical convergence. In the case of a steady state model, recycling of modelled heads (and/or concentrations) and rerunning of the model in an iterative manner can enable a modeller to achieve a converged solution that also provides a satisfactory mass balance.

A model should be documented *as built*. Preparation of documentation can be very time-consuming. The degree of detail required should be agreed in advance. It is generally more important to highlight any deviations from common practice for model construction, rather than to provide details that could be considered to be common practice.

5 Calibration and sensitivity analysis

In this chapter:

- Introduction
- Fundamental concepts
- Calibration methodologies
- Challenges and solutions
- Sensitivity analysis
- Verification.

Guiding principles for calibration and sensitivity analysis

Guiding Principle 5.1: All available information should be used to guide the parameterisation and model calibration. All parameters should initially be considered to be uncertain.

Guiding Principle 5.2: The calibration process should be used to find model parameters that prepare a model for use during predictions of future behaviour, rather than finding model parameters that explain past behaviour.

Guiding Principle 5.3: The modeller should find a balance between simplicity (parsimony) and complexity (highly parameterised spatial distribution of some properties). Non-uniqueness should be managed by reducing the number of parameters or by regularisation, which is a way of ensuring that parameter estimates do not move far from initial estimates that are considered to be reasonable.

Guiding Principle 5.4: Performance measures should be agreed prior to calibration, and should include a combination of quantitative and non-quantitative measures. The scaled root mean squared error (SRMS) is a useful descriptor of goodness of fit when the only objective is to fit historical measurements of heads, but is less useful when automated calibration methods are used. A target SRMS of 5% or 10% is only meaningful when those setting the target know that it is achievable for a particular kind of problem and a particular environment with a known density of informative data.

Guiding Principle 5.5: Sensitivity analysis should be performed to compare model outputs with different sets of reasonable parameter estimates, both during the period of calibration (the past) and during predictions (in the future).

Guiding Principle 5.6: A formal verification process should only be attempted where a large quantity of calibration data is available and it is possible to set aside a number of key observations that could otherwise be used for calibration.

5.1 Introduction

This chapter provides an introduction to model **calibration**—a subject considered by some to be the most important step in modelling. Calibration is a process, following model design and construction, by which parameters are adjusted until model predictions fit historical measurements or observations, so that the model can be accepted as a good representation of the physical system of interest. Calibration is often followed by **sensitivity analysis**, to test the robustness of the model to changes in parameters during the calibration period.

The process of calibration is also known as model fitting, history matching, parameter estimation and the inverse problem. It is during calibration that the modeller first gains an understanding of how changes in model parameters affect a model's capability to simulate the groundwater system and fit historical measurements.

Calibration is an inherently complex process. A deep understanding of calibration requires knowledge of advanced mathematics and statistics. A number of software packages are available to assist with calibration, and while they become ever more accessible, some aspects require highly specialised knowledge and skills.

Calibration can be undertaken with many levels of sophistication. Much of the complexity surrounding calibration depends on the way parameters are defined, and the way data is perceived and utilised as measurements of model inputs and outputs. The number of measurements is important, that is, the quantity of data. But individual measurements can be more or less valuable, depending on the accuracy of measurements, the sensitivity of model predictions to parameters, and redundancy (i.e. duplicate measurements which are not equally valuable). What really matters is the amount of information contained in the measurements about parameters.

Sometimes there is insufficient data to calibrate a model. In these circumstances, a model may still be useful as a predictive tool, especially if sensitivity analysis is undertaken.

5.2 Fundamental concepts

5.2.1 Model parameters and calibration

A model is a method for converting or transforming the values of model parameters (model inputs) into predictions of state variables (model outputs) (refer Figure 5-1). A model includes many details that are not model parameters, for example, the geometry and discretisation of the model domain. In a groundwater flow model:

- **Parameters** include coefficients that describe the spatial distribution of hydrogeological properties and the spatial and temporal distribution of boundary conditions, where the latter include recharge, pumping and all other stresses on the system.
- **State variables**, which represent the state of a groundwater flow system, are the heads at all locations and times.
- Fluxes within the model domain and through boundaries are **derived quantities** because they are computed from the parameters and state variables.

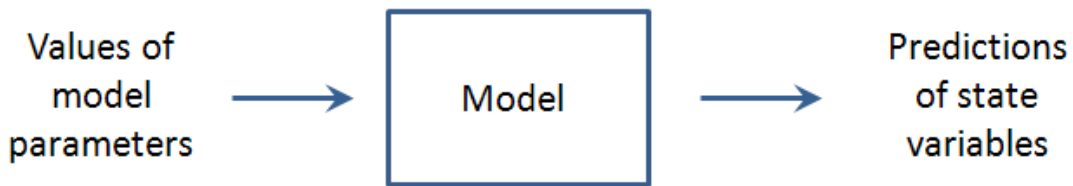


Figure 5-1: Transforming model parameters to predictions

All model parameters must be defined to prepare a model for making predictions. Initial estimates can be made using **measurements** (data) that relate directly to the quantities being represented by parameters. However, when historical measurements of state variables are also available, an opportunity arises for this data to be used to improve the estimates of model parameters.

Calibration tests many sets of model parameters to find the set that best fits historical measurements.

The modeller develops an in-depth understanding of the behaviour and responsiveness of a hydrogeological system through a modelling project. During calibration, the modeller begins to understand the effect of changes in model parameters on how well a model predicts historical measurements. This learned intuition about the groundwater system is a valuable (though fundamentally qualitative) outcome of the modelling process.

5.2.2 The past versus the future

Modelling is generally undertaken in two stages, covering two distinct periods of time (refer Figure 5-2):

- **a period in the past**, during which historical measurements are available of the state of the system, for example, watertable elevations or piezometric heads at depth, or of derived quantities such as discharge to streams
- **a period in the future**, during which predictions will be made.

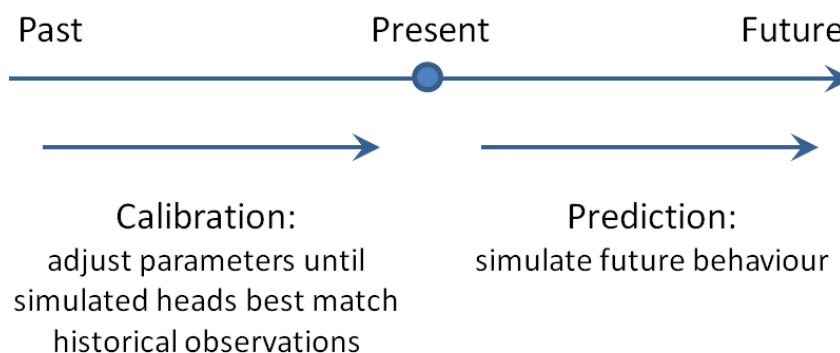


Figure 5-2: Distinction between calibration and prediction

Most models are designed with an expectation that they will be used to predict future behaviour. Model parameters that represent aquifer properties and some attributes of boundary conditions are generally time-invariant, and can be expected to be the same in the future as they were in the past.

Example 5.1 describes calibration of an analytical model that is frequently used to infer the properties of aquifers.

Example 5.1: Interpretation of an aquifer test using Theis's solution

Interpretation of field data following an aquifer test is an example of model calibration with an analytical model.

Consider a single borehole drilled into a confined aquifer, in conditions that are assumed to be homogeneous and isotropic, and where the aquifer is believed to have constant thickness. Suppose an observation bore has been drilled at some distance (radius) from the bore that is pumped. During the aquifer test, measurements of piezometric head are taken in the observation bore at designated increasing time intervals, and results are later analysed using an analytical model known as Theis's solution (Theis 1935).

An aquifer test can be analysed graphically by hand, on log-log paper or log-linear paper, by comparing the time series of observations with so called Type curves. Today it is more common to use one of a number of software packages to estimate model parameters (aquifer transmissivity and storage coefficient (refer section 1.5.1)) by minimising a least squares objective function that is essentially the sum of squared differences between observations and model predictions. The Theis equation is a constraint, because it is assumed (believed) that the relationship between heads and parameters must obey this analytical solution. In other words, it is assumed that site conditions are consistent with the assumptions that underlie the Theis solution. This assumption of model correctness is implied and fundamental in any calibration exercise.

Such an approach is a routine application of model calibration by practising hydrogeologists, even though they may not always realise the analogue with calibration of more general numerical models.

Even with such a simple textbook example, there are many subtleties:

- If the observation bore is not at an appropriate distance from the pumped bore, or if observations started too late (relative to this distance), the information contained in the observations may be insufficient to provide an estimate of the aquifer storage coefficient with a low level of uncertainty, as measured by its estimation variance.
- If the thickness of the aquifer is not known accurately, subsequent estimates of horizontal hydraulic conductivity or specific storativity (refer section 1.5.1) will be more uncertain, as measured by their estimation variances.
- If fitting is performed using log drawdown, there is a question relating to whether weights on measurements should vary with time, because constant weights may assign too much importance to measurements at early time in the aquifer test.

Numerous experiments with students at universities around the world have shown enormous variability between the parameter estimates obtained, even when they use the same measurements and apparently the same methodology. Model calibration is useful, and necessary, but requires care and experience.

Calibration requires a calibration dataset; a set of historical measurements or observations that show how the groundwater system behaved in the past. Data typically includes measurements of watertable elevation or piezometric head at different times at a number of locations within the model domain. Data can also include measurements of flows in rivers or streams and solute concentrations in groundwater or surface water. These are measurements of the state of a system, the so-called state variables, or of quantities derived from those state variables.

Calibration relies on earlier measurements or estimates of model parameters. Some types of data can be used in a formal mathematical calibration methodology, while others can be described as soft data, in the sense that they provide guidance about likely ranges of parameters, and cannot be used directly to assign model parameters.

Figure 5-3 illustrates how a model is used repeatedly as part of model calibration, simulating the past and, later, to predict the future. When a model is set up with parameters that describe the system in the past, it is capable of simulating how the system would have responded in the past. A calibration methodology compares these simulations with historical measurements and provides estimates of model parameters that fit historical data. During calibration, the simulations of the past are repeated many times, until the best estimates of parameters are found. When these parameter estimates are combined with additional model parameters that describe the forcing on the system in the future, the model predicts the behaviour of the system in the future.

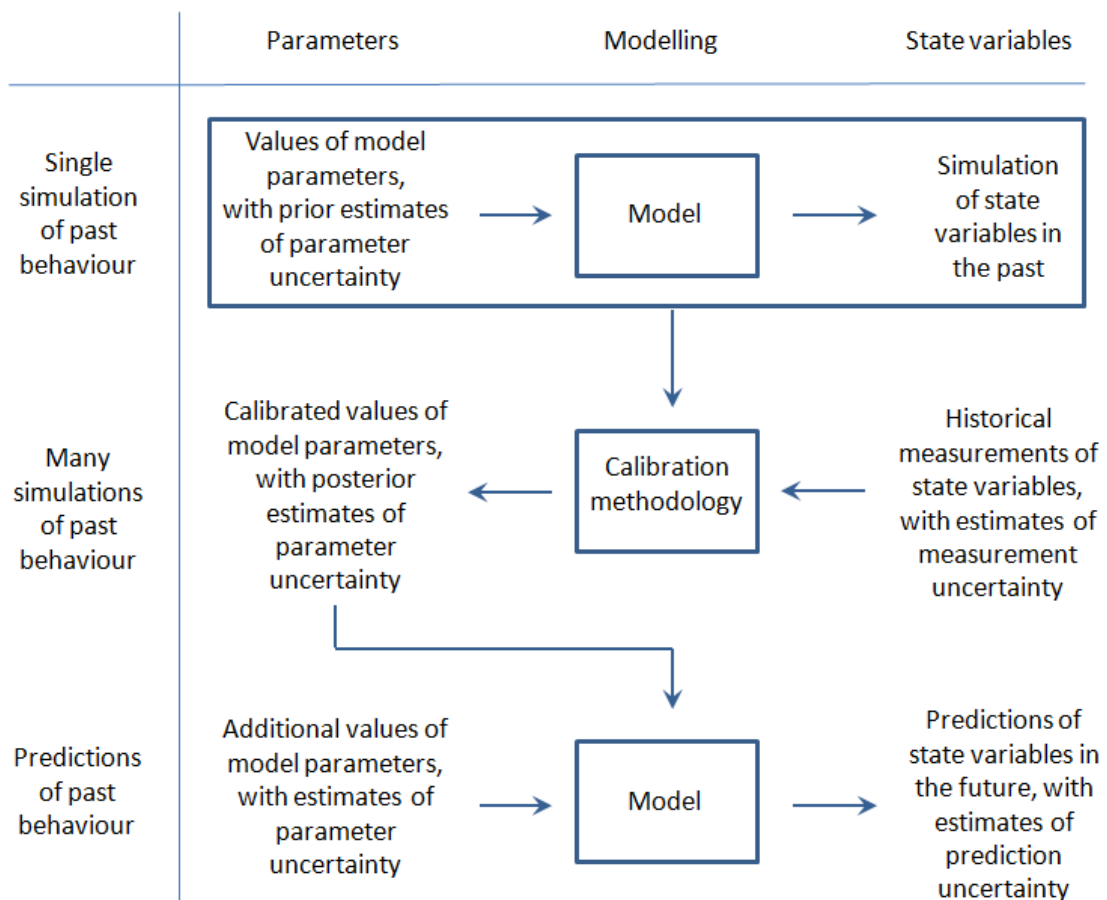


Figure 5-3: How a model is used during calibration and for prediction

5.2.3 Parameterisation

Since calibration is aimed at estimating model parameters, it is important to understand how many parameters there are in a model.

Parameterisation is the process by which model parameters are defined. The process starts during conceptualisation (refer section 3.6.2), and continues through design and construction (refer section 4.7) of a model. Since modelling is iterative, and all steps from conceptualisation onwards can be revisited based on the results of calibration and subsequent predictions, parameterisation can also change throughout a modelling project.

In the case of hydrogeological properties, parameterisation involves making choices about how the spatial distribution of aquifer properties will be represented. Ways in which hydrogeological properties can be assigned are listed in section 4.7.

Similar choices are possible for spatially varying boundary conditions. A small number of parameters can be assigned for one or more large zones, or a large number of parameters can be assigned at the smallest level of discretisation in the description of the boundary conditions.

Different values of boundary conditions at different times can also be considered to be different model parameters, for example, recharge can be assumed to be constant with a long-term average value, or varying year to year as a percentage of annual rainfall, or varying month to month.

Parameterisation may need to be revised during model calibration, when it becomes clear how much information historical data contain about model parameters, or during the predictive phase of modelling if it becomes clear that predictions may require more spatial definition in aquifer properties.

5.2.4 Using all available data

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 (refer to section 5.4.1).

It is generally believed that calibration of groundwater flow models is much more robust when historical measurements of fluxes are also available. This is because the sensitivity of fluxes to parameters is different from the sensitivity of heads to fluxes. Measurements of fluxes therefore contain new and important information about parameters, which helps to resolve non-uniqueness issues (refer section 5.4.1).

In principle, there is no reason to exclude any data from the model calibration process, but it is important that data be studied in detail and quality assured before attempting calibration. For example, for any measurement of head, the modeller chooses a cell or node in a particular model layer in order to compare the modelled head with the observation. This can only occur if the elevation of the screened interval in the observation bore and the hydrostratigraphic unit in which the screen is located are known.

Some types of data can be described as soft data in the sense that they provide guidance about likely ranges of parameters and cannot be used directly to assign model parameters. Soft data can be very useful as a way of guiding model calibration.

5.2.5 Initial estimates of model parameters

Guiding Principle 5.1: 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.

It is not necessary to estimate all model parameters by calibration. However, by assuming all model parameters to be uncertain, all parameters can be estimated by a systematic process and analysis of prediction uncertainty will include the effects of errors in all parameters. During the course of calibration, some parameters can be fixed by assigning zero uncertainty to the current estimates, so that the current estimates cannot change. However, by allowing all parameters to be uncertain with appropriate levels of uncertainty and appropriate estimates of correlation between parameters, all model parameters can be adjusted by calibration.

Box 5A: CAUTION regarding parameterisation.

Hydrogeological properties estimated during earlier modelling studies should be used with caution. If groundwater flow modelling has been undertaken in the same location several times over a period of 10 or more years it is likely that the models have become increasingly detailed, with more and more cells or elements of decreasing size. Hydrogeological properties estimated for large cells in the past may average out details that may need to be included in higher-resolution models. Parameters representing aquifer properties may be grid-dependent.

5.2.6 Objectives of calibration

Guiding Principle 5.2: The calibration process should be used to find model parameters that prepare a model for use during predictions of future behaviour, rather than finding model parameters that explain past behaviour.

The first and obvious objective of calibration is to find values of model parameters that allow a model to fit historical measurements of various kinds. The ultimate and less obvious objective is to find model parameters that allow a model to predict future behaviour with as much confidence as possible. In other words, a model of the past is calibrated in order to give confidence in a model of the future.

It is important at the outset to consider how **goodness of fit** will be measured, but it is not always necessary to define a target for goodness of fit. A target for goodness of fit may be useful for a model that is similar to other models developed previously in the same geographical area. A target may be less useful for models of regions or situations that have never previously been modelled, where there is considerable uncertainty and a lack of data, and where there is no way of knowing whether the available data will contain sufficient information to ensure a good fit between the model and measurements. The options available for measuring goodness of fit depend on the method by which calibration will be carried out.

A model that is calibrated against historical data can be quite different from the model used for prediction, because the hydrogeological system and the stresses applied to it may be quite different when proposed projects are undertaken in the future. Nevertheless, an objective of calibration is to learn as much as possible about model parameters that may have a significant influence on predictions.

Seeking to minimise a measure of goodness of fit during the calibration period, or to achieve a specific predefined value of goodness of fit, may or may not be the best way to increase confidence in predictions. This is because the parameters that have the greatest impact during the calibration period, and to which historical measurements may be most sensitive, may have less impact on predictions. Predictions may be less sensitive to these parameters, and more sensitive to others. It is possible, therefore, that a good outcome from model calibration is a set of estimates of model parameters that results in a larger (at first glance worse) measure of goodness of fit than the minimum.

Heads and fluxes can be sensitive or insensitive to specific model parameters during the calibration and prediction periods (Hill and Tiedeman 2007, Figure 8-2):

- If heads and fluxes are sensitive to parameters during calibration, predictive modelling may be successful, regardless of sensitivity to those parameters during prediction.
- If heads and fluxes are insensitive to parameters during both calibration and prediction periods, predictive modelling may or may not be successful.
- If heads and fluxes are insensitive to model parameters during calibration and sensitive to those parameters during prediction, there is a risk that prediction uncertainty may be high.

The approach taken to model calibration must be linked to the questions that all groups of stakeholders (project proponents, regulators and modellers) are trying to answer. It is important at the start of model calibration to understand the purpose of the model, that is, what the model is intended to predict. It is the desire for accuracy in future predictions that must drive the choices that are made during model calibration.

5.3 Calibration methodologies

5.3.1 Theory and practice

The theory of model calibration relies on an understanding of hydrogeology, mathematics, numerical analysis and statistics. Putting the theory into practice also relies on software engineering to embed algorithms and procedures in computer software.

Useful introductions to calibration methods are provided by Hill and Tiedeman (2007) and Doherty and Hunt (2010).

Nearly all modern approaches rely to some extent on the concept of weighted least squares estimation (WLSE). This approach can be developed heuristically, based on common-sense arguments, and does not rely on formal statistical theory. However, similar approaches can also be developed based on a number of different but related statistical philosophies: Bayesian estimation, Maximum Likelihood (ML) estimation, Maximum a Posteriori (MAP) estimation, pilot points in combination with geostatistics (kriging) (refer section 4.7 and many more (e.g. McLaughlin and Townley 1996).

In principle it is possible to fit a model to data by trial and error. Possible measures of goodness of fit are discussed below. Measures that include a sum of weighted squares of deviations are related to WLSE, and are therefore related to all statistical methods that use the concept of variance as a measure of spread. Other measures of goodness of fit are less likely to be supported by any kind of statistical theory.

In practice, apart from trial-and-error calibration, there are only options for automating the search for best estimates of model parameters, which include (also refer Table 4-1):

- PEST (Watermark Numerical Computing 2005; <www.pesthomepage.org>)
- UCODE (Poeter and Hill 1998; Poeter et al. 2005)

As shown in Figure 5-3, calibration is related to prediction and uncertainty analysis. When best estimates of model parameters are found by a formal calibration procedure, it is possible to estimate the covariance of these estimates. The propagation of uncertainty based on parameter uncertainty relies on a statistical description of this kind. In addition to the references given above, Doherty et al. (2010a, 2010b) describe calibration methods in the context of prediction uncertainty (refer Chapter 7).

5.3.2 Modelling without calibration

In some circumstances, groundwater models are needed to predict future behaviour in regions where there are no historical measurements. Without a calibration dataset, it is impossible to calibrate a model. This does not mean that modelling is not worthwhile. It simply means that there is a lower degree of confidence in models that are not supported by robust calibration.

Uncalibrated models can be useful to design field investigations, and to gain a general understanding of time and spatial scales, in the context of a specific field site or as a generalisation that may apply at many field sites. They are sometimes described as idealised models.

Even without calibrating a model, model parameters can still be considered to be uncertain. Simplifying Figure 5-3 to Figure 5-4 shows that for uncalibrated models, predictive scenarios and uncertainty analysis can be undertaken based on initial estimates of all model parameters and their uncertainty.

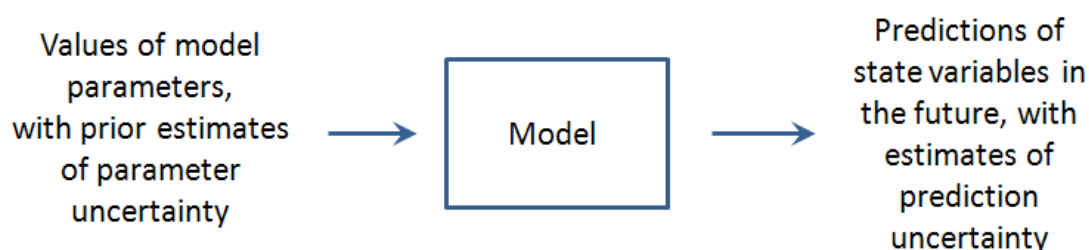


Figure 5-4: Prediction and prediction uncertainty without calibration

5.3.3 Calibration by trial and error

While automated calibration using computer software has been available for decades, it is still common for calibration to be attempted by trial and error. The model is run initially, using initial estimates of all model parameters, for the period of time during which historical data is available. Modelled heads and possibly fluxes are compared with observations, either numerically, graphically or spatially on a map. The following methods are commonly used:

- A scatter graph (see Figure 8-2a) can be used to show all predicted heads on the vertical axis and corresponding measured heads on the horizontal axis. Ideally, the data points in the graph should fall along a straight line through the origin with slope 1. Visual examination of a scatter graph is sometimes a good indication of progress towards successful calibration, but a scatter graph alone is inadequate in all but the simplest of steady state models. A scatter graph may provide an indication about which parts of a model need further attention, especially if points on the scatter graph are represented using different symbols in different regions or layers. A scatter graph can also be used for fluxes or any other quantities that are both predicted and measured.
- Goodness of fit is often measured using a simple statistic. Options include:

RMS: The root mean squared error.

$$RMS = \sqrt{\frac{1}{n} \sum_{i=1}^n [(z_{hi} - h_i)]^2} \quad \text{Eqn 5.1}$$

where z_{hi} are measurements of heads h_i at n locations and times.

SRMS: The scaled root mean squared error is the RMS divided by the range of measured heads and expressed as a percentage. Weights are sometimes introduced to account for different levels of confidence in different measurements.

$$SRMS = \frac{100}{\Delta H} \sqrt{\frac{1}{n} \sum_{i=1}^n [W_i (z_{hi} - h_i)]^2} \quad \text{Eqn 5.2}$$

where W_i are weights between 0 and 1, and ΔH is the range of measured heads across the model domain.

MSR: The mean sum of residuals uses absolute values of errors and is sometimes preferred because it places less weight on measurements that appear to be outliers. It can also include weights.

$$MSR = \frac{1}{n} \sum_{i=1}^n W_i |z_{hi} - h_i| \quad \text{Eqn 5.3}$$

When weights are 1, the MSR can be visualised as the average of all vertical deviations between points in a scatter graph and the 1:1 line. It is also visually related to the goodness of fit between hydrographs of predicted and measured heads.

SMSR: The scaled mean sum of residuals is the MSR scaled by the range of measurements and expressed as a percentage:

$$SMSR = \frac{100}{\Delta H} \frac{1}{n} \sum_{i=1}^n W_i |z_{hi} - h_i| \quad \text{Eqn 5.4}$$

- It is useful to compare time series of heads at specific locations, showing modelled heads as continuous lines (perhaps linearly interpolated, rather than smoothed, between modelled time steps) and observed heads as individual points.
- It is useful to compare the spatial distribution of heads, in plan or even in cross-section, comparing contours of modelled heads with point values of observed heads at specific times. Experienced hydrogeologists argue that contours of modelled heads can also be compared with hand-drawn contours based on observed heads, because experience can allow a hydrogeologist to infer the location of contours based on knowledge of geological structure and properties. In general, it is less useful to compare contours with contours, when contours between sparse measurements of heads have been obtained using contouring software that knows nothing about how heads need to vary in space to satisfy water balance equations. In principle, contouring software used for plotting predictions should be perfectly consistent with the spatial interpolation implicit within the model. This is possible for linear triangular finite element models, where there is an assumption of linear variation in head between nodes, but is not possible for finite difference models, since there is no explicit assumption of linear gradients between cells.

Trial-and-error calibration relies on the modeller's ability to assess the changes in modelled heads, relative to how one would expect the groundwater system to respond. It is a kind of sensitivity analysis (see below) in which changes in parameter values are chosen by the modeller and differences in modelled heads are compared using the measures described above (Eqns 5.1 to 5.4).

After each model run, with each new set of parameter values, the modeller considers the differences between runs, and attempts to choose new parameter values that will in some sense bring the model predictions closer to all available measurements. For example:

- when hydraulic conductivities are increased, heads and gradients tend to decrease, and response times (lags) decrease.
- when storage coefficients are increased, the response to recharge or pumping is less, and response times increase.
- when recharge is increased, heads and gradients increase.

It is not unusual for modellers to find that the calibration does not allow all aspects of historical measurements to be reproduced. Sometimes absolute values of heads are too high or too low, suggesting that hydraulic conductivities and recharge are not in balance, but trends are reasonable, suggesting that the relationship between hydraulic conductivity and storage coefficient is reasonable, or that the relationship between perturbations in recharge and specific yield are reasonable (refer section 5.4.1). In such cases calibration may be considered reasonable if differences in heads seem to be reasonable. There may be no theoretical reason to support this conclusion, but sometimes there appears to be no alternative.

5.3.4 Automated calibration

Powerful software is available to assist in model calibration. Through the use of software, the calibration process is partially automated, with software doing much of the work on behalf of the modeller, and a rigorous mathematical methodology is applied that increases the reproducibility of the calibration process compared to trial-and-error calibration. Given the complexity of the mathematical methods involved, the modeller needs a clear understanding of what the software is doing for meaningful results to be obtained.

All model parameters can and should be considered to be uncertain. Some parameters are more uncertain than others. A parameter that is known with certainty can be considered to be an estimate with zero variance. A parameter that is unknown can be considered to have virtually any mean and infinite variance. Between these extremes, parameters can be considered to have a prior estimate, based on hydrogeological investigations and context, with some finite variance that limits how far the parameter is likely to move from the prior estimate. This representation of 'prior information' allows a large number of model parameters to be estimated concurrently, with observations being used to inform the best choice of model parameters.

Software that assists during model calibration is 'optimisation' software, which searches for an optimal set of model parameters that are considered best, in some agreed sense.

All optimisation methods require:

- selection of a number of decision variables, that is, the parameters to be estimated
- an objective function, that is, a function of the decision variables, defined such that its value is to be minimised
- constraints that somehow limit the possible choices for the values of decision variables.

At the end of a successful search, the final set of values of the decision variables results in a minimum value of the objective function, and all of the constraints are met. The objective function is generally some kind of weighted least squares objective function that measures how well model predictions fit the historical observations, and sometimes how far estimated model parameters deviate from initial or prior estimates of the parameters. The RMS error defined above is closely related to an objective function, which both trial-and-error and automated calibration methods try to minimise. In automated calibration, a systematic mathematical search algorithm is adopted to find the minimum of the objective function (subject to constraints). Description of the methods used in this is beyond the scope of these guidelines. Suffice to note that the software tests different sets of parameter values until the optimum set is found.

The shape of the objective function can be complex. Rather than having a single minimum like a parabola, it can have many local minima. Setting out to find the minimum of a function with many minima is challenging, both from a computational point of view (if the objective is to find the global minimum) and from a philosophical point of view (because if many local minima have almost the same value, it may be hard to argue why local minima should be less significant than the global minimum).

Constraints include the fundamental requirement for mass balances (for water and solute), that is, that the predicted heads be a valid solution of the groundwater equations. In other words, the model itself provides a critically important set of constraints. Constraints may also include assumed upper and lower bounds on parameter values, for example, the physical requirement that hydrogeological properties should not be negative, or that specific yield and porosity cannot exceed 1. Some model parameters are transformed during automated calibration by taking the logarithm of the parameter values, so that it is never possible to estimate a negative value for a physical property that must have a value greater than zero.

5.4 Challenges and solutions

5.4.1 Identifiability and non-uniqueness

One challenge in model calibration is commonly described as the non-uniqueness problem; the possibility that multiple combinations of parameters may be equally good at fitting historical measurements. Model parameters can be non-identifiable or non-unique if the mathematical equations that describe a situation of interest depend on parameters in combination, rather than individually, in such a way that the product or ratio of parameters may be identifiable, but not the individual parameters themselves.

In the context of formal parameter estimation, whenever there is a tendency for parameters to be non-unique, the objective function ($J(\underline{u})$) is not a simple function in multidimensional parameter space with an obvious minimum. Rather, the objective function tends to have long narrow valleys, with gently sloping bottoms, and individual parameters are not uniquely identifiable (refer Figure 5-5).

These issues arise every time the aquifer flow equation (in two dimensions (2D)) or the groundwater flow equation (in three dimensions (3D)) are solved (refer example 5.2).

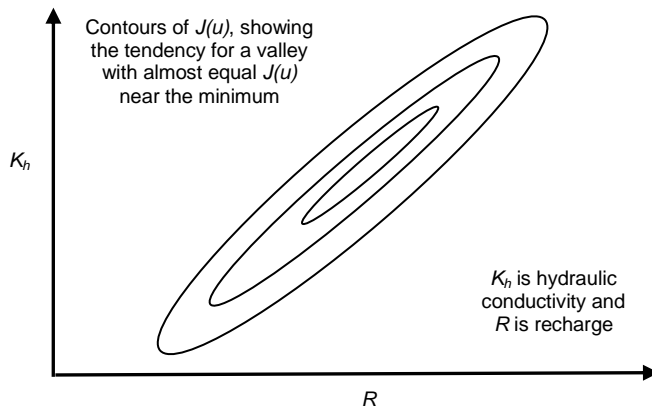


Figure 5-5: Valley in objective function with two model parameters

Example 5.2: The aquifer flow equation and identifiability.

Consider the case of flow in a homogeneous unconfined aquifer, where the watertable elevation, $h(x,y,t)$, satisfies:

$$S_y \frac{\partial h}{\partial t} = T \left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \right) + R \quad \text{Eqn 5.5}$$

where S_y is specific yield [-], T is transmissivity [L^2T^{-1}] and R is recharge [LT^{-1}].

1. In steady state, or in an almost steady state when the time derivative is negligibly small, or by averaging seasonal fluctuations over the course of a year, the steady head h_s satisfies:

$$\frac{\partial^2 h_s}{\partial x^2} + \frac{\partial^2 h_s}{\partial y^2} \approx \frac{R}{T} \quad \text{Eqn 5.6}$$

In this case, observations of $h_s(x,y)$ support estimation of the ratio R/T , but neither R nor T independently. Observations provide no information about S_y .

2. In the near field of a pumping bore, for example, during a short-term aquifer test, when recharge can be assumed to be zero or negligible:

$$\frac{\partial h}{\partial t} \approx \frac{T}{S_y} \left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \right) \quad \text{Eqn 5.5}$$

In this case, it is the aquifer diffusivity T/S_y that becomes identifiable in general, but not necessarily T or S_y independently. Observations provide no information about R .

3. In a regional flow system far from drainage boundaries, where seasonal watertable fluctuations can be explained by recharge in the wet season and evapotranspiration in the dry, the fluctuation in head, that is, the deviation of head from the long-term average, satisfies:

$$\frac{\partial(h-h_s)}{\partial t} \approx \frac{R}{S_y} \quad \text{Eqn 5.6}$$

In this case, the ratio R/S_y becomes identifiable, rather than R or S_y individually. Observations provide no information about T .

This simple exploration of the aquifer flow equation shows that in different circumstances, when any two of the three terms in the aquifer flow equation dominate the third, the three parameters of the equation are not themselves identifiable. Rather, the response of an aquifer depends on ratios of model parameters. In general, there is a tendency for all these ratios to influence the system response. To estimate all three parameters, observations are needed during periods when all three parameters influence the behaviour of the system.

5.4.2 Over-determined and under-determined systems

Another challenge relates to the number of available measurements and the number of parameters to be estimated, or more precisely, the amount of information contained in measurements and the effective number of parameters to be estimated.

In many fields of endeavour, large quantities of data are collected, and relatively simple models are required to explain the data. Such systems are **over-determined**, in the sense that there is more than enough data to allow accurate estimation or determination of model parameters. An example is classical linear regression, in which two parameters define a straight line that approximately fits large numbers of measurements.

Groundwater flow models, however, are often **under-determined**, for example, when hydraulic conductivity and other hydrogeological properties vary from point to point, at very small spatial scales, leading to a very large number of unknown model parameters relative to the likely number of measurements. When setting out to estimate a large number of model parameters, the objective function is unlikely to have a single global minimum, so it is difficult to obtain robust estimates of parameter values using automated methods. There are two main approaches to managing underdetermined systems:

- revising the parameterisation to reduce the effective number of parameters, for example using the pilot point method (De Marsily et al. 1984; Certes and de Marsily 1991). In essence, instead of attempting to estimate hydraulic conductivity for every cell in a finite difference grid, estimates are obtained at a number of pre-defined points and an interpolation method is used to interpolate or extrapolate from these pilot points to all cells, using an assumption about statistics that describe the nature of spatial variability
- regularising the problem by including additional information, including correlation between parameters. Even though hydraulic conductivity may be estimated for every cell, the spatial correlation means that the effective number of estimates is smaller.

In both cases, the modeller is attempting to make the calibration more robust.

5.4.3 Parsimony versus highly parameterised models

Guiding Principle 5.3: The modeller should find a balance between simplicity (parsimony) and complexity (highly parameterised spatial distribution of some properties). Non-uniqueness should be managed by reducing the number of parameters or by regularisation, which is a way of ensuring that parameter estimates do not move far from initial estimates that are considered to be reasonable.

With respect to model calibration, there are two broadly accepted schools of thought on this subject:

- proponents seek parsimony—the notion that the best model should have the smallest possible number of parameters (Hill and Tiedemann 2007). The parameterisation is chosen so that the model is overdetermined or if underdetermined, as close to determined as possible
- proponents believe that spatial variability should be allowed in all parameters, so as to avoid relatively arbitrary assumptions about the spatial distribution of parameters. The model is underdetermined, but as described above, the effective number of model parameters can be reduced. The best results will be obtained by taking advantage of all available data, including soft data, to regularise the objective function (Doherty and Hunt 2010).

Each of these has its place, depending on the objectives of modelling:

- The principle of parsimony is applied every time an aquifer test is used to estimate local values of transmissivity and storage coefficient.
- In regional problems where the focus is on predicting flow, predictions depend on large-scale spatial averages of hydraulic conductivity rather than on local variability. Moreover, in large regions there may be insufficient data to resolve or support a more variable representation of hydraulic conductivity. A parsimonious approach may be reasonable, using constant properties over large zones, or throughout a hydrostratigraphic unit.
- In local scale contaminant transport problems, flow paths and travel time may be significantly affected by heterogeneity at small scales, and efforts must be made to represent the spatial variability of hydrogeological properties that affect the predictions. A highly parametrised model may be required.

Groundwater-modelling software allows aquifer properties to be specified by layer, in zones and for individual elements and cells. Increasingly, it supports the pilot point method in which parameters are assigned (and ultimately estimated) at a small number of points within each material type and interpolated between those points to all elements or cells. The pilot point method allows representation of complex spatial distributions, using a reduced number of model parameters. By reducing the number of model parameters, it helps to solve the non-uniqueness problem, which sometimes occurs when a large number of model parameters individually have little effect on predictions.

The number of model parameters is not on its own a measure of the difficulty of calibration. If the number is large, and the system is underdetermined, there are a number of possible remedies to solve the non-uniqueness problem:

- **The pilot point method**, in which parameters are estimated at a small number of points and interpolated between those points to all elements or cells, allows representation of complex spatial distributions, using a reduced number of model parameters. The number of independent model parameters is effectively reduced.
- **Regularisation**, which means adding additional structure to the calibration problem so that it is more likely to have a unique global minimum, expands the objective function with additional terms that include prior estimates of all model parameters, their variances and possibly covariances. A model with hydraulic conductivity individually assigned at hundreds of thousands of cells could be equivalent to a model with one unknown hydraulic conductivity, if the individual values for each cell were considered to be perfectly correlated.

5.4.4 Information

Based on the notion that measurements contain information, and that the ultimate objective is to make the best possible use of all information, minimising the uncertainty in estimated parameters is equivalent to maximising the information contained in estimated parameters. Information has a common everyday meaning, but there is also a well-established discipline known as information theory.

Uncertainty and information are in many respects the inverses of each other. The information content of a measurement (e.g. of head) about a model parameter (e.g. hydraulic conductivity) depends on the sensitivity of the state variable being measured to that parameter.

Provided that a measurement is sensitive to a parameter, a good way to reduce uncertainty is to take more measurements. Not all measurements are equally useful, and it is not simply the number of measurements that matters. For example:

- If a piezometric head has been measured at a specific location in a steady flow system, taking another 100 measurements will do little to reduce uncertainty. Measurements that are clustered in space or time should be reduced to a smaller number of representative measurements prior to using the data in model calibration, or appropriately weighted to reduce the reliance on each measurement.
- If piezometric heads have been measured at two locations in a uniform flow field, an additional measurement half way in between may allow further resolution in the spatial distribution of hydraulic conductivity, but may do little to change an estimate of uniform hydraulic conductivity for the whole region.

The usefulness of data depends on parameterisation, the choice of parameters being estimated and the sensitivity of measured state variables to those parameters.

5.4.5 Performance measures and targets

Guiding Principle 5.4: Performance measures should be agreed prior to calibration and should include a combination of quantitative and non-quantitative measures. The SRMS is a useful descriptor of goodness of fit when the only objective is to fit historical measurements of heads, but is less useful when automated calibration methods are used. A target SRMS of 5% or 10% is only meaningful when those setting the target know that it is achievable for a particular kind of problem and a particular environment with a known density of informative data.

A number of performance measures have been proposed in the past to indicate when a model fits historical measurements 'well enough' to be acceptable for use in predictions. These include RMS, SRMS, MSR and SMSR (refer section 5.3.3). It has been suggested that performance measures, for example, $SRMS < 5\%$, should be agreed prior to a modelling study and that these should be included in acceptance criteria. However, experience has shown that it is not always desirable to specify a target value of some performance measure in advance. For instance:

- If there is insufficient information contained in available data to estimate model parameters that fit the available measurements, this should be interpreted as a limitation imposed by lack of data rather than a failure in modelling.

- If a performance measure is chosen, such as an SRMS error of 5% comparing all available measured and simulated heads, it is always possible for a modeller to achieve that target by introducing more model parameters. One can always modify the hydraulic conductivity and storage coefficient near an observation bore until the SRMS is small. The number of parameters can be increased in such a way that calibration appears to be robust and the SRMS becomes negligibly small, but there may be no rational hydrogeological basis to support the degree of detail (the number of parameters) added to the model. This phenomenon is known as ‘overfitting’. Overfitting should not be preferred relative to a larger SRMS with rational relationships between model parameters.
- If a regulator or other stakeholder has experience in a particular geographic region with particular types of aquifers with a particular density of data and with particular modelling objectives, it may be possible, after the successful completion of several modelling studies, to know that an SRMS of 5% (comparing all available measured and simulated heads) is achievable. In this case, setting a target of 5% SRMS prior to calibration may be reasonable.

The difficulty with predefined performance measures is that they may prevent a modeller from obtaining the best possible calibration, based on the information contained in all available data, and in some cases they may pervert the process by encouraging inappropriate parameterisation. A performance measure such as SRMS of heads, for example, cannot take into account the SRMS of fluxes or the goodness of fit with prior estimates of parameters (prior information).

All measures are less useful when measurements vary over many orders of magnitude, for example, for concentrations of solutes, or even when considering drawdown following aquifer tests. This leads to the temptation to take logarithms of the measured values. The deviations are differences of logarithms, which are effectively multiplying factors.

Model acceptance should be based on a number of measures that are not specifically related to model calibration (Table 5-1). These are required to demonstrate that a model is robust, simulates the water balance as required and is consistent with the conceptual model on which it is based. Many of these measures can be applied during the calibration and prediction phases of modelling.

Table 5-1: Performance measures and targets

<i>Performance measure</i>	<i>Criterion</i>
<p>Model convergence</p> <p>The model must converge in the sense that the maximum change in heads between iterations is acceptably small.</p>	<p>The iteration convergence criterion should be one or two orders of magnitude smaller than the level of accuracy required in head predictions. Typically of the order of centimetres or millimetres.</p>
<p>Water balance</p> <p>The model must demonstrate an accurate water balance, at all times and in steady state. The water balance error is the difference between total predicted inflow and total predicted outflow, including changes in storage, divided by either total inflow or outflow and expressed as a percentage.</p>	<p>A value less than 1% should be achieved and reported at all times and cumulatively over the whole simulation. Ideally the error should be much less. An error of >5% would be unacceptable, and usually indicates some kind of error in the way the model has been set up.</p>

<i>Performance measure</i>	<i>Criterion</i>
<p>Qualitative measures</p> <p>The model results must make sense and be consistent with the conceptual model. Contours of heads, hydrographs and flow patterns must be reasonable, and similar to those anticipated, based either on measurements or intuition.</p> <p>Estimated parameters must make sense, and be consistent with the conceptual model and with expectations based on similar hydrogeological systems.</p>	<p>Qualitative measures apply during calibration, when comparisons can be made with historical measurements, but also during predictions, when there is still a need for consistency with expectations.</p> <p>There is no specific measure of success. A subjective assessment is required as to the reasonableness of model results, relative to observations and expectations. The modeller should report on relevant qualitative measures and discuss the reasons for consistency and inconsistency with expectations.</p>
<p>Quantitative measures</p> <p>The goodness of fit between the model and historical measurements can be quantified, using statistics such as RMS, SRMS, MSR and SMSR for trial-and-error calibration and the objective function in automated calibration.</p>	<p>Quantitative measures only apply during calibration.</p> <p>Statistics of goodness of fit are useful descriptors but should not necessarily be used to define targets.</p> <p>Goodness of fit of heads is only one part of a regularised objective function—the other relates to agreement between parameter estimates and prior estimates, so in this situation, the two components of the objective function should both be reported.</p> <p>Targets such as $SRMS < 5\%$ or $SRMS < 10\%$ may be useful if a model is similar to other existing models and there is good reason to believe that the target is achievable. Even if a formal target is not set, these measures may provide useful guides.</p>

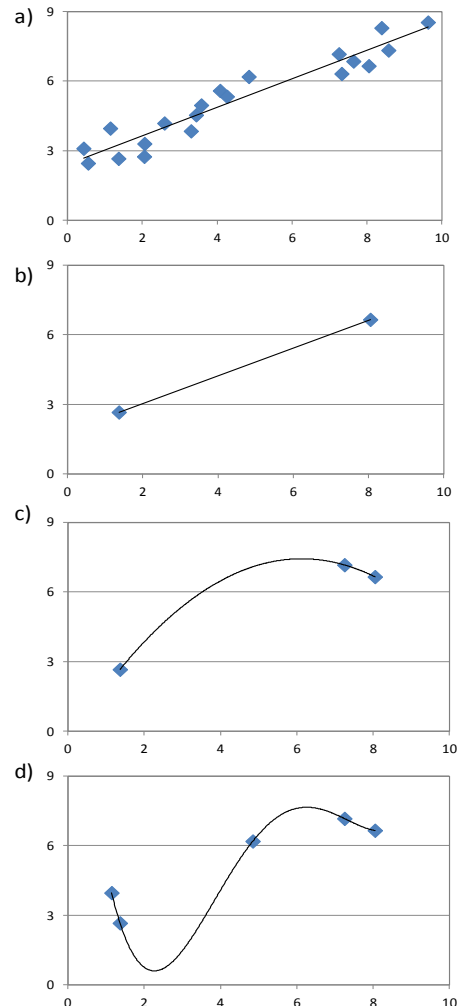
Example 5.2: The risk of over-fitting.

Many people are familiar with the concept of fitting a curve to data. The simplest and most common form of curve fitting is 'linear regression'. If a dependent variable y is believed to depend on an independent variable x , and if many combinations of x and y are measured and plotted, it is common to seek the equation of a straight line that best fits the data (plot a)). The line of best fit, often written $y = ax + b$, depends on two coefficients or parameters. In many senses, the equation of the straight line is a model; a simple functional representation of the relationship between y and x .

It is not uncommon for there to be many measurements of x and y , yet there are only two model parameters. Such a system is said to be overdetermined. When the line of best fit is plotted, very few if any of the measurements lie perfectly on the line, but overall the line appears to fit the data reasonably well. The differences between measurements and the line are known as 'residuals'. The method by which the line of best fit is chosen seeks to minimise the sum of the squared residuals, yet there is no way of knowing a priori, before the parameters a and b are computed, how small the residuals will be, or how small the sum of squared residuals will be. In spite of not being able to specify the goodness of fit a priori, the line of best fit would often be used to predict y for other values of x .

Consider what would happen if there were only two measurements of x and y . In such a case the line of best fit would pass through those two measurements perfectly (plot (b)). The line of best fit could be used to predict y for other values of x , but with so few data, that is, with such limited 'support' for the model, there may be less confidence than if more data had been available.

If there were exactly three measurements of x and y , a quadratic curve could be found that would pass through the measurements perfectly (plot (c)). If there were n measurements, a polynomial of order $n-1$ could be found that would pass through the measurements perfectly (plot (d)). However, there is no guarantee that such a polynomial would allow one to predict with confidence.



A numerical groundwater model is neither linear nor polynomial. The water balance equations that are solved analytically or numerically define the relationship between model parameters and the state variables (e.g. heads) predicted by the model. If there are more independent measurements of state variables than parameters, it is possible to estimate the parameters, for example by minimising the sum of squared residuals, but it is impossible to say a priori how small that sum will be. If the number of parameters is increased to equal the number of independent measurements of state variables, the sum of squared residuals can be driven to zero. But just as with a higher order polynomial, with many parameters, the level of confidence in predictions is less when an unjustifiably large number of parameters is estimated.

5.5 Sensitivity analysis

Guiding Principle 5.5: Sensitivity analysis should be performed to compare model outputs with different sets of reasonable parameter estimates, both during the period of calibration (the past) and during predictions (in the future).

In strict mathematical terms, a sensitivity measures how fast one quantity changes when another changes. A sensitivity is the derivative, or slope, of a function. In groundwater modelling, the term sensitivity analysis has several meanings, some quite rigorous and others much simpler.

During trial-and-error calibration, sensitivity analysis involves changing a model parameter by a small amount to establish how model predictions are affected by that change. Manual sensitivity analysis requires changing a single model parameter, re-running the model to obtain a new set of predicted heads and fluxes and observing the effect of the change, either by eye or numerically by differencing. In this context, a true sensitivity (derivative) is never calculated. The emphasis is on determining how sensitive the model is to each parameter, using a non-technical interpretation of 'sensitive'.

A similar interpretation applies when best estimates of parameters have been found, by trial and error or automated calibration. At this time, the same approach can be applied to predictions, either during the calibration period (in the past) or during predictive scenarios (in the future). Time-series plots of heads or fluxes, contour plots and tabulations of any kind of model predictions can be prepared using values of model parameters that are slightly higher or lower than the best estimates. These are compared visually with those based on the best estimates of parameter values. Hydrographs of predicted heads can include measurements of heads to provide a visual indication of goodness of fit with different parameter values. Care should be taken to choose increments in parameters that are sensible. It is not uncommon to vary hydraulic conductivity by an order of magnitude (a factor of 10), but each parameter should only be adjusted by an amount commensurate with its likely range.

During automated model calibration, the search algorithm computes sensitivities of the objective function to changes in all parameters and uses them to guide the search. When the best estimates are found, these sensitivities are used to estimate the uncertainty in the best estimates. This type of sensitivity can be examined using PEST and similar software to gain insights into the calibration process. If a particular sensitivity is small, the available data used in calibration provides no information about that parameter. If a modeller tries to estimate specific yield in a steady state problem, the sensitivity of the objective function will always be zero. This is a clear indication that calibration will provide no information about specific yield.

Sensitivity analysis is related to uncertainty analysis, which is carried out following the stage of predicting future behaviour of a system. In uncertainty analysis, sensitivities of predictions to model parameters are combined with a (statistical) description of parameter uncertainty, leading eventually to quantitative estimates of prediction uncertainty (refer Chapter 7 for more discussion on uncertainty). As a form of analysis following model calibration, using observations in some historical period, there could be justification for combining sensitivities and prior estimates of uncertainty to illustrate the uncertainty of the system during the calibration phase.

5.6 Verification

Guiding Principle 5.6: A formal verification process should only be attempted where a large quantity of calibration data is available and it is possible to set aside a number of key observations that could otherwise be used for calibration.

The terms verification and validation are not used consistently in the field of groundwater modelling, or in other fields. In some contexts, verification would mean comparing the results of a numerical model with an analytical solution to confirm that the numerical algorithm has been implemented correctly, while validation would mean checking the model against an independent set of data. Anderson and Woessner (1992) use verification in the same sense as in these guidelines and validation to describe what is described in Chapter 9 as a post-audit.

Verification involves comparing the predictions of the calibrated model to a set of measurements that were not used to calibrate the model. The aim is to confirm that the model is suitable for use as a predictive tool. Choosing not to use some data, and reserving it for verification, is a good idea in principle, but may not make the best use of available data.

Verification of a model is difficult. Some people argue that groundwater modelling has dubious value because models cannot be verified. But without modelling, it will never be possible to predict the future behaviour of groundwater systems.

6 Prediction

In this chapter:

- Introduction
- Predictive model time domain
- Modelling extraction from wells
- Climate stresses in prediction
- Particle tracking
- Predicting pore pressures
- Predicting groundwater responses to underground construction
- Annual aquifer accounting models
- Checking model results.

Guiding principles for predictive modelling

Guiding Principle 6.1: All model predictions are uncertain. The modelling process should acknowledge and address uncertainty through an appropriate uncertainty analysis (refer to Chapter 7).

Guiding Principle 6.2: The net impacts of future climate stresses (or changes in future climate stresses) should be obtained from the difference between predictions that include climate change assumptions and a null scenario that includes historic or current climate assumptions.

Guiding Principle 6.3: Particle tracking in groundwater flow models should be considered as an alternative to computationally demanding solute transport models in situations where advection is the dominant process controlling solute movement.

Guiding Principle 6.4: Caution should be exercised in accepting model results without first checking that they do not include any obvious errors or are influenced by model artefacts.

6.1 Introduction

Guiding Principle 6.1: All model predictions are uncertain. The modelling process should acknowledge and address uncertainty through an appropriate uncertainty analysis (refer to Chapter 7).

Predictions are used to obtain the outputs required to meet the project objectives. Accordingly, this is an appropriate time for the modellers and key stakeholders to revisit both the project *and* the modelling objectives (refer Chapter 2).

Output from predictive scenarios help answer the questions framed by the modelling objectives, which in most cases will involve a modification of the calibration model to implement changes to stresses (such as groundwater extraction or recharge) or changes to boundary conditions that represent future perturbations to the groundwater system. Predictions must be formulated in such a way as to provide the key outcomes being sought. The aim is to construct predictive models that will yield the required information with minimal uncertainty (even though uncertainty can be large).

This chapter provides a discussion and advice on commonly used approaches for dealing with a range of issues that arise during the development and use of predictive models. It includes advice on the implementation of future climate conditions and how to run such models in a manner that reduces predictive uncertainty. It also provides advice on how best to achieve convergence on required outputs for projects where optimised groundwater extraction rates are required.

Predictive models must be formulated in a manner that will provide the answers to those questions posed by the modelling objectives. They should include the appropriate representations of (future) boundary conditions, stresses and any other model features that are appropriate for the questions at hand. To some extent there is a need to revisit or consider aspects of the model design as the model time domain and discretisation, boundary conditions and the stresses to be included in the predictions may vary from the model used for calibration. For example, the predictions can be run in either transient or steady state mode irrespective of the temporal domain chosen for calibration. Even the hydrogeological properties may be different, for example, when modelling the effect of an underground tunnel or a sheet pile.

The groundwater flow model will predict groundwater heads and solute transport models predict concentrations at all nodes within the model grid or mesh of elements. In addition, fluxes of water and solutes are calculated between all adjoining model nodes and between model nodes and the defined boundary conditions. In steady-state models the calculations are presented as a single set of heads and/or concentrations that relate to the equilibrium condition for the particular combination of stresses and boundary conditions. When the model is run in transient mode, heads and/or concentrations are calculated at all nodes a number of times to provide a time series of model outputs.

The calculated model mass balance at each calculation interval is an important output that is often used to illustrate key model predictions. The mass balance includes a summation of all fluxes into and out of the model, including those defined as model inputs and those calculated by the model. The principle of conservation of mass (a constraint imposed by the groundwater equations) dictates that the difference between all fluxes into the model and those out of the model equals the change in storage

All groundwater models are uncertain. It is the modeller's obligation to, first, acknowledge uncertainties in modelling outcomes and to address this uncertainty through an appropriate confidence level classification for the model (refer to Chapter 2). The confidence level classification of the model predictions can be expressed quantitatively in a formal model uncertainty analysis, which is discussed in detail in Chapter 7.

Predictive scenarios can be formulated to quantify groundwater behaviour in absolute terms or in relative terms. In the latter, the particular modelling outcome is obtained by subtracting one model result from another (null scenario²) result.

² A null scenario is a predictive model that has no future changes in the stresses that are being investigated. For example, for a resource management model it may assume no groundwater extraction in the future or it may assume that current levels of extraction continue into the future.

Predictions in absolute terms are affected by uncertainties not only associated with the model itself but also with our inability to predict future groundwater stresses with any certainty. For example, a mine dewatering model must provide predictions of groundwater drawdown in the future as the mine is developed and grows. However, if there is an interruption to mining operations that causes a significant departure from the assumed mine development plan, the predictions of mine dewatering are compromised because the real mine development schedule differs from that assumed in the model. As a result, most groundwater model forecasts in absolute terms require frequent updating to allow for deviation from assumed conditions.

Model outputs obtained from calculating differences between two model simulations (e.g. the difference between a stressed and unstressed or 'null scenario' model) can reduce the predictive uncertainty associated with model outcomes.

The confidence level classification (refer to section 2.5) provides an indication of the relative confidence of the predictions. Indeed, the manner in which the predictions are formulated has a bearing on the classification as illustrated in Table 2-1. Both the period over which the predictions are run and the levels of stresses applied in the predictive models have a direct impact on some of the quantitative indicators that can be used to determine a relevant confidence level classification. The underlying assumption is that if the time frames and stresses used in a prediction are close to those of the calibration, the confidence of the prediction will be higher than when predictive time frames and stresses are significantly different from those of calibration.

6.2 Predictive model time domain

The term 'time domain' refers to the time frames in which the model is to be run. The modeller must determine whether predictive scenarios will be run in steady state or transient mode. Transient predictive models are used where groundwater trends with time are an important model outcome or if the stresses in the model are not constant in time.

Steady state models are particularly useful where the model is required to predict long-term groundwater responses and if the stresses and boundary conditions can be adequately represented as being constant with time. Steady state models are often useful in resource management where long-term impacts are required to assess sustainability of various assumed levels of extraction. Advantages of running steady state predictive scenarios are the short model run times and the outcomes not being clouded by seasonal fluctuations or trends leading up to steady state realisation.

If transient predictive scenarios are used it is important to consider the model simulation time period and an appropriate time discretisation for the calculations. Selection of the simulation time may be obvious. For example, mine dewatering scenarios will need to be run for the duration of the mining operations. However, sometimes the selection of an appropriate timeframe for model predictions is not trivial. Selection of the duration of a predictive model of the groundwater-level recovery following mine closure, for example, may not be immediately obvious and some trial runs (or application of analytical models) may be needed. Transient water resource management models will be run for the duration of the planning period. Where long-term sustainability is a management objective, the model should be run over a longer time frame than the immediate planning period, or possibly be run in steady state mode.

The temporal discretisation of predictive scenarios should be based on both the dynamic nature of the groundwater system and the desired outcomes. If a fine temporal resolution is not a requirement from the point of view of desired outcomes, fewer stress periods or time steps can be used so that model run times and output file sizes remain within reasonable limits. If the nature of the groundwater system is such that temporal features like tidal oscillations, seasonal recharge or pumping patterns exert a strong control on the water levels, a temporal discretisation that matches or is finer than the frequency of groundwater-level fluctuation is required.

Box 6A: CAUTION regarding the predictive model time frame.

The length of time that a transient predictive scenario is run compared to the length of time over which the model has been calibrated can influence the confidence-level classification of the prediction. When the predictive model duration substantially exceeds the period of transient calibration the uncertainty associated with the prediction increases. Accordingly, the ratio of predictive model duration to calibration model duration may become an important indicator of the confidence-level classification for predictive scenarios.

Limiting the duration of predictive model runs to less than five times the duration of the calibration is recommended wherever possible.

6.3 Modelling extraction from wells

Many predictive scenarios aim to identify the optimum distribution and rate of groundwater extraction that will result in drawdown or changes in fluxes that meet design or management criteria and are best considered as optimisations. Such scenarios are often needed for projects such as:

- **sustainable yield assessments**, where the model is required to help identify the maximum level of groundwater extraction that can be sustained by an aquifer. In this optimisation the maximum level of extraction is sought within maximum limits assigned to drawdown and other impacts
- **mine dewatering projects**, where the pumping rates and locations of individual pumping wells must be determined. For these models the optimisation is aimed at identifying the minimum pumping rate required to achieve a minimum desired drawdown.

Groundwater extraction from pumping wells is usually included in groundwater models as an input dataset, and those models aimed at determining optimum groundwater extraction rates usually involve a trial and error approach. In general, these predictive scenarios include a set of target responses that help to identify acceptable groundwater behaviour. For example, for a mine dewatering scenario a set of groundwater head criteria within the mine are defined as maximum head (or minimum drawdown) targets that indicate that the mine is effectively dewatered. The model is run with an assumed distribution of extraction wells and the model-predicted heads are compared to the dewatering targets. Groundwater extraction rates are varied until the targets are reached, usually with a minimum number of wells and minimum total extraction required.

Box 6B: CAUTION regarding the pumping rates included in predictions.

When groundwater extraction is modelled as point sinks, modelling artefacts may arise as the rate of extraction assigned to individual bores exceeds the rate at which water can be delivered by the aquifer at that point. Most model codes will automatically implement changes in the rate or location at which groundwater is taken from the model where the defined extractions cannot be sustained.

The modeller must understand how the particular model code will cope with over-extraction defined in individual wells and carefully check the model outputs to ensure that the actual modelled extraction rates are known and reported as opposed to those defined in the model inputs.

In some circumstances the model can be structured to allow the calculation of the extraction rate. To this end, the model can be formulated with Type 1 or Type 3 boundary conditions (refer section 4.5) to force the piezometric head to meet the target drawdown or groundwater head levels. The model can be run once and the required extraction rate is a calculated model output. This type of model formulation is particularly useful in mine dewatering predictions where the target dewatering heads can be clearly defined for the volume of the mining pit. The principal advantage of using this approach is that it provides an estimate of the dewatering pumping requirements in a single model run and avoids a trial-and-error process to estimate optimum groundwater extraction. The disadvantage is that it does not provide any information on the number and location of dewatering wells required. In practice, both approaches are often used. First, the model is run with boundary conditions enforcing the required drawdown. The model is run with individual extraction wells. The choice of pumping rates assigned to the extraction wells is informed by the predicted extraction rates obtained from the initial model run. In this manner the trial-and-error convergence to the optimum solution is accelerated by the initial estimate of optimum extraction rate.

Box 6C: CAUTION regarding modelling extraction wells.

A predictive groundwater model will generally not adequately represent those processes occurring in and immediately around extraction wells (commonly referred to as 'well losses'). As such, there is no guarantee that pumping wells constructed at the site will be able to deliver the pumping rates included in the model.

To address this issue the modeller should take account of any pumping tests or pumping trials that have been undertaken at the site to ensure that a realistic maximum pumping rate is adopted for individual extraction wells.

6.3.1 Spatial distribution of extraction wells

Choosing an appropriate spatial distribution for groundwater extraction wells included in prediction models will impact on the outcomes obtained from the model. This issue is particularly relevant for simulations formulated to help define the sustainable yield of a regional aquifer³. The manner in which the problem is addressed usually involves an initial definition of sustainability criteria in which water resource managers and other stakeholders create rules for assessing the acceptability of estimated impacts of extraction (Richardson et al. 2011). Sustainability criteria will typically include resource-condition limits that relate to groundwater levels, salinity, baseflow reduction in rivers or springs or reduction in evapotranspiration representing a loss in water availability to vegetation that accesses groundwater. The specified model extraction rates can be iteratively refined in order to determine the maximum level of extraction that can be applied without violating or breaching the sustainability criteria. The process may be run manually, or it can be managed through an automated optimisation routine.

The following issues should be understood when running models to support a sustainable yield assessment:

³ It should be recognised that groundwater models do not, by themselves, provide a value of sustainable yield.

- The sustainable yield of an aquifer, as indicated by groundwater modelling, depends on the arrangement of extraction wells included in the predictive scenarios. In many cases the predictive model will be set up with existing extraction wells only. This approach is valid when the aquifer in question has a history of extraction. In this case it can reasonably be assumed that the water users have optimised their extraction to take account of water availability, water quality and other socioeconomic drivers. Provided these factors do not change substantially over time it can be assumed that these are the locations best suited for future extractions from the aquifer. However, in aquifers or areas that have not been exploited in the past it may be necessary to define a distribution of extraction wells that represent the potential locations of future pumping wells.
- Optimisation schemes can be set up to automate the convergence to a maximum sustainable yield given a set of criteria such as trigger levels identified at key indicator sites in the aquifer. A number of software tools provide optimisation routines that facilitate the inclusion of such runs in a predictive modelling format. In many instances such models will overestimate the sustainable yield simply because the distribution of extraction wells resulting from the optimisation process cannot be replicated in reality. It is recommended that optimisation schemes be used with some caution in predictions to ensure that unrealistic distributions of extraction wells are avoided.
- Resource managers often develop adaptive management plans to manage groundwater resources. These plans involve reducing seasonal groundwater allocations in times of drought. Often a set of observation wells will have trigger levels assigned to them and the management rules are implemented at times when the trigger levels are breached. This problem is not easily modelled. It requires the outputs at each model calculation step to be interrogated during simulation and, if a trigger level is breached, a reduction in groundwater extraction is implemented and maintained until piezometric levels recover to the original or alternative trigger level. At that time the model will allow extractions to revert to their previously defined levels. Model codes have recently been developed that allow the use of adaptive management rules in predictive model scenarios and it is likely that such models will be regularly used in the future. Under this type of management regime it is not always necessary to define a sustainable yield for a resource and the maximum level of acceptable extraction will vary with time and climatic conditions.

6.3.2 Dewatering wells

The modeller should be aware of limitations with dewatering-well performance when an excavation is planned to the base or near the base of an aquifer unit. Problems arise when dewatering wells are designed to only extract water from the aquifer that must be dewatered. Dewatering pumping in this case will eventually cause a decrease in the saturated thickness and transmissivity (refer section 1.5.1) of the aquifer at the well location. Eventually the decrease in transmissivity will lead to a reduction in the possible pumping rate as the remaining saturated sediments are unable to transmit the required fluxes of water to the dewatering well. As a result, it can be shown that an aquifer cannot be dewatered to its base level by pumping from bores that extract water from that aquifer alone.

This problem can be avoided by ensuring that dewatering wells are designed to extract water from the aquifer itself as well as from formations or sediments beneath the aquifer that is to be dewatered. Alternatively, dewatering can be achieved by a combination of pumping from dewatering wells and from drains and sumps constructed in the pit floor. This strategy can be modelled through the combined use of dewatering extraction wells and Type 1 or Type 3 boundary conditions (refer section 4.5) applied to the excavation to represent in-pit drainage and pumping. In this case, the modeller should ensure that the assumed drainage of the mine floor represented in the model is realistic and can be achieved in practice.

In some cases a mine-dewatering design may include the use of horizontal drains or wells constructed on benches in the mine pit. These features are best modelled as head-dependent boundary conditions (Type 1 and Type 3 boundary conditions) that are able to extract water from the model when the calculated heads exceed the specified head (e.g. the drain elevation). In this type of model it may be necessary to limit the boundary flux to ensure that modelled extraction rates do not exceed the maximum possible flow through a drain of the specified dimensions. Care should also be taken to prevent the boundary condition acting as a recharge source once heads fall below the specified head. This can be achieved by selecting an appropriate type of boundary condition (e.g. one that only allows groundwater discharge).

6.4 Climate stresses in predictions

Guiding Principle 6.2: The net impacts of future climate stresses (or changes in future climate stresses) should be obtained from the difference between predictions that include climate change assumptions and a null scenario that includes historic or current climate assumptions.

Climate stresses are defined as the removal and addition of water from and to an aquifer through processes such as rainfall and evapotranspiration, related to interactions of the groundwater system with the atmosphere. As most predictive models are aimed at predicting future groundwater behaviour, it is often necessary to determine or assume future climate stresses when formulating model predictions. Where the climate stresses are not an important component of the model water balance (e.g. in mine dewatering predictions) it is acceptable to include historic recharge and evapotranspiration stresses in the prediction models. In other cases, such as in regional models for sustainable yield estimation, recharge and evapotranspiration are major components of the water balance and it is often necessary to take account of future climate variability in prediction models.

Assessing the impacts of future climate change on groundwater behaviour has become an important aspect of many groundwater modelling studies in recent years. In these scenarios climate change assumptions must be implemented. Typically, these assumptions include future changes in recharge and evapotranspiration and may also involve changes in boundary conditions that represent water levels in surface water features such as lakes and rivers or the ocean. Where models are required to predict impacts due to future climate change, the prediction model results are generally represented as the difference between the climate change scenario and a null scenario that has been formulated with historic climate.

Climate change assumptions may involve a simple assumed shift in hydrogeological condition (e.g. a uniform and arbitrary reduction in recharge), a statistical analysis of historic climate to generate synthetic climate stresses or more complex assessment of global climate model results with associated modelling of unsaturated zone processes to provide time series changes in recharge, evapotranspiration and river stage data.

Box 6D: CAUTION regarding the use of recharge models to develop climate change scenarios.

Recharge modelling is often undertaken in isolation to groundwater modelling. For example, recharge investigations undertaken at a national scale, such as those described by Crosbie et al. (2011), provide recharge estimates for current and possible future climates. There will most likely be discrepancies between the recharge model predictions and the recharge fluxes included in the groundwater model. Where the recharge model is used to assess climate change impacts, the use of recharge scaling factors obtained from the recharge modelling to scale up or down the groundwater model recharge can provide an effective modelling approach. For example, if the recharge model suggests that the future climate will, on average, lead to a reduction in recharge of 5% compared to current or recent historic recharge, the groundwater model should be run with a 5% decrease in recharge to capture the impacts of a future drier climate. In other words, the groundwater model should reflect relative changes in recharge and not necessarily the absolute recharge rates obtained by the recharge model.

6.5 Particle tracking

Guiding Principle 6.3: Particle tracking in groundwater flow models should be considered as an alternative to computationally demanding solute transport models in situations where advection is the dominant process controlling solute movement.

Predictive particle-tracking scenarios using model codes such as MODPATH provide a useful means of estimating the maximum travel distance of solutes in the groundwater model. These models assume that solute movement is controlled entirely by advection and that density-dependent flow, dispersion and diffusion are of minor significance. The method involves identifying specific particles at locations of interest in the model domain and defining a release time for these particles. The model code estimates the location of the particles at each calculation step based on the modelled flow field and develops a trace that defines the particle trajectory through the model domain.

Particle-tracking models provide a simple means of assessing potential water quality impacts without the need for the added sophistication and computational effort of a solute transport model. Models may be run with transient or steady state groundwater models and calculation can be forward in time (i.e. particles are traced as they move after the time of release) or backward in time (i.e. particle locations are plotted at times leading up to the 'release time' or reference time).

Forward-tracking models are often used to determine the maximum likely extent of water migration over a defined period. Examples of the use of forward-tracking models include the estimate of the maximum likely extent of contamination given an assumed time and location of contaminant release or the estimate of the extent of water movement from a seawater–freshwater interface due to increased extraction of fresh groundwater near a coastline.

Backward tracking is particularly useful for estimating groundwater-source protection zones and may be considered as defining the locations of particles at defined times prior to arriving at a particular location. For example, backward tracking can be used to identify the distances that particles will travel to a proposed water supply well over the period of one year or other relevant time frame. In this manner, an exclusion zone surrounding a water-supply well can be estimated such that particles entering the aquifer outside the exclusion zone will take more than a certain time to appear at the extraction well.

6.6 Predicting pore pressures

When groundwater models are used to investigate the flow of groundwater to and around excavations below the watertable they are often required to provide input to geotechnical stability studies aimed at assessing the risk of pit wall and pit floor failure. Pit stability concerns arise from the fact that, under some circumstances, high hydraulic gradients can build up immediately behind pit walls and under the floor of a pit or underground mine. Slope stability assessment will require the model to provide estimates of pore pressure in the formations immediately behind pit walls and beneath the pit floor. Most groundwater model outputs are in the form of hydraulic heads. The pore pressure in each node is related to the head and can be estimated by the following equation:

$$P = \rho g(h - z) \quad \text{Eqn 6.1}$$

Where: P = pore pressure (Pa)

ρ = water density (on the order of 1000 kg/m^3)

g = gravitational acceleration (9.81 m/s^2)

h = modelled head (m)

z = elevation of the node (m)

The use of 2D vertical slice models is recommended for predicting pore pressures in and around deep excavations so that the detailed geometry of the pit shape can be incorporated. Model location and orientation should be carefully chosen to ensure that representative slices can be assessed as well as those that include the worst case from a stability point of view.

Box 6E: **CAUTION** regarding models used to assess pit stability.

Pit wall stability issues in deep excavations often arise where there are anomalously low-permeability sediments (e.g. clay layers in a sand aquifer) close to the excavation. While substantial layers of clays, for example, may be included as a feature in a groundwater model, less-significant layers or lenses may be equally significant in terms of pit wall stability but may not be included explicitly in the model. In other words, the local variation of the hydraulic conductivity distribution that gives rise to pit stability problems may be at a scale that is not adequately captured or represented in the groundwater model. The modeller should clearly articulate the issue so that geotechnical engineers and mine operators are fully aware of the limitations arising from simplifications included in the groundwater model.

6.7 Predicting groundwater responses to underground construction

These predictive scenarios are run to assess groundwater responses that may occur during the construction and operation of underground structures, including tunnels and underground mines. In particular, they are used to assess temporary and long-term inflow rates to drains used to control groundwater levels in and around underground facilities, and to assess the impacts that these inflows may have on regional groundwater levels, fluxes to and from surface water bodies, and groundwater availability for groundwater dependent ecosystems. Predictions are also often aimed at estimating the impacts of a relatively impermeable structure, such as a concrete-lined tunnel, on the groundwater flow system.

The principle usually adopted for modelling a tunnel is to assume that at certain times it acts as a drain that removes groundwater from its surroundings. Tunnels are generally designed to either be:

- **fully drained**, in which case water is pumped from drains at the base of the tunnel so that the piezometric head will remain near the base of the tunnel during normal tunnel operation, or
- **tanked**, in which case the piezometric head is able to rise above the tunnel level during operation. In this case, the tunnel is designed to withstand the hydrostatic pressures that develop when it is submerged below a piezometric head that may be many metres above the tunnel level.

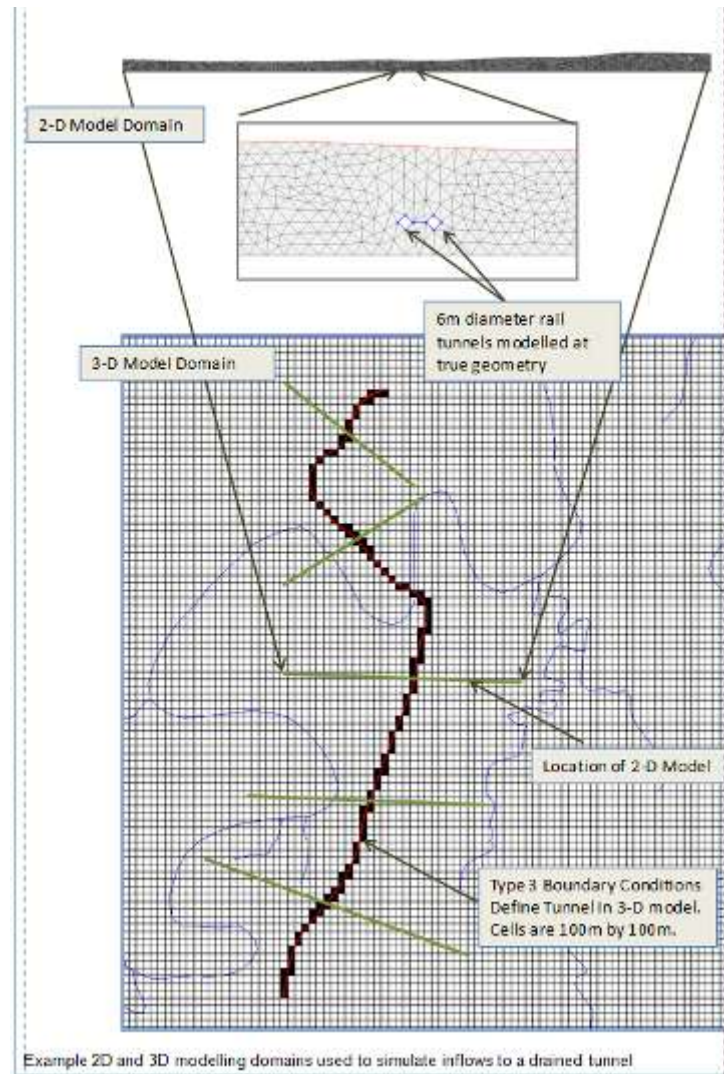
For tanked tunnels the primary question often posed to a model is: *how much water is pumped from the site during construction when temporary dewatering is often required to control inflows? A second question is: what will be the impact on groundwater flows of the emplacement of a near-impermeable tunnel liner below the watertable?* For fully drained tunnels the question is often: *how much water will be drained from the tunnel during operation to maintain the required piezometric head condition at the tunnel location? And what are the impacts of this water extraction?* In both cases the modelling scenario generally involves the use of Type 1 or Type 3 boundary conditions that force the piezometric head at the tunnel location to the tunnel-invert level at times when it is drained. Models may also require the introduction of impermeable barriers to replicate the changes in hydraulic conductivity provided by the tunnel lining.

Often the model is designed to assess environmental impacts of the tunnel construction and operation and, as a result, the model domain is often large compared to the tunnel cross-section. The modeller must either design the model grid to be able to provide fine-scale resolution at the tunnel (e.g. using a finite element mesh) or allow for model cell sizes that represent a larger volume of aquifer than the volume that will be drained around the tunnel. Where the problem is modelled in three dimensions and the model discretisation is too coarse, model cells may be substantially larger than the tunnel itself. Attempts to force the piezometric head to the tunnel-invert level will result in the draining of a much larger volume in the model compared to that in reality. The problem can be solved through the use of a series of 2D slice models oriented perpendicular to the tunnel axis. In this arrangement it is possible to accurately represent the shape and size of the tunnel cavity in the model. Scenarios can be run with appropriate boundary conditions that control piezometric heads in the tunnel cavity and tunnel inflow results should be reported in terms of flux per unit of tunnel length. A number of different models may be required to account for variation in stratigraphy and tunnel depth below the piezometric surface.

If necessary the results from the 2D models can be used to control or moderate inflows to the tunnel when modelled in three dimensions. In this case the tunnel inflows are modelled in the 3D model as Type 3 boundary conditions and the boundary condition conductance term is adjusted to ensure that the inflows are equivalent to those predicted by the 2D model under a set of standard conditions.

Example 6.1: Models used to investigate groundwater inflows to a tunnel and the associated impacts

The figure below shows an example of how a number of 2D finite element models (five in total) have been used in combination with a 3D finite difference model to assess changes in both groundwater levels and fluxes to nearby surface water features during construction and operation of a drained rail tunnel (consisting of two parallel tunnels each of 6 m diameter). The 2D models include the rail tunnels with their true geometry. The 3D finite difference model has grid cells that are 100 m by 100 m in size. The tunnel is included as a linear arrangement of Type 3 boundary condition cells with the conductance term adjusted so that the inflows to the tunnel match those predicted by the 2D models.



Example 2D and 3D modelling domains used to simulate inflows to a drained tunnel

6.8 Annual aquifer accounting models

Groundwater models are sometimes used to support annual water balance estimates for important regional aquifers. Often termed *accounting models*, they are formulated with groundwater extractions, climatic stresses and river-stage levels all estimated from measurements and records made for the year in question. The initial conditions for accounting models are obtained from the final heads predicted by the previous year's model. The model is run and mass balance time-series results are extracted to illustrate the aquifer behaviour over the course of the year. The models can also be used to illustrate changes in groundwater levels that may have occurred over the duration of the year and these can be related to changes in aquifer storage over the same period. The account itself can be presented in a variety of formats, including one that is similar to an annual financial statement in which assets (water available in storage) and liabilities (water extracted) are quantified.

The principal objectives of this type of model are to review the impacts of the groundwater allocation for a particular year and thereby help to improve the allocation process in future years. In many regards this type of model run is not a prediction; rather it is a progressive validation of the model by periodic simulation of historic groundwater behaviour. It represents an opportunity to continually update model currency and to periodically review or validate the model calibration. It is recommended that predicted groundwater behaviour (in particular groundwater levels) in each annual model run be compared against observations so that an informed decision can be made on when model recalibration may be required.

6.9 Checking model results

Guiding Principle 6.4: Caution should be exercised in accepting model results without first checking that they do not include any obvious errors or are influenced by model artefacts.

All model results should be checked to ensure that there are no obvious errors. A series of checks are suggested that are equally applicable to all model runs (not only predictive runs). Checks should not be limited to those model results that are of direct importance or significance to the particular problem being addressed. In fact, it is the spurious model features, or so-called artefacts in parts of the model, that are not being directly reported that are commonly missed. It is important to assess, and if necessary remove, modelling artefacts, as they can significantly reduce the value or accuracy of the result being sought.

The model mass balance should be reviewed to check:

- **Groundwater extraction rates are as specified in the model input files.** If cells that host groundwater extraction go dry during a model run, the extraction from such cells may cease or may be moved to another location (depending on the software package being used). Where this occurs, it identifies areas where the applied extraction exceeds the model's ability to deliver the required water. In some cases the outcome can be noted as an important finding from the model run. In other cases it may be necessary to redistribute the groundwater extraction to avoid excessive drawdown.
- **The predicted net seepage to or from a riverbed does not exceed measured or expected river flow.** Most model codes do not limit the water exchange between groundwater and a river or other surface water body. The modeller should use the tools available within the chosen model code or GUI to restrict the mass fluxes when model results are physically untenable.

- **The presence of anomalous boundary fluxes.** Sometimes the superposition of head-dependent sinks (e.g. evapotranspiration) on head-dependent boundary cells (Type 1 or Type 3 boundary conditions) can lead to unreasonably large fluxes through the individual boundary cells. Avoid superimposing such conditions.
- **Recharge due to rainfall does not exceed rainfall.** Such outcomes may arise if recharge is modelled as a head-dependent boundary condition. The problem can be solved by using a groundwater source term or flux boundary condition to model rainfall derived recharge.
- **Model storage changes are not dominated by anomalous head increases in cells that receive recharge but are isolated from other cells or boundary conditions.** Predicted groundwater heads in model cells or groups of cells that become isolated from model boundary conditions will rise without limit in response to applied recharge fluxes. The problem can be overcome by either de-activating these cells or by re-designing the model to avoid the cells becoming isolated.
- **Mass balance closure error.** In numerical models the solutions to the groundwater equations are numerical approximations and, as a result, there is always a small closure error in the mass balance. A cumulative mass balance error of not more than 1% of the total mass balance is considered acceptable. Errors larger than this value point to some inconsistency or error in the model⁴. Closure errors can be minimised by using small numerical values for the *head change* and *residual* criteria for defining numerical solution.

Contours of the predicted groundwater levels should be reviewed and compared against the conceptual understanding of groundwater flow directions. They should also be checked to ensure that the predicted heads are within reasonable limits. In some cases extreme and untenable groundwater heads can be generated in a model when cells dry out during a model run. As indicated above, extremely high heads can sometimes be predicted in cells or groups of cells that become isolated from the rest of the model and there is no mechanism for the removal of water that recharges these cells. Similarly, when shallow layers dry and are not re-wetted, underlying cells can become confined and generate anomalously high heads. In many cases such problems do not impact significantly on the important model results and hence the issue can be ignored. Conversely, the anomalies may have a direct impact on the modelling outcomes being sought and the problem must be solved by reconsidering the model design.

Individual predictions should be checked by comparing the predicted groundwater responses to analytical solutions where possible. It is expected that, if the model has been developed and calibrated in a sound manner, it will yield more accurate predictions than an analytical solution (in fact, this is one of the reasons for developing a numerical model in the first place). However, in many cases analytical solutions can provide a benchmark for a sanity check on numerical modelling outcomes.

⁴ While a maximum level of the global mass balance closure error has been set as a requirement for a high-confidence-level classification, it does not by itself indicate a good model. It should also be noted that there may be significant mass balance errors within specific locations of a model even when the global mass balance error meets the agreed criterion.

7 Uncertainty

In this chapter:

- Introduction
- The concept of uncertainty
- Sources of model uncertainty
- Relation of model calibration to model uncertainty
- Common approaches for estimating uncertainty
- Communicating uncertainty to decision makers.

Guiding principles for uncertainty analysis:

Guiding Principle 7.1: Because a single ‘true’ model cannot be constructed, modelling results presented to decision-makers should include estimates of uncertainty.

Guiding Principle 7.2: Models should be constructed to address specific objectives, often well-defined predictions of interest. Uncertainty associated with a model is directly related to these objectives.

Guiding Principle 7.3: Analysis of uncertainty should recognise that the uncertainty of predictions increases with the level of dependence on knowledge of small-scale system detail. Model predictions that integrate larger areas are often less uncertain because characterisation methods are well-suited to discern bulk properties, and field observations directly reflect bulk system properties.

Guiding Principle 7.4: Analysis of uncertainty should recognise that there is more uncertainty when reporting confidence intervals around an absolute model output, and less uncertainty when a prediction can be formulated as a subtraction of two model results.

Guiding Principle 7.5: When appropriate for the prediction of interest, linear uncertainty methods should be considered a primary tool for conveying the modelling estimate of uncertainty, because they are less computationally intensive than other methods.

Guiding Principle 7.6: Uncertainty should be presented to decision-makers with visual depictions that closely conform to the decision of interest.

7.1 Introduction

Management decisions will often be directly informed by model predictions. However, we now know there can be no expectation of a single ‘true’ model; thus, model results are uncertain. Understandable reporting of underlying uncertainty provides necessary context to decision-makers, as model results are used for management decisions. This, in turn, forms a mechanism by which groundwater models inform a risk-management framework because uncertainty around a prediction provides the basis for estimating the probability or likelihood of some event occurring. Given that the consequences of management decisions vary, it follows that the extent of and resources devoted to an uncertainty analysis may depend on the consequences. For events with low impact, a qualitative, limited uncertainty analysis may be sufficient for informing a decision. For events with a high impact, on the other hand, the risks might be better assessed and associated decisions made using a more robust and comprehensive uncertainty analysis.

The purpose of this chapter is to provide guidance on uncertainty analysis through discussion of concepts and approaches, which can vary from heuristic (i.e. the modeller's assessment of prediction uncertainty based on trial and error and experience) to a comprehensive, sophisticated, statistics-based uncertainty analysis. Most of the material presented here is taken from Doherty et al. (2010) if not otherwise cited. Although the treatment here is necessarily brief, the reader can find citations for the source material and additional references within this chapter.

7.2 The concept of uncertainty

Guiding Principle 7.1: Because a single 'true' model cannot be constructed, modelling results presented to decision-makers should include estimates of uncertainty.

Guiding Principle 7.2: Models should be constructed to address specific objectives, often well-defined predictions of interest. Uncertainty associated with a model is directly related to these objectives.

Doherty et al. (2010) describe an ideal model in the following thought experiment: suppose that the complexity of a numerical model is such that the model's ability to simulate environmental processes at a site is perfect. Such a model would need to be as complex as the salient natural processes it simulated. Furthermore, it would need to account for all spatial and temporal variability of hydraulic and other properties of the system that it is to simulate. If these properties were all known and the model was parameterised accordingly, the model would predict with perfect accuracy the response of the system to a set of user-supplied inputs.

Although this exercise defines the ideal, models are *defined* as a simplification of the natural world. Simplifications—short cuts that underpin solvable models—deviate from this ideal and thus can impart unintended and unquantified artefacts to the model simulation, which may or may not affect the model's ability to simulate a prediction of interest. Common simplifications required by the model design are assumptions of steady state, or practical limitations in model size. Even the model assumption that the natural world is invariant within a model node blurs natural-world detail, yet is required of all lumped-parameter hydrologic models. Moreover, even if a model is transient, time-stepping schemes require temporal averaging of model inputs and associated time-varying parameters.

A model's inability to represent spatial and temporal heterogeneity is rarely the primary driver of uncertainty, especially in modern computing environments that allow many nodes or time steps. Instead, the potential for model predictive uncertainty is set by an inability on the part of the modeller to supply accurate parameterisation detail at the fine spatial and temporal scale that most models are capable of accommodating. Finally, the *field observations* we use to constrain the world of possible models have inherent error associated around their measurement. Therefore, all models contain uncertainty, no matter how much effort and expense has been brought to bear to have it be otherwise.

Box 7A: Model uncertainty in a decision-making context—modified from Doherty 2011 and Hunt and Welter 2010

A decision often must address the fact that something bad may happen. We may be willing to pay a price to reduce the likelihood of its occurrence. How much we are prepared to pay depends on the cost of its occurrence and the amount by which its likelihood can be reduced through pre-emptive management. The role of modelling in this process is to assess likelihood. This must not be confused with predicting the future. Modelling should constitute a scientific expression of our ignorance rather than a claim to knowledge that we do not possess. When it makes a prediction, a model cannot promise the right answer. However, if properly constructed, it can promise that the right answer lies within the uncertainty limits that are its responsibility to construct. Obviously these limits should be as narrow as possible, given local expert knowledge and the information content of site-specific data. Extraction of maximum information from that data during the history-matching process through which uncertainty limits are constrained through replication of historical system behaviour is therefore an integral part of the modelling process.

Groundwater model uncertainty also interacts with the decision-making process in less-obvious ways. As noted by many, the model-construction process organises and formalises potential conceptual models of a groundwater system. This in and of itself has utility because it raises the discussion of contrasting professional opinions to discussion of reasonableness of process and ranges of model inputs. Even models that fail provide useful insight into the utility (or futility) of the conceptual model—an insight that often is more useful than partially successful model results. Moreover, quantitative hydrologic models often feed less quantitative ecological, economic and societal elements of decision-making. Without admittedly heuristic insights gained from these groundwater models, what instead could be used to inform these elements? Finally, although we cannot calculate hard and fast error bars around a model prediction, attempts at such calculations can still have value; perhaps the most under-appreciated utility of models is for calculating the reduction in prediction uncertainty resulting from different actions such as data collection. By subtracting the prediction uncertainty for various scenarios of future monitoring and data collection, for example, we can extract insight that is more resilient to the confounding effects of unknown unknowns. This type of model output facilitates focusing on efficient use of current and future monitoring resources—something valued by many decision-makers, regardless of background, system managed and social context.

Because all models have uncertainty, it follows that no model output should be reported as a *single* model result unless that single result is accompanied by a due-diligence effort at estimating the associated expected uncertainty. Indeed, Doherty (2011) points out that after all sources of uncertainty are considered, the very best any model can hope for is to:

- report a representative uncertainty for a prediction
- minimise that uncertainty to the extent possible given the time, effort, and field data available
- provide the calculation of representative uncertainty in a time frame consistent with the speed of decision-making.

One desirable adjunct to uncertainty analysis is the mechanism to quantitatively identify which factors contribute most to the prediction uncertainty. This, in turn, allows formulation of cost-benefit analyses that can facilitate the most cost-effective strategy of data-gathering and/or modelling to reduce predictive uncertainty (see Examples 7.1 and 7.2).

As pointed out in section 5.5, uncertainty analysis builds upon, but is distinct from, sensitivity analysis. Whereas sensitivity simply evaluates how model outputs change in response to changes in model input, uncertainty analysis is a more encompassing assessment of quality of model predictions. In uncertainty analysis, sensitivities of predictions to model parameters are combined with a statistical description of model error and parameter uncertainty. Thus, the uncertainty associated with a prediction depends on both the sensitivity of the prediction to changes in the model input, and on the uncertainty of the inputs, parameters, observations and conceptual model itself.

Example 7.1: Parameter sensitivity versus prediction uncertainty

Suppose a regional groundwater model calibrated solely on head data is used to predict a long-term groundwater-derived stream flux. A sensitivity analysis would show that the modelled heads are appreciably sensitive to both changes in aquifer transmissivity and recharge; the simulated heads will be different if you change either parameter. However, as detailed by Haitjema (1995; 2006), calibration to head data can only tell us the *ratio* of recharge to transmissivity, not the recharge rate or transmissivity itself. That is, an infinite number of possible increases/decreases in recharge can be offset by corresponding increases/decreases in transmissivity, resulting in an identical simulated head field. Because the long-term stream flux prediction is directly proportional to the recharge rate, the inability of head-only calibration data to constrain recharge rate makes the model's predicted stream flux relatively uncertain, even though the recharge model parameter was appreciably sensitive.

Taking this example further, the model described above can be used to assess reductions in uncertainty in the groundwater-derived stream flux prediction given different data-gathering or modelling strategies. For example, expanding the heads-only calibration to include a field measurement of river flow (an observation of the same type as the prediction of interest) breaks the correlation of recharge and transmissivity inherent to heads-only calibration, thus reducing the uncertainty in the recharge parameter and the associated predicted stream flux (e.g. Poeter and Hill 1997).

7.3 Sources of model uncertainty

In general, uncertainty associated with predictions (Figure 7-1) made by a model results from two components:

- Effects of error in field measurements—Exact estimation of appropriate parameter values is not possible because of noise inherent in measurements used for calibration. If more effort is directed to increase the accuracy of field data (e.g. taking more measurements, improving the quality of the measuring point elevation), the measurement error will be reduced but some error associated with the field data remains. Thus, uncertainty in predictions that depend on calibrated parameters can never be eliminated—it can only be reduced.
- Failure to capture complexity of the natural world salient to a prediction—This component represents the contribution to error that results from the conceptual, spatial and temporal simplifications made during modelling and model calibration. Predictive uncertainty from uncaptured complexity reflects heterogeneity that is beyond the ability of field measurements, and thus the ability of the calibration process, to discern.

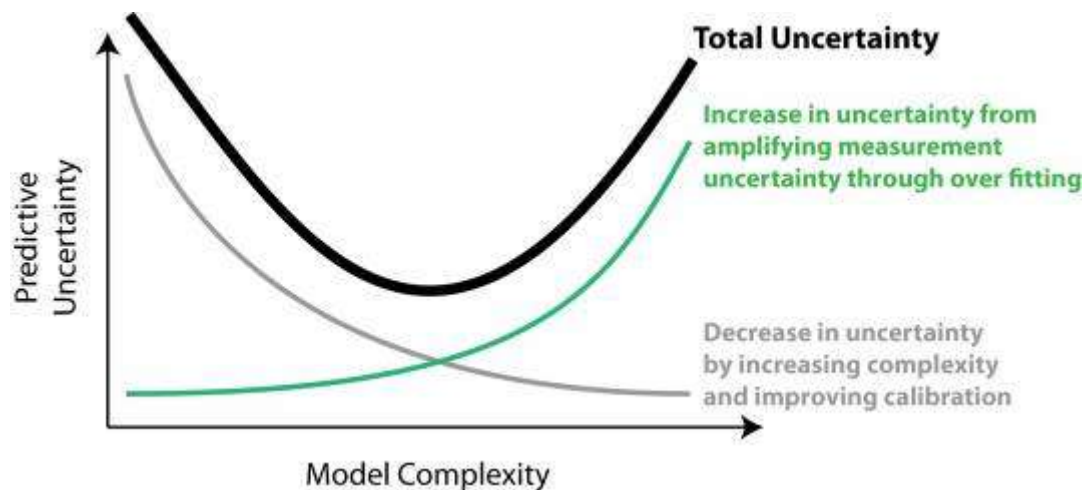


Figure 7-1: Conceptual sources of uncertainty and their relation to model complexity and predictive uncertainty

Increasing complexity results in traditional measurement error-related uncertainty. Very simple models, on the other hand (left-hand portion of the figure) are also characterised by relatively high prediction uncertainty because the model’s ability to predict is adversely effected by oversimplification (after Moore and Doherty 2005).

The effects of field measurement error by itself is widely understood and can be considered a more traditional approach to model uncertainty, in which measurement error drives much of the calculation of uncertainty. The failure to capture salient complexity is often called a model’s ‘structural error’ as it is inherent to the simplifications in model spatial and temporal structure needed to develop a tractable model. Rigorous assessments of structural error are a relatively new addition to model uncertainty estimation, but are now known to be of primary importance because structural error is often the dominant contributor to model errors in predictions that are sensitive to system detail (Gaganis and Smith 2001; Moore and Doherty 2005; Ye et al 2010).

Example 7.2: Importance of avoiding model oversimplification in uncertainty analysis—modified from Fienen et al. (2010; 2011)

One robust approach for extracting the greatest value from limited monitoring resources is linear analysis of the difference in prediction uncertainty with or without future data collection. There is a concern, however, that misapplication of an overly simple model can confound assessments of the worth of data collection, because artefacts in the calculated sensitivities that result from oversimplification can cloud insight resulting from inclusion of data that is sensitive to unrepresented detail. The concern is that outcomes of data worth in such cases may be more reflective of parameter-simplification devices than of the true information content of hypothetical data collected. To illustrate the potential for oversimplification, Fienen et al. (2010) optimised future data-collection locations with a model with the goal of maximising the reduction in the uncertainty of a prediction regarding the amount of groundwater-level decline in area of interest containing an endangered species. The water-levels decline in response to pumping (500 gal/min) situated near a headwater stream and within the ecologically sensitive area (pink circle, Figure 7-2). The objective of the uncertainty analysis is to identify locations of future groundwater monitoring that would most reduce the uncertainty in predicted drawdown in the ecologically sensitive area. The worth of future data collection was investigated using three different levels of parameterisation (columns in Figure 7-2).

The results of data-worth calculations pertaining to the addition of new bore observations (bottom row, Figure 7-2) demonstrate that counterintuitive artefacts are encountered in the low level and intermediate levels of parameterisation—artefacts that result from model structure error. These results are considered counterintuitive because the areas reported as most important for reducing the prediction uncertainty are distant from both the stress and the ecologically sensitive area of interest. When the same data-worth analysis is performed by using a more highly parameterised model, locations of higher values of data worth are in places where intuition suggests—the area that outlines a groundwater divide near the stress and prediction.

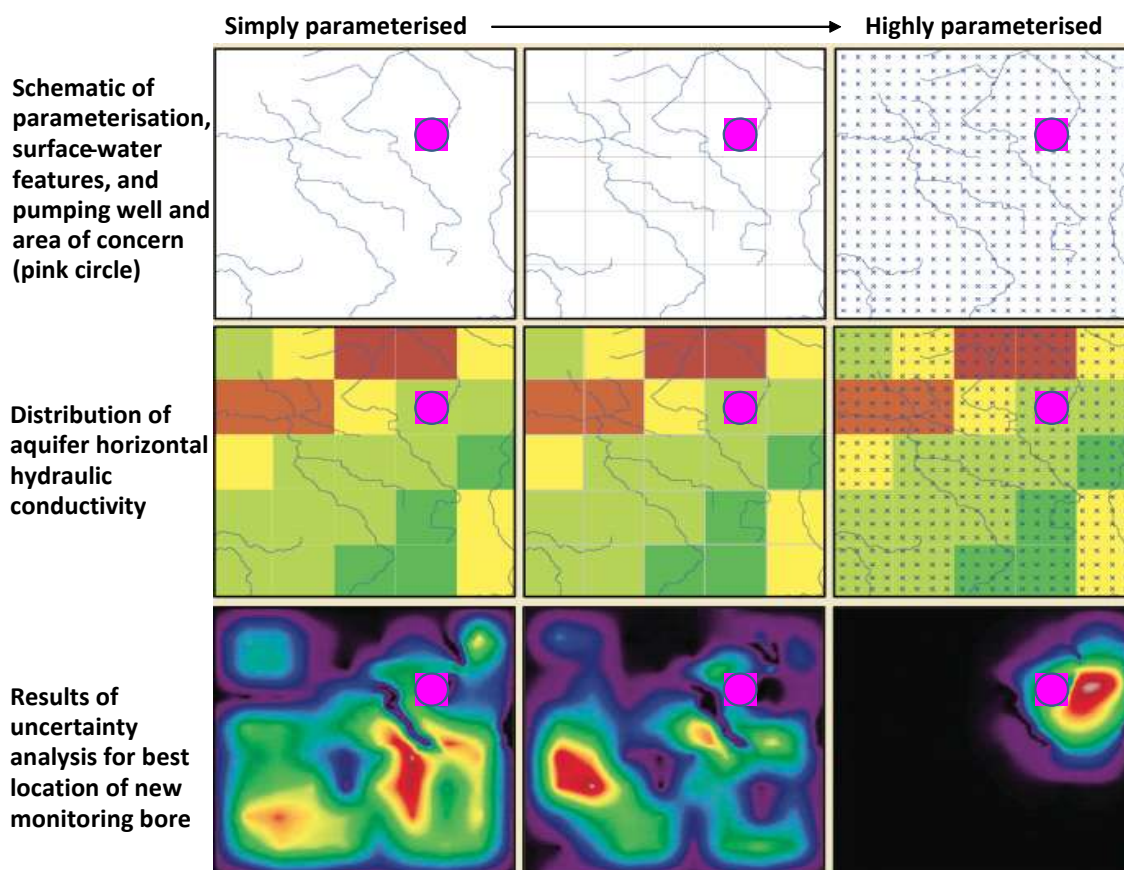


Figure 7-2: Schematic layout (top row), hydraulic conductivity distribution (middle row), and results of uncertainty analysis used to discern the best location to collect new data to reduce the uncertainty of predicted drawdowns near the pumping well (bottom row)

The value of future data is estimated by quantifying the reduction in prediction uncertainty achieved by adding multiple potential observation wells to an existing model. Potential bore locations can be ranked (bottom row) with regard to their effectiveness for reducing uncertainty associated with the drawdown prediction of interest where warmer colors represent locations of more uncertainty reduction. When the underlying model is appropriately parameterised (rightmost column) reasonable results are obtained. When oversimplified the uncertainty analysis is confounded by artefacts resulting from the coarseness of underlying model parameterisation, and provide unreasonable locations for future monitoring. (Modified from Fioren et al. 2010; 2011).

7.4 Relation of model calibration to model uncertainty

Guiding Principle 7.3: Analysis of uncertainty should recognise that the uncertainty of predictions increases with the level of dependence on knowledge of small-scale system detail. Model predictions that integrate larger areas are often less uncertain because characterisation methods are well-suited to discern bulk properties and field observations directly reflect bulk system properties.

Guiding Principle 7.4: Analysis of uncertainty should recognise that there is more uncertainty when reporting confidence intervals around an absolute model output, and less uncertainty when a prediction can be formulated as a subtraction of two model results.

Automated calibration techniques minimise an objective function, commonly expressed as the weighted sum of squared residuals, where the residuals are the difference between observations and equivalent model outputs (see section 5.3.3). When the objective function includes data very similar to the prediction or when data greatly informs the system needed to make this prediction, calibration can reduce predictive uncertainty appreciably. On the other hand, if the prediction is sufficiently dissimilar in type, time or condition to the data used to construct the objective function, a well-calibrated model cannot ensure that prediction uncertainty was reduced.

Example 7.3: Difference between calibration fit and prediction uncertainty

A potential discrepancy between calibration fit and prediction uncertainty is seen by considering the importance of head and flux observations to constrain a prediction of travel time: values of hydraulic conductivity and recharge are constrained by such field data, but porosity—a system characteristic inversely proportional to the travel time prediction—is not directly constrained by simple head and flux observations. Therefore, travel time will always be relatively uncertain, regardless of how well the model calibrates to head and flux observations.

In most modelling, field observations can neither eliminate all uncertainty in model parameters, nor inform us of all costs of simplifications. Rather, calibration to typical field data reduces the uncertainties associated with a number of broad-scale combinations of model parameters that collectively describe bulk or spatially averaged system properties (Doherty and Hunt 2009a;b). The uncertainties associated with other combinations of parameters, especially those that pertain to small-scale detail in system processes dealing with space and time, will not be reduced through the calibration process. To the extent that a prediction of interest depends on bulk properties constrained by calibration, the model may perform well. In cases where a prediction of interest is driven by small-scale detail uncaptured by calibration, the effectiveness of the model as a predictor is expected to be reduced (e.g. Moore and Doherty 2005). This understanding underscores a primary point of model purpose and model uncertainty—in many ways model uncertainty directly results from the stated objective for building the model. Some types of model predictions (e.g. contaminant breakthrough, travel time) are directly dependent on system detail, and inherently more uncertain than predictions that depend on bulk system properties (water balance, capture zones).

Likewise, there is more uncertainty when reporting confidence intervals around an absolute model output and less uncertainty when the prediction can be formulated as a subtraction of two model results (because focusing on output change largely removes model bias).

As such, discussion of uncertainty flows directly from the discussion of model objective as much, if not more, than the degree of model calibration. Furthermore, the presence of multiple disparate predictions of interest suggests the need for different estimates of uncertainty, if not different models, developed to represent uncertainty around each prediction of interest—that is, because development of one true model is not possible, the goal becomes one of reducing the family of possible models to a subset of those that provide the minimum uncertainty around each prediction of interest.

Box 7B: A Bayes perspective on uncertainty

Within the family of non-unique possible models, not all are equally likely. Therefore, parameter sets that do not allow the model to replicate historical measurements of system state should have their probabilities reduced in comparison with those that do. This concept of calibration-constrained parameter variability is formally expressed by the widely used Bayes equation (e.g. Gaganis and Smith 2001). In Bayes equation, an estimate of parameters for a model is expressed as a probability distribution, meaning that uncertainty is formally included in the expression of all values. The estimate of parameter values and their uncertainty prior to model calibration (a priori) is *updated* by gaining new information (calibration), resulting in an updated (a posteriori) estimate of parameters and their uncertainty. This updating process is generally assumed to result in reduced uncertainty.

It is noteworthy that Bayes equation makes no reference to the term ‘calibration’, even though ‘calibrated model’ is often a fundamental tool of environmental decision-making. The updating could be performed in a variety of ways (literature research, new direct information etc.), but in practicality the process of calibration—matching historical observations—is a common way to perform the updating. Owing to the expression of all values as probability distributions, Bayes equation suggests that use of a single parameter set to make an important model prediction should be avoided, because this practice does not reflect the degree of parameter and predictive uncertainty inherent in most modelling contexts. Nevertheless, if done correctly, use of a single parameter for a model prediction of interest can be justified on the premise that this set is of minimum uncertainty (Doherty et al. 2010). Note, however, minimum uncertainty does not necessarily mean small uncertainty (e.g. Moore and Doherty 2005).

7.5 Common approaches for estimating uncertainty

Model parameter and predictive uncertainty is an extensively researched topic and a vast body of literature is available, together with numerous techniques and methodologies to assess uncertainty. Descriptions of uncertainty, as well as specific uncertainty tools, methods and mathematical foundations include, but are not limited to, the following: Beven (1993; 2009), Beven and Binley (1992), Moore and Doherty (2006), Hunt and Welter (2010), and Doherty (2011). Detailed description of guidelines and software tools currently available for groundwater uncertainty analysis are given by Doherty et al. (2010). Description of the highly parameterised approach for maximising information extracted from field data and minimising model structural error during groundwater model calibration is given by Hunt et al. (2007) and Doherty and Hunt (2010). A detailed example of the use of models for assessing the worth of data collection for reducing model uncertainty, and the importance of avoiding model oversimplification, is given by Fienen et al. (2010) and Fienen et al. (2011). Detailed description of the theoretical basis of an uncertainty approach to groundwater modelling can be found in Moore and Doherty (2005), Christensen and Doherty (2008), Tonkin et al. (2007), Tonkin and Doherty (2009), Doherty and Hunt (2009a;b), Doherty and Hunt (2010), Doherty and Welter (2010), Moore et al. (2010), and the Appendix 4 of Doherty et al. (2010).

A comprehensive coverage of all approaches used to estimate uncertainty is not possible in general guidelines. Therefore, this chapter focuses on examples of tools and approaches for characterising uncertainty with a short description of their associated strengths and weaknesses. Given the many possible methods to estimate uncertainty, the best approach to estimate model uncertainty is itself uncertain. However, as Doherty and Welter (2010) discuss, this is theoretically expected, and correct interpretations of uncertainty include quantitative elements as well as more qualitative modelling common sense. Therefore, the goal of uncertainty analysis is more focused on conveying the best estimate of a modeller's judgement of uncertainty to decision-makers, regardless of the specific method employed.

7.5.1 Quick uncertainty estimates: linear methods

The outputs from groundwater models themselves can be characterised as linear (e.g. confined groundwater flow like the Darcy experiment) or non-linear (e.g. unconfined flow with an ephemeral/perennial stream). In addition, the calculation of uncertainty can also be linear or non-linear, where the degree of linearity in the underlying groundwater model may or may not influence the degree of linearity in an uncertainty calculation using that model (Mehl 2007). The nonlinearity of the uncertainty calculation model differs from that of the groundwater model itself because the function of interest is not the head solution but the *derivative* of the head solution with respect to some parameter (these derivatives are the sensitivities). These derivatives and observations can be used to estimate uncertainty if the sensitivities are sufficiently linear with respect to the model parameters employed.

Linear uncertainty analysis is attractive because:

- in general, it is computationally far less costly than nonlinear analysis
- the outcomes of the analysis provide significant insights into the sources of parameter and predictive uncertainty
- the results of the analysis are independent of the specific value of model parameters; this makes results of the analysis particularly useful in assessing such quantities as the worth of observation data, for the data whose worth is assessed do not need to have actually been gathered.

The foundation for most methods of linear uncertainty analysis is the Jacobian matrix, a matrix that simply relates the sensitivity of changes in model parameters to changes in model outputs. Model outputs are those for which field measurements exist, or are potentially available for use in the calibration process. The uncertainty is considered linear because it assumes that the sensitivity calculated by the parameters specified and encapsulated in the Jacobian matrix applies for all possible values that the parameters might attain. This may not be true, of course, but the artefacts that result from violations of the linearity assumption are commonly small. Moreover, because these methods are quick (only one Jacobian matrix need be calculated), and the ever-present nature of unknowable structural error precludes hard-and-fast calculation of true uncertainty in any event, linear methods are often attractive as a quick means to provide a illustrative portrayal of the expected representative model uncertainty.

Modellers must formulate the expected uncertainty associated with parameters to include some consideration of the often-dominant structural error component of uncertainty. As discussed by Doherty and Welter (2010), this structural error can, in fact, never be known, but instead is estimated as a result of professional judgment made by those with knowledge of the site modelled (Gaganis and Smith 2001). This information is encapsulated in a matrix of innate parameter variability—a matrix that reflects the fact that exact parameter values are unknown but some expert knowledge exists concerning the range of reasonable values for these properties. Predictive uncertainty can be calculated from parameter uncertainty through linear propagation of error. The importance of this step, the specification of the modeller’s estimate of innate parameter variability, cannot be overstated—it is critical for ensuring uncertainty methods include the structural error component of uncertainty. An example of a linear uncertainty is shown in Figure 7-3. Detailed explanation of tools for calculating linear estimates of uncertainty, and the underlying mathematical formulation, is given in Doherty et al. (2010), among others.

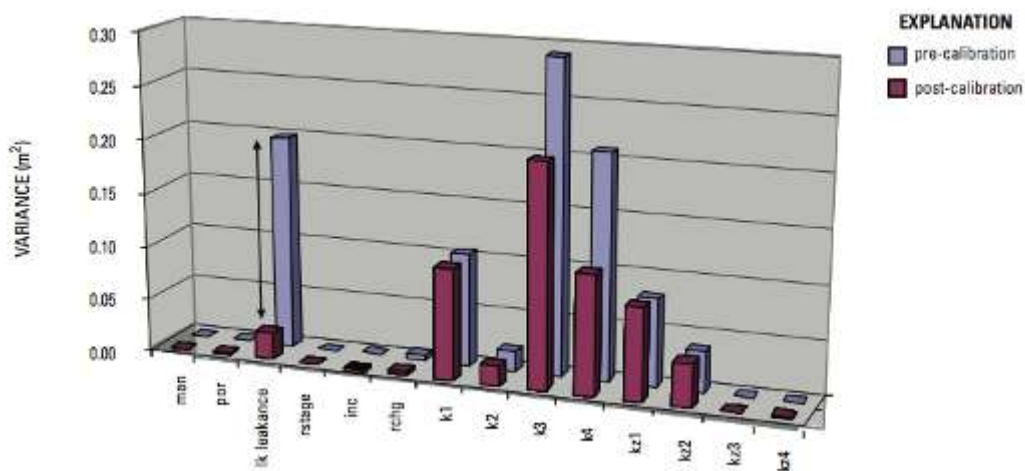


Figure 7-3: Pre-calibration and post-calibration contribution to uncertainty associated with a lake-stage prediction under drought conditions calculated using linear uncertainty methods

Parameter types used in the model are the following: man = Manning’s n, por = porosity, lk leakage = lakebed leakage, rstage = far-field river stage boundary, inc = stream elevation increment boundary condition, rchg = recharge, k1 through k4 = Kh of layers 1 through 4, kz1 through kz4 = Kz of layers 1 through 4. Note that post-calibration reduction in the prediction uncertainty accrued through calibration was due primarily to reduction in uncertainty in the lakebed leakage parameter. Thus, less gain is expected from future data collection activities targeting only this parameter (modified from Hunt and Doherty 2006; reproduced with permission)

7.5.2 Encompassing uncertainty estimates: non-linear methods

Guiding Principle 7.5: When appropriate for the prediction of interest, linear uncertainty methods should be considered a primary tool for conveying the modelling estimate of uncertainty because they are less computationally intensive than other methods.

Non-linear methods for calculating uncertainty are attractive in that the linearity restrictions no longer apply, but are characterised as exceedingly computationally intensive. Two overarching formulations of the nonlinear uncertainty are covered here. In the first, post-calibration predictive uncertainty analysis can be posed as a constrained maximisation-minimisation problem (Figure 7-4) in which a prediction is maximised or minimised subject to the constraint that the objective function rises no higher than a user-specified value (Vecchia and Cooley 1987; Cooley and Christensen 1999, 2006; Tonkin et al. 2007). This value is normally specified to be slightly higher than the minimum value of the objective function achieved during a previous model calibration exercise.

Monte Carlo analysis (e.g. Figure 7-6) is based on many different parameter sets, generated on the basis of the modeller's estimate of reasonable parameter variability. To make the sampling of parameter combinations more run-efficient, parameter combinations that give a reasonable fit are favoured, such as in Markov Chain Monte Carlo simulation—a common tool for formal Bayesian analysis. Null-space Monte Carlo (Tonkin and Doherty 2009) is another run-efficient version of Monte Carlo analysis, where the list of possible runs is reduced to those that do not have adverse effect on calibration before the Monte Carlo process begins.

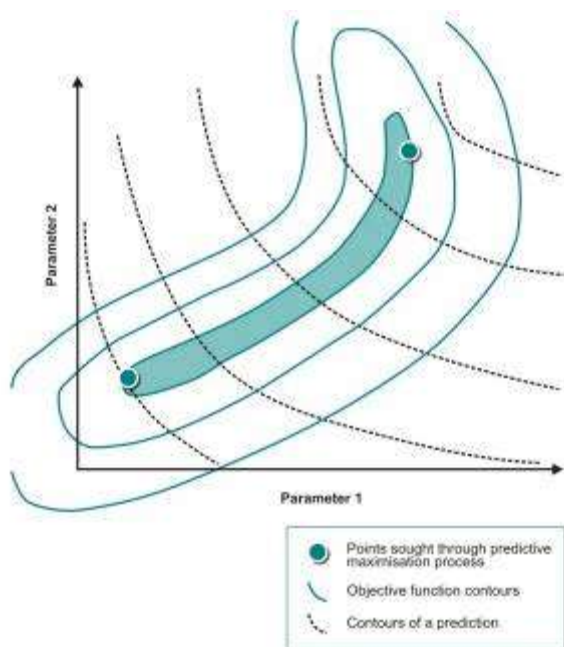


Figure 7-4: Schematic description of 2-parameter calibration-constrained predictive maximisation/minimisation (from Doherty et al 2010)

7.5.3 Other methods: ensemble, global and heuristic uncertainty estimation

The uncertainty methods described previously are based on alternative parameterisations, with associated searches in parameter space using an assumed site geometry or structure. Although alternative parameterisations might be considered alternative models, alternative models can also encompass those conceptualisations that are plausible but cannot be readily described or accommodated via alternative parameterisations of the same model structure. For example, these might include presence or absence of a fault in a groundwater flow model or contrasting chemical transport characteristics. To accommodate uncertainty associated with different conceptual models, multiple conceptual models might be included in a more encompassing view of uncertainty.

The general likelihood uncertainty estimation (GLUE—Beven and Binley 1992; Beven 2009) approach used in surface water hydrologic modelling explicitly recognises that there are multiple models that simulate an observed natural process equally well. These equally acceptable models explicitly recognise that natural observations can be reached through many possible means; these models are deemed ‘equifinal’. GLUE techniques evaluate the family of possible outcomes between equifinal models and assess how good the associated representations of uncertainty are. Maximum likelihood Bayesian model averaging (MLBMA) combines predictions from several competing models and assesses their joint predictive uncertainty using statistical information criteria. Because it uses a Bayesian approach, MLBMA updates both model probabilities and parameter estimates/parameterisation schemes, which in turn can be updated as new information of the system becomes available.

When undertaking an uncertainty analysis using a multi-model type of approach, the goal is to retain and weight or rank in terms of likelihood all the models that are somehow ‘behavioural’ (i.e. that reproduce historic observations within some tolerance and contain features consistent with the conceptual model); and to reject models that are not behavioural. This can be accomplished using formal methods such as the Bayes equation or informal, more heuristic methods that the GLUE method can accommodate.

Unfortunately, an inherent difficulty with the multi-model assessments of uncertainty is that assessing the (relative) likelihood of each alternative model is difficult and, as a result, cannot readily be cast in a traditional statistical framework. Moreover, these and other global or heuristic methods are currently not widely used to describe model uncertainty in groundwater modelling practice due to the computational burden that these methods generally incur. Further information is available in Keating et al 2010; Vrugt et al 2008; Pappenberger and Beven 2006; and references cited there.

7.6 Communicating model uncertainty to decision makers

Guiding Principle 7.6: Uncertainty should be presented to decision-makers with visual depictions that closely conform to the decision of interest.

Regardless of method(s) used to estimate uncertainty, its presentation to decision-makers is one of the most important aspects of model uncertainty. That is, just as there is no reasonable expectation for a true model, there is no expectation for the true model uncertainty estimation. Therefore, the goal is to present, in as clear a fashion as possible, the modeller’s estimate of the representative uncertainty given what is known about the system, the type of prediction(s), and the modeller’s experience with the model and model calibration.

Visual presentations (graphs, figures) are preferred over tables and text descriptions. When possible, the visual depiction should highlight the fact that the model prediction is more than a single result or set of results, thus underscoring the inherent non-unique nature of groundwater modelling.

A modeller should not assume that decision-makers and others not trained in the field will be able to translate an academic uncertainty metric in an optimal fashion. Rather, it is incumbent on the modeller to provide a presentation of uncertainty that most directly aligns, approximates or conforms to the decision of interest. For example, a probabilistic figure of spring capture portrays the high and low confidence of simulated spring recharge (Figure 7-5).

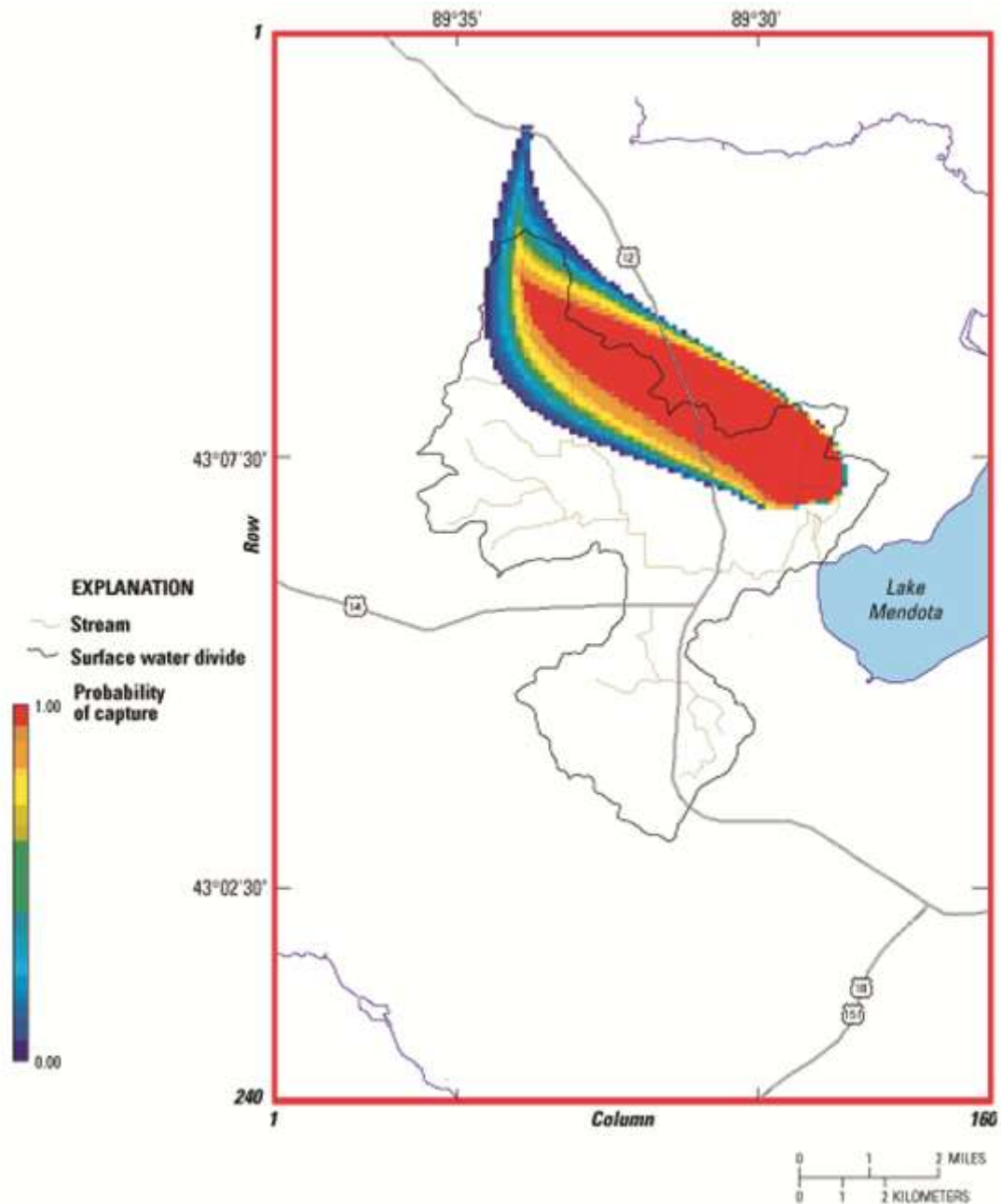


Figure 7-5: Example of visualising uncertainty through a Monte Carlo probabilistic capture zone for a spring

Rather than one result, multiple results are shown ranging from low (blue) to high (red) probability of capture (modified from Hunt et al. 2001; reproduced with permission).

A Pareto Front portrayal of a prediction versus degradation of model fit underscores the fact that multiple models might be considered ‘reasonable’ and provides the decision-maker with a view of how much model fit would need to be lost in order to meet a specific model outcome. For example, a model may have been developed to assess if a solute travel time to reach a receptor is shorter than an actionable arrival time threshold. Multiple runs of the model allow the creation of the Pareto Front (Figure 7-6), which allows the decision-maker to use the degradation of model fit to assess the likelihood of attaining the threshold. Such visual representations relate uncertainty in metrics that can directly feed societal decision making.

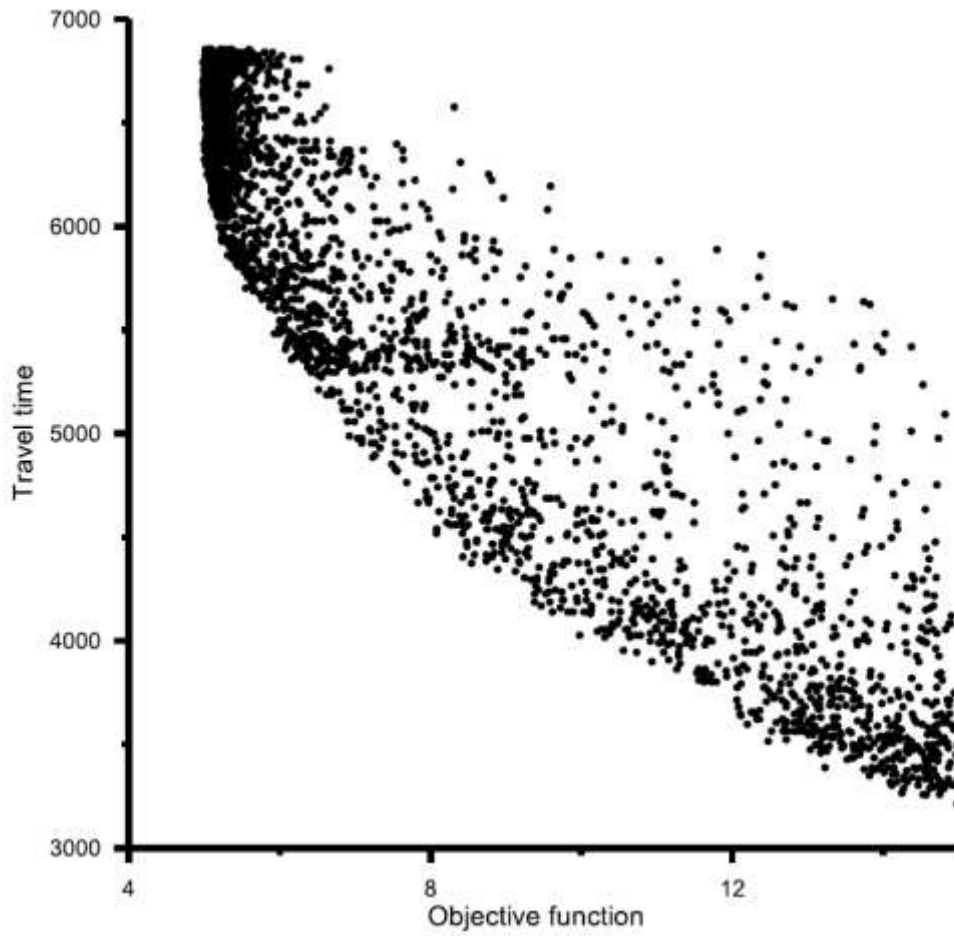


Figure 7-6: A Pareto Front plot of the trade-off between best fit between simulated and observed targets (objective function, x-axis) and a prediction of a particle travel time. A subset of the black dots that define the leftmost edge of the Pareto Front may be considered a 'reasonable' model prediction (modified from Moore et al. 2010; reproduced with permission).

8 Reporting

In this chapter:

- Introduction
- Staged reporting
- Target audience
- Structure
- Visualisation
- Archiving.

Guiding principles for reporting in the groundwater modelling process

Guiding Principle 8.1: Reports should be prepared following the conceptualisation and design stage, after the calibration stage, and after predictive modelling and uncertainty analysis.

Guiding Principle 8.2: Reporting should be tailored to its target audience, so a report should consist of an executive summary section for a non-technical audience and a detailed section for a technical audience.

Guiding Principle 8.3: Model data and results should be presented using clear approaches to visualisation, with appropriate graphing, mapping and colour scheme.

Guiding Principle 8.4: A model archive should be created that allows the model results to be reproduced exactly, while at the same time acts as a repository for data and knowledge of the system. It is recommended that GUI-independent standard file formats be used.

8.1 Introduction

Model reporting encompasses all communication of the conceptualisation, model design, construction, its performance and outputs from predictions. This is traditionally achieved through a written technical document, often supported by a number of presentations at workshops. While the guidelines focus on the written report, the concepts are applicable to any communication of the model and results.

The model, all data collected and information created through the modelling process need to be archived in the report, so the results presented can be reproduced and the model can be used in future studies. The quality of the model is always judged on the basis of the information presented in the technical report, together with the accompanying electronic files.

This chapter focuses on the written report and model archiving, and addresses two important issues—the timing of reporting and the target audience.

8.2 Staged reporting

Guiding Principle 8.1: Reports should be prepared following the conceptualisation and design stage, after the calibration stage, and after predictive modelling and uncertainty analysis.

Rather than producing a single model report at the end of the model project, it is recommended that a staged reporting approach is used. Staged reporting implies writing progress reports and organising meetings with clients and stakeholders after each major stage in the modelling project.

As a minimum, three such stages can be considered:

- after conceptualisation and model design
- after calibration and sensitivity analysis
- after predictive modelling and uncertainty.

Staged reporting of key model aspects not only makes it possible to change or remediate the direction of the project, it also allows the model team to align the expectations of the client and a stakeholder with what is achievable within the project. It also allows the overall report to be prepared progressively throughout the study, with opportunities for progressive reviews, which should benefit the quality of the final report.

All steps and assumptions should be clearly and thoroughly detailed in each report to render the information accessible to all stakeholders and any other interested parties.

8.3 Target audience

Guiding Principle 8.2: Reporting should be tailored to its target audience, so a report should consist of an executive summary section for a non-technical audience and a detailed section for a technical audience.

Model reports should be tailored to technical and/or non-technical audiences. A non-technical audience may be more interested in a plain-English style that describes the model predictions, while a technical audience will require details of conceptualisation, assumptions and calibration.

It is therefore recommended that at each stage the model report consist of two sections; an executive summary-style section for the non-technical audience and a detailed model report section for the technical audience.

The executive summary-style section should provide a summary overview of the issues tackled by the particular report. For example, the executive summary of the final model report should summarise the understanding of the aquifer system and list the key assumptions used in the modelling process, but the focus needs to be on the model outcomes and predictions.

The detailed model report for a technical audience on the other hand needs to provide a detailed description and justification of all aspects of the modelling so that a peer review is possible from this document.

8.4 Structure

Detailed guidance for reporting of all types of groundwater modelling applications is not possible. Site-specific model reports will probably deviate from the structure suggested in these guidelines; however, most reports will need to touch on some or all of the elements that are described, to be of practical use to the intended audience(s).

The structure of these guidelines itself can be used as a template for reporting many modelling projects and Table 8-1 gives an example of a model-report structure. Some of the important aspects that need to be addressed in a model report include:

- model objectives
- hydrogeological conceptualisation
- model code, design and construction
- calibration and sensitivity analysis
- predictive modelling
- uncertainty analysis
- model capabilities and limitations
- conclusions and recommendations
- references.

Modelling objectives should have a prominent place in the report, preferably a separate chapter or section at the beginning of the document. As discussed in Chapter 2, the objectives play a major role in the model design and calibration, and are therefore essential when assessing whether the model is fit for purpose.

The conclusions are linked to the objectives and describe the degree to which the modelling succeeded in meeting the objectives along with highlights from the results. Conclusions can lead to recommendations for preferred management options. The conclusions and recommendations section is also an opportune place to describe the capabilities and limitations of the model, which can be the basis for recommendations for further research or data collection.

Solute transport or surface water–groundwater interactions can be key processes in the model. The implementation of these processes should be discussed in separate chapters if they are very important, otherwise their implementation can be discussed in the design and calibration chapters.

The model report should contain sufficient information to enable a technical peer review, which means any supporting non-modelling information should be referenced and accessible to a reviewer.

The capabilities and limitations section is intended to explicitly describe the capabilities and limitations of the model. This section states what the model should and should not be used for, so that expectations of the model can be managed.

Table 8-1: Example final model report structure (modified after MDBC, 2001)

<i>Item</i>	<i>Title</i>	<i>Description</i>
1	Report title	The title should reflect the model and project objectives rather than just the study location.
2	Executive summary	The detailed model report includes a brief executive-style report to summarise the major findings of the study for non-technical audiences.
3	Model objectives	The objectives state how the groundwater model will be used to address the project objectives and the target confidence level.
4	Conceptualisation	This section describes the current level of understanding of the aquifer system and how this is translated into a conceptual model to address the model objectives. Include reference to a data inventory.
5	Model design	The model design section specifies the model confidence level and the technical details of the groundwater model such as spatial and temporal discretisation, parameter distributions, implementation of stresses and boundary conditions, and model code and software.
6	Model calibration	Summary of how model parameters are changed within predefined constraints to match observations. This requires a clear description of the parameterisation, objective function and constraints as well as the calibration methodology and sensitivity analysis.
7	Predictive modelling	Description of the use of the model to address the model objectives by exploring aquifer behaviour under different stresses.
8	Uncertainty analysis	Presentation of the uncertainty associated with the predictions, based on, at least, heuristic descriptions of measurement uncertainty associated with parameters, stresses and calibration targets and structural model uncertainty, associated with the conceptual and mathematical model.
9	Model limitations	States the limitations of data and code, the reliability of different outcomes of the model and how further data collection or research may improve reliability.
10	Conclusions and recommendations	Summary of model findings and recommendations for further analysis.
11	References	Full references of cited literature and data sources.
12	Appendices	Maps, graphs and tables containing detailed information on the model that is important to fully document the model.

8.5 Visualisation

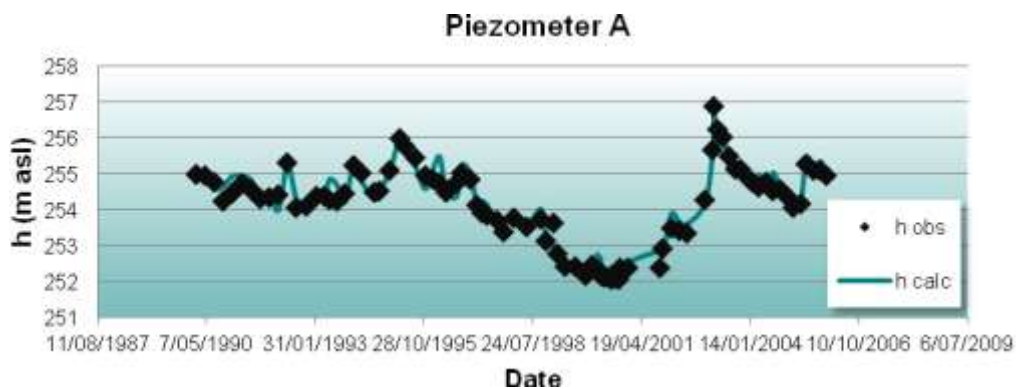
Guiding Principle 8.3: Model data and results should be presented using clear approaches to visualisation, with appropriate graphing, mapping and colour scheme.

The groundwater modelling process collects or generates a large amount of spatial and temporal data and information. The visualisation of such large datasets (and their associated uncertainty) can be a daunting task, but is nevertheless essential in communicating and reporting model results.

Traditional graphics, such as time series and scatter plots, maps, cross-sections and schematic sketches or diagrams of conceptual models, are often the most suited and intuitive tools to communicate groundwater data. The modeller is, however, encouraged to look beyond the often limited capabilities of spreadsheet software and graphical user interfaces. Specialised graphing software, such as plotting toolkits in scripting languages or graphical design software, allow modellers to customise graphs and maps and tailor them to the target audience. An excellent review and guidance on data visualisation for environmental science is provided in Kelleher and Wagener (2011). A few of their guidelines relevant to groundwater modelling are discussed and illustrated in the following sections.

8.5.1 Keeping the graph simple

Figure 8-1 shows two versions of the same data, an imaginary observed hydrograph and the calculated equivalent. The upper graph is created using the default settings of mainstream spreadsheet software. The lower graph minimises the data-ink ratio, defined by Tufte (2001) as the ratio of ink used to represent the data over the ink needed for the entire graph. Reducing this ratio will simplify the graph and focus attention on the data.



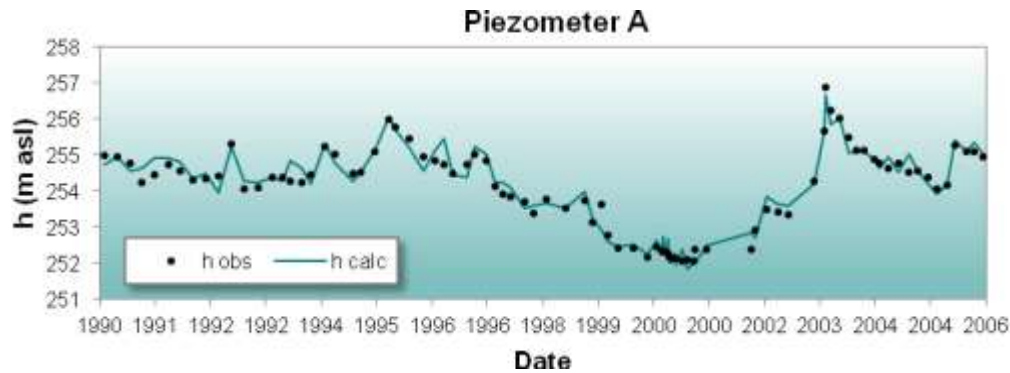


Figure 8-1: Keep the graph simple by using appropriate density of ink and symbol styles (h (m asl) – metres of head above mean seal level; h obs – head on an observation well; h calc – head calculated by the model)

8.5.2 Select an appropriate graph type

Figure 8-2 shows four different graphs used to evaluate the goodness of fit between observed and calculated values of groundwater levels. Figure 8-2a is the traditional, and sometimes the only, graph used to indicate the quality of fit between observed and modelled values. For most groundwater models, especially if the range in observed groundwater levels is large, most data points will plot along the 1:1 line and will give the impression of a good fit. However, this is very often misleading.

To evaluate the goodness of fit, the residuals, observed minus calculated values are far more important (see discussion in Chapter 5). Figure 8-2b), c) and d) show three ways of depicting the distribution of the residuals. The magnitude and any systematic bias in the residuals are much easier to identify in these kinds of plots.

It has to be stressed, however, that these are only summary plots and that they are not sufficient to judge the quality of a model. They should be accompanied by statistical performance measures (see Chapter 5), maps showing the spatial distribution of residuals, hydrographs for the temporal distribution (such as in Figure 8-1), the water balance and the direction and magnitude of head gradients, for example.

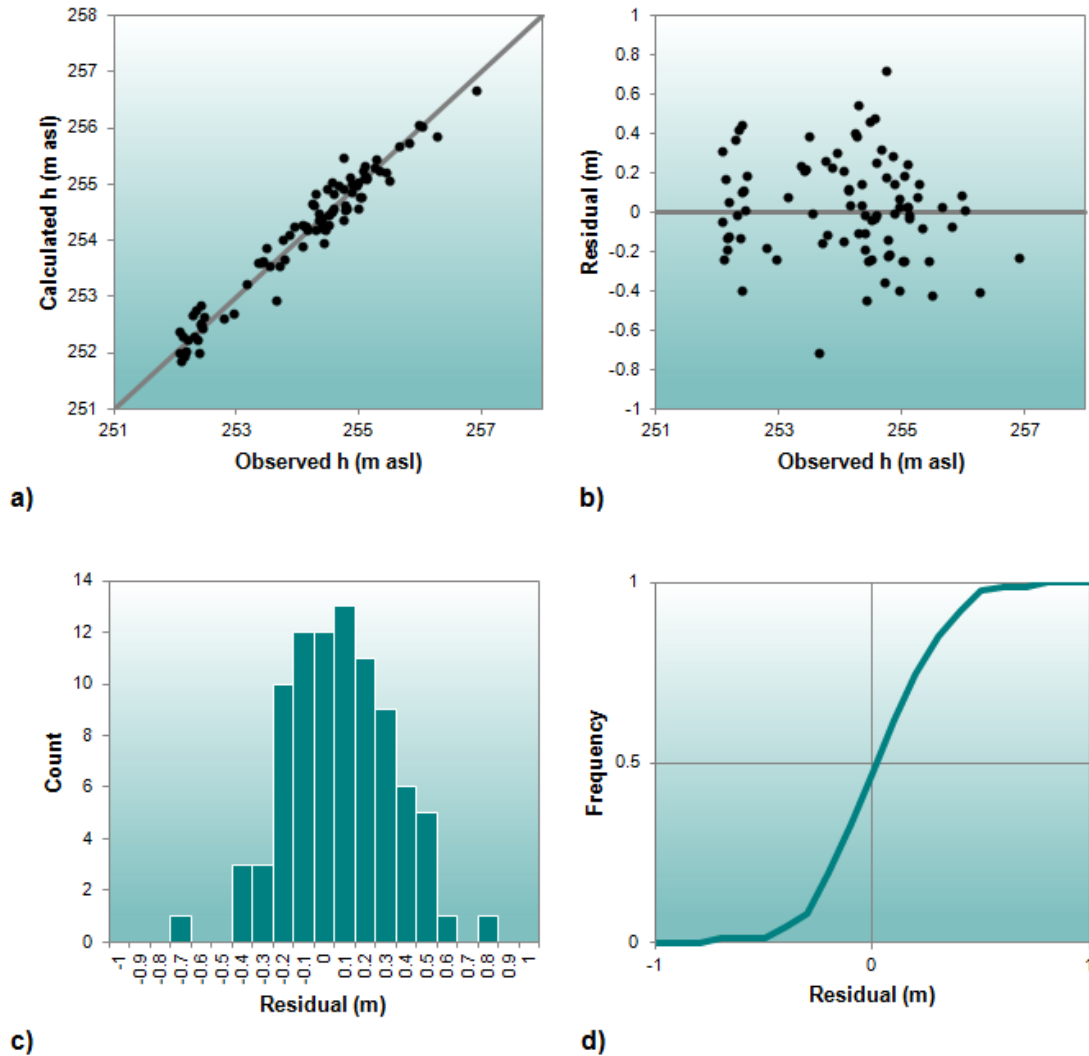


Figure 8-2: Select an appropriate graph type to evaluate calibration (h (m asl) – metres of head above mean seal level)

8.5.3 Select meaningful axes

The selection of meaningful axes is always an important issue in graphs, but especially so for cross-sections and 3D visualisations. As aquifer systems usually have a much larger horizontal than vertical extent, vertical exaggeration is needed to visualise the geometry. It is, however, very useful to include in the report a cross-section with no or very small vertical exaggeration to emphasise that groundwater flow in most aquifers occurs mostly in a 2D horizontal plane (Figure 8-3).

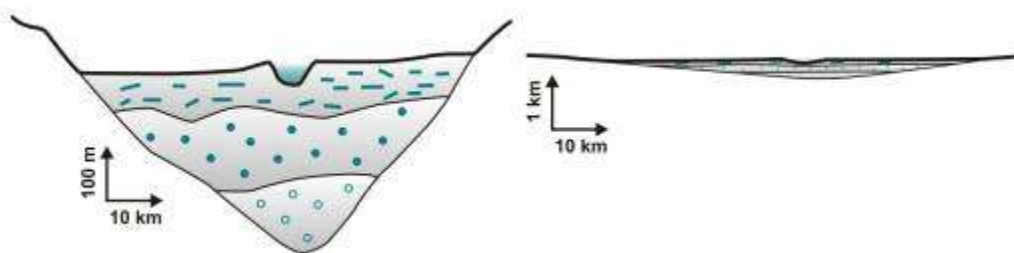


Figure 8-3: Select meaningful axes

8.5.4 Plot overlapping points in scatter plots in a way that density differences become apparent

When plotting large datasets in scatter-plots, individual points will often overlap. This entails a loss of information in the display as the visual appearance of a single outlier will be almost equal to that from a cluster of points (Figure 8-4a). One way to alleviate this is to make the data points partly transparent (Figure 8-4b). In this plot darker regions indicate zones of high data density.

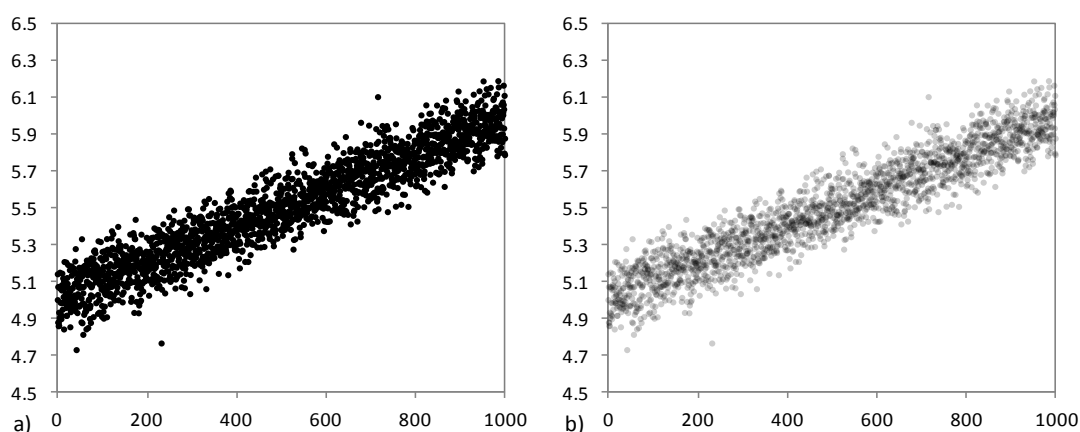


Figure 8-4: Plot overlapping points in scatterplots in a way that density differences become apparent

8.5.5 Select an appropriate colour scheme

One of the most used colour schemes is the spectral or rainbow colour scheme, which varies from violet over blue, green, yellow and orange to red (Figure 8-5). This scheme is available as default for visualisation of continuous data in many software packages. Light and Bartlein (2004) advise strongly against using this scheme as there is no intuitive magnitude attribute attached to the colours, that is, green is not intuitively perceived as being larger than yellow and some of the colour combinations, such as red and violet or yellow-green and yellow-orange, are hard to distinguish, confusing the interpretation of the map.

Sequential schemes gradually vary one colour from light to dark and are much more suited to represent continuous data, such as a piezometric head surface. If it is important to highlight departures from a mean value, such as the difference in piezometric head surface between two simulations, a diverging colour scheme is preferred. These schemes use a light, neutral colour to represent average values and contrasting dark hues for the extremes of the data. Categorical data is best represented by contrasting colours without reference to magnitude.

More guidance on colour scheme selection and example schemes can be found at <http://colorbrewer2.org>. (Cynthia A. Brewer, Geography, Pennsylvania State University).

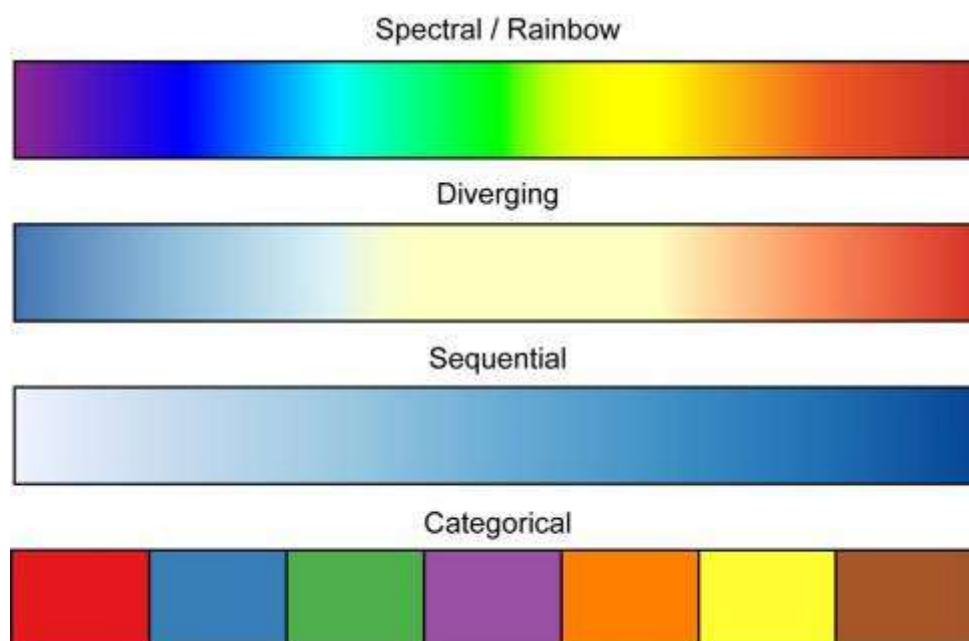


Figure 8-5: Different colour schemes used for presenting data

8.5.6 3D visualisation

As mentioned in section 3.8, 3D (or 4D if temporal data is included), geo-databases have become increasingly available to groundwater modellers and are invaluable tools to manage and analyse hydrogeological data. The visualisation options provided as front-end to these databases allow practitioners to interactively change the viewpoint on the data, cut away sections from aquifer models or create animations to show how a property changes with time or depth. The ability to interactively change the visualisation can provide additional insight into the aquifer system. A snapshot of such a visualisation, however, usually yields an impressive graphic, but often fails to convey the full details of the 3D/4D database. A modeller therefore has to be very careful in selecting an appropriate visualisation if it is included in the report. Presentations or workshops on the other hand provide an ideal platform to fully exploit the possibilities of interactive or animated 3D and 4D visualisations.

8.5.7 Visualising uncertainty

The visualisation of uncertainty is almost as important as the method used to obtain the uncertainty. Simultaneous representation of uncertainty, that is, in the same graph as the prediction, is most insightful and most appropriate for decision making (Viard et al. 2011).

For single predictions or time series, uncertainty can be expressed using traditional error bounds or 95% confidence intervals. To visualise uncertainty estimates that are not normally distributed, a colour scale can be used to express the probability of a prediction. For single predictions, histograms are ideal to convey the details of a distribution.

Visualising uncertainty for 2D spatial predictions is often not straightforward. Maps with probability shown through a colour scale can be used in some special cases, such as the probability that a grid cell belongs to the catchment area of a well or the probability that the groundwater level decline in a grid cell will be greater than a threshold value. A more generic way to visualise uncertainty associated with spatial data is by varying the transparency to indicate uncertainty (Figure 8-6). Figure 8-6a) and b) show an interpolated piezometric surface and the associated uncertainty, while Figure 8-6c) combines both. The general trends in piezometric surface are still apparent, while no data is displayed for the areas with high uncertainty. An added advantage of making the uncertainty an integral part of the map, is that when the map is isolated, for instance, in a summary report or presentation, the uncertainty of the results are still apparent.

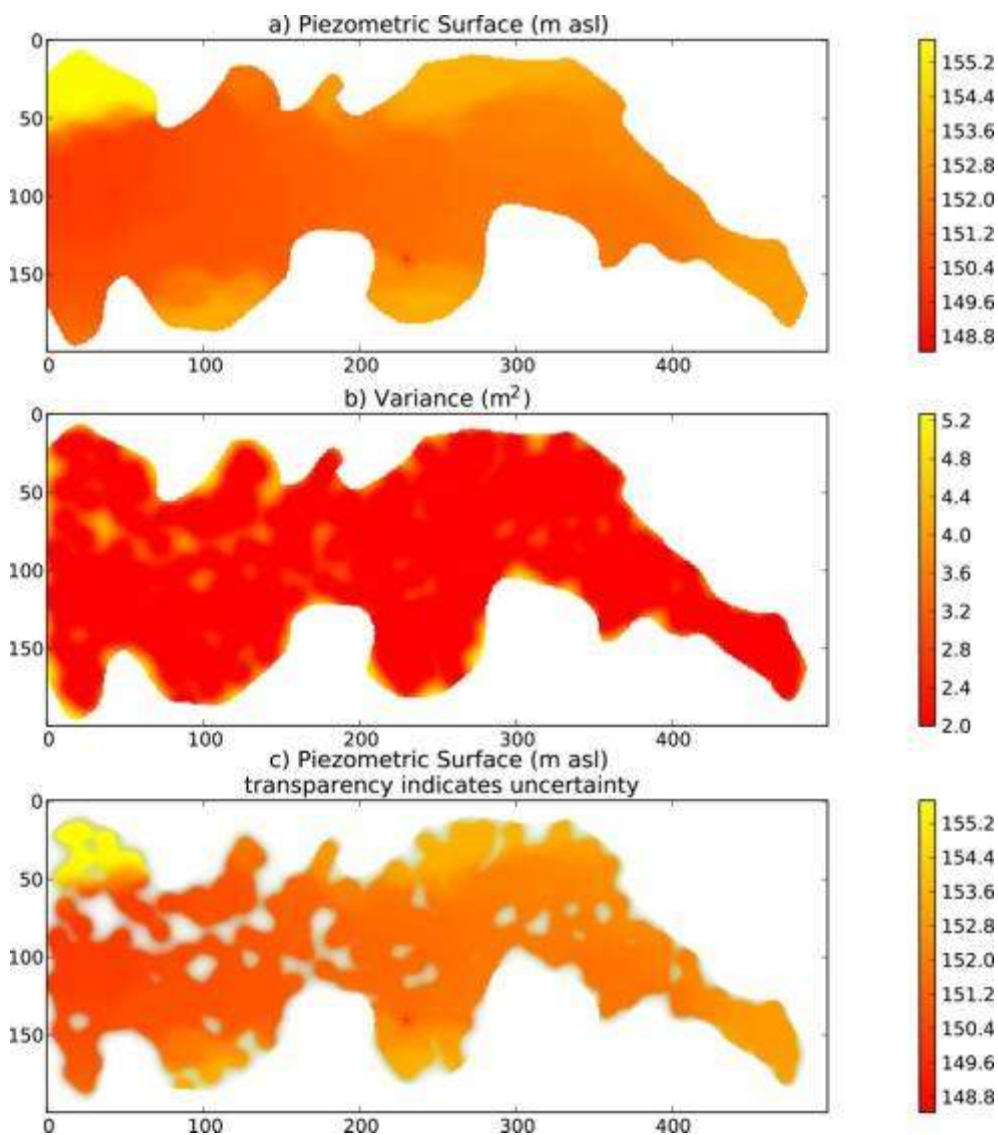


Figure 8-6: Visualising spatial uncertainty with transparency (h (m asl) – metres of head above mean seal level)

8.6 Archiving

Guiding Principle 8.4: A model archive should be created that allows the model results to be produced exactly, while at the same time act as a repository for data and knowledge of the system. It is recommended that GUI-independent standard file formats be used.

The goal of archiving is twofold; first, it must allow for the exact reproduction of the results presented in the model report, and, second, it serves as a repository for all data, information and knowledge accumulated through the modelling process to facilitate future analysis of the aquifer system. The model archive should be accompanied with a report describing the archive structure and the metadata.

The first type of archive should contain all data used to create the model and the associated metadata, such as the data source and date of capture. The data can be stored in a spreadsheet, a database, a GIS or even in a groundwater modelling GUI.

For all data in the archive, the metadata should clearly list the source of the data, the uncertainty or confidence level associated with the data and any processing done in the project to create or modify the dataset. The latter is often required to convert the original data into a format suited for groundwater modelling or to summarise and visualise model outcomes. The use of customised scripts or software in pre- and post-processing and visualisation is especially encouraged, as it allows for an easier reproduction of the reported results. These scripts can be provided as part of the delivered report and archive.

The model archive or the model log should document the software used in the modelling process, including the version of the software. If possible, the software itself or the model executables should be included in the archive, especially in the case of commercial groundwater modelling software, as forward and backward compatibility issues can occur. This, unfortunately, can lead to the situation where it becomes very hard to access a large amount of data and model results because they are stored in a format that is no longer supported.

The latter issue is especially cumbersome when reusing or revisiting earlier modelling projects. It is recommended to archive data in software or GUI-independent, standard file formats.

The most versatile and accessible format to save data tables and grids is in ASCII text files. The last couple of years have seen the development and implementation of a number of international standard file formats and frameworks. Examples are the OpenMI standard for data interchange between models <www.openmi.org>, the Open Geospatial Consortium (OGC) for geospatial data <www.opengeospatial.org/> or the OpenDocument format for office applications (<http://opendocument.xml.org/>). Within Australia, the Bureau of Meteorology has adopted the Water Transfer Data Format (WTDF) as standard for the exchange of water data (Walker et al. 2009).

It is not the intention of these guidelines to provide a scheme for groundwater model archiving. A good example of such a scheme can be found in the groundwater model-archiving standard for South Australia (Yan et al. 2010).

9 Reviews

In this chapter:

- Introduction
- Review process
- Example checklist (for model appraisal and review).

Guiding principles for model review

Guiding Principle 9.1: A review should take place after each reporting milestone.

Guiding Principle 9.2: Three levels of review should be undertaken: a model appraisal by a non-technical reviewer to evaluate model results; an in-depth peer review by experienced hydrogeologists and modellers; and a post-audit involving a critical re-examination of the model when new data is available or when the model objectives change. The post-audit may happen long after the modelling project has taken place.

9.1 Introduction

Model reviews occur to provide the modelling team (and the model owner) with a check on whether the model is fit for purpose when judged against the modelling objectives and the guidance provided in this document. This chapter provides an overview of the review process and provides a checklist which is recommended as a tool for the review process. Flexibility in the review process is encouraged, and so scoring or ranking systems in the checklist have been avoided.

9.2 Review process

Guiding Principle 9.1: A review should take place after each reporting milestone.

Guiding Principle 9.2: Three levels of review should be undertaken: a model appraisal by a non-technical reviewer to evaluate model results; an in-depth peer review by experienced hydrogeologists and modellers; and a post-audit involving a critical re-examination of the model when new data is available or when the model objectives change. The post-audit may happen long after the modelling project has taken place.

Chapter 8 outlined the need to tailor the model report to the target audience. Likewise, the level of review of a model should be commensurate with the background of the reviewers. Three levels of model review are suggested:

- appraisal
- peer review
- post-audit.

A **model appraisal** is a model evaluation by a reviewer with a basic to intermediate level of understanding of groundwater modelling but with a sound understanding of the overall project and how the groundwater model is expected to contribute to that project. A **peer review** is a thorough in-depth review of the groundwater model by both experienced hydrogeologists and groundwater modellers. The third level is the **post-audit**, which is a critical re-examination of the model when new data become available or when the objectives of the model change, which again is undertaken by experienced hydrogeologists and groundwater modellers.

A groundwater model used for groundwater management can be updated annually, incorporating newly observed rainfall, river-stage and groundwater level data. A model audit based on the accumulated data is carried out every five years to assess if the conceptual model is still valid. If conceptualisation is still adequate, the model should be recalibrated/validated as more data is available to constrain the parameter estimates.

The different options for review need to be discussed with the client and the review process needs to be agreed upon before the start of the project. The staged reporting suggested in Chapter 8 also implies staged reviewing. The reviewers should be involved early in the project, at the planning stage, especially to evaluate key modelling decisions. A review and discussion of the conceptual model and design before construction and calibration allows the opportunity to alter model assumptions. Discussion between modeller and client at this stage can also reveal whether the model objectives can be attained within the available data and budget. This can result in an adjustment to the model confidence level classification or trigger collection of additional data needed to make predictions at the original confidence level.

Notwithstanding the formal review process discussed above, modellers should seek a formal or informal internal review during the modelling project. This internal quality control can, of course, also be communicated to the client.

A panel of reviewers should have complementary skills and experience with the intricacies of numerical groundwater modelling, with the hydrogeology of the studied aquifer system and with the project to which the groundwater model is to contribute. All data and reference material should be easily accessible for review.

A detailed peer review of a groundwater model might require the reviewer to carry out additional model runs independent of the model team. This requires the complete disclosure of the model and associated files and scripts to the reviewing panel.

Section 9.3 provides a checklist for both a model appraisal and peer review. The checklist contains no guidance for a model audit. As mentioned earlier, this process should be invoked when a substantial amount of new data is available or when a model is considered for use with a different model objective.

Example 9.1: Assessing model suitability for addressing alternative modelling problems

A groundwater model is developed to design a new well field. Later the same model is used to assess the influence of climate change on a groundwater dependent ecosystem. A model audit is carried out to assess the level of confidence of the original model in the area of the groundwater dependent ecosystem and whether all relevant processes are included. If the model is suited, the audit assesses what additional data is required to meet the new objective.

9.3 Review checklists

The primary task of the reviewer is to provide advice on whether the model is fit for purpose. The model's purpose/objectives and how these have been decided by the model team and client should have been documented. A checklist of review questions can help in judging whether a model is fit for purpose.

Table 9-1 provides a generic compliance test for groundwater models. The 10 questions are essential aspects that any groundwater model needs to satisfy independent of model objectives or confidence-level classification. This compliance test can be used to summarise and communicate the results of the peer review.

Table 9-1: Compliance checklist

<i>Question</i>	<i>Yes/No</i>
1. Are the model objectives and model confidence level classification clearly stated?	
2. Are the objectives satisfied?	
3. Is the conceptual model consistent with objectives and confidence level classification?	
4. Is the conceptual model based on all available data, presented clearly and reviewed by an appropriate reviewer?	
5. Does the model design conform to best practice?	
6. Is the model calibration satisfactory?	
7. Are the calibrated parameter values and estimated fluxes plausible?	
8. Do the model predictions conform to best practice?	
9. Is the uncertainty associated with the predictions reported?	
10. Is the model fit for purpose?	

Table 9-2 provides a more detailed checklist for model review based on this guidelines document. The checklist elements are grouped by chapter of the guidelines and consist of two levels of questions. The first level is general, with questions that can be addressed during both appraisal and peer review. The second level provides more detailed questions or model aspects that need to be assessed. These questions are typically part of a peer review.

The questions in the checklist are intended to be generic and widely applicable. A scoring system is purposefully not included in the checklist. Reviewers should apply their experienced judgement on whether a question is applicable or to what degree the question needs to be satisfied in the context of the stated model purpose/ objectives based on the model objectives and model confidence level. This does not preclude reviewers commenting on issues that may be outside the scope of the study, but the fitness for purpose of the model should be judged in relation to the stated scope and objective of the study.

Table 9-2: Review checklist

<i>Review questions</i>	<i>Yes/No</i>	<i>Comment</i>
1. Planning		
1.1 Are the project objectives stated?		
1.2 Are the model objectives stated?		
1.3 Is it clear how the model will contribute to meeting the project objectives?		
1.4 Is a groundwater model the best option to address the project and model objectives?		
1.5 Is the target model confidence-level classification stated and justified?		
1.6 Are the planned limitations and exclusions of the model stated?		
2. Conceptualisation		
2.1 Has a literature review been completed, including examination of prior investigations?		
2.2 Is the aquifer system adequately described?		
2.2.1 hydrostratigraphy including aquifer type (porous, fractured rock ...)		
2.2.2 lateral extent, boundaries and significant internal features such as faults and regional folds		
2.2.3 aquifer geometry including layer elevations and thicknesses		
2.2.4 confined or unconfined flow and the variation of these conditions in space and time?		
2.3 Have data on groundwater stresses been collected and analysed?		
2.3.1 recharge from rainfall, irrigation, floods, lakes		
2.3.2 river or lake stage heights		
2.3.3 groundwater usage (pumping, returns etc)		
2.3.4 evapotranspiration		
2.3.5 other?		
2.4 Have groundwater level observations been collected and analysed?		
2.4.1 selection of representative bore hydrographs		
2.4.2 comparison of hydrographs		
2.4.3 effect of stresses on hydrographs		
2.4.4 watertable maps/piezometric surfaces?		
2.4.5 If relevant, are density and barometric effects taken into account in the interpretation of groundwater head and flow data?		
2.5 Have flow observations been collected and analysed?		
2.5.1 baseflow in rivers		
2.5.2 discharge in springs		
2.5.3 location of diffuse discharge areas?		
2.6 Is the measurement error or data uncertainty reported?		
2.6.1 measurement error for directly measured quantities (e.g. piezometric level, concentration, flows)		
2.6.2 spatial variability/heterogeneity of parameters		
2.6.3 interpolation algorithm(s) and uncertainty of gridded data?		

<i>Review questions</i>	<i>Yes/No</i>	<i>Comment</i>
2.7 Have consistent data units and geometric datum been used?		
2.8 Is there a clear description of the conceptual model?		
2.8.1 Is there a graphical representation of the conceptual model?		
2.8.2 Is the conceptual model based on all available, relevant data?		
2.9 Is the conceptual model consistent with the model objectives and target model confidence level classification?		
2.9.1 Are the relevant processes identified?		
2.9.2 Is justification provided for omission or simplification of processes?		
2.10 Have alternative conceptual models been investigated?		
3. Design and construction		
3.1 Is the design consistent with the conceptual model?		
3.2 Is the choice of numerical method and software appropriate (Table 4-2)?		
3.2.1 Are the numerical and discretisation methods appropriate?		
3.2.2 Is the software reputable?		
3.2.3 Is the software included in the archive or are references to the software provided?		
3.3 Are the spatial domain and discretisation appropriate?		
3.3.1 1D/2D/3D		
3.3.2 lateral extent		
3.3.3 layer geometry?		
3.3.4 Is the horizontal discretisation appropriate for the objectives, problem setting, conceptual model and target confidence level classification?		
3.3.5 Is the vertical discretisation appropriate? Are aquitards divided in multiple layers to model time lags of propagation of responses in the vertical direction?		
3.4 Are the temporal domain and discretisation appropriate?		
3.4.1 steady state or transient		
3.4.2 stress periods		
3.4.3 time steps?		
3.5 Are the boundary conditions plausible and sufficiently unrestrictive?		
3.5.1 Is the implementation of boundary conditions consistent with the conceptual model?		
3.5.2 Are the boundary conditions chosen to have a minimal impact on key model outcomes? How is this ascertained?		
3.5.3 Is the calculation of diffuse recharge consistent with model objectives and confidence level?		
3.5.4 Are lateral boundaries time-invariant?		
3.6 Are the initial conditions appropriate?		
3.6.1 Are the initial heads based on interpolation or on groundwater modelling?		
3.6.2 Is the effect of initial conditions on key model outcomes assessed?		

<i>Review questions</i>	<i>Yes/No</i>	<i>Comment</i>
3.6.3 How is the initial concentration of solutes obtained (when relevant)?		
3.7 Is the numerical solution of the model adequate?		
3.7.1 Solution method/solver		
3.7.2 Convergence criteria		
3.7.3 Numerical precision		
4. Calibration and sensitivity		
4.1 Are all available types of observations used for calibration?		
4.1.1 Groundwater head data		
4.1.2 Flux observations		
4.1.3 Other: environmental tracers, gradients, age, temperature, concentrations etc.		
4.2 Does the calibration methodology conform to best practice?		
4.2.1 Parameterisation		
4.2.2 Objective function		
4.2.3 Identifiability of parameters		
4.2.4 Which methodology is used for model calibration?		
4.3 Is a sensitivity of key model outcomes assessed against?		
4.3.1 parameters		
4.3.2 boundary conditions		
4.3.3 initial conditions		
4.3.4 stresses		
4.4 Have the calibration results been adequately reported?		
4.4.1 Are there graphs showing modelled and observed hydrographs at an appropriate scale?		
4.4.2 Is it clear whether observed or assumed vertical head gradients have been replicated by the model?		
4.4.3 Are calibration statistics reported and illustrated in a reasonable manner?		
4.5 Are multiple methods of plotting calibration results used to highlight goodness of fit robustly? Is the model sufficiently calibrated?		
4.5.1 spatially		
4.5.2 temporally		
4.6 Are the calibrated parameters plausible?		
4.7 Are the water volumes and fluxes in the water balance realistic?		
4.8 has the model been verified?		
5. Prediction		
5.1 Are the model predictions designed in a manner that meets the model objectives?		
5.2 Is predictive uncertainty acknowledged and addressed?		
5.3 Are the assumed climatic stresses appropriate?		
5.4 Is a null scenario defined?		
5.5 Are the scenarios defined in accordance with the model objectives and confidence level classification?		

<i>Review questions</i>	<i>Yes/No</i>	<i>Comment</i>
5.5.1 Are the pumping stresses similar in magnitude to those of the calibrated model? If not, is there reference to the associated reduction in model confidence?		
5.5.2 Are well losses accounted for when estimating maximum pumping rates per well?		
5.5.3 Is the temporal scale of the predictions commensurate with the calibrated model? If not, is there reference to the associated reduction in model confidence?		
5.5.4 Are the assumed stresses and timescale appropriate for the stated objectives?		
5.6 Do the prediction results meet the stated objectives?		
5.7 Are the components of the predicted mass balance realistic?		
5.7.1 Are the pumping rates assigned in the input files equal to the modelled pumping rates?		
5.7.2 Does predicted seepage to or from a river exceed measured or expected river flow?		
5.7.3 Are there any anomalous boundary fluxes due to superposition of head dependent sinks (e.g. evapotranspiration) on head-dependent boundary cells (Type 1 or 3 boundary conditions)?		
5.7.4 Is diffuse recharge from rainfall smaller than rainfall?		
5.7.5 Are model storage changes dominated by anomalous head increases in isolated cells that receive recharge?		
5.8 Has particle tracking been considered as an alternative to solute transport modelling?		
6. Uncertainty		
6.1 Is some qualitative or quantitative measure of uncertainty associated with the prediction reported together with the prediction?		
6.2 Is the model with minimum prediction-error variance chosen for each prediction?		
6.3 Are the sources of uncertainty discussed?		
6.3.1 measurement of uncertainty of observations and parameters		
6.3.2 structural or model uncertainty		
6.4 Is the approach to estimation of uncertainty described and appropriate?		
6.5 Are there useful depictions of uncertainty?		
7. Solute transport		
7.1 Has all available data on the solute distributions, sources and transport processes been collected and analysed?		
7.2 Has the appropriate extent of the model domain been delineated and are the adopted solute concentration boundaries defensible?		
7.3 Is the choice of numerical method and software appropriate?		
7.4 Is the grid design and resolution adequate, and has the effect of the discretisation on the model outcomes been systematically evaluated?		
7.5 Is there sufficient basis for the description and parameterisation of the solute transport processes?		

<i>Review questions</i>	<i>Yes/No</i>	<i>Comment</i>
7.6 Are the solver and its parameters appropriate for the problem under consideration?		
7.7 Has the relative importance of advection, dispersion and diffusion been assessed?		
7.8 Has an assessment been made of the need to consider variable density conditions?		
7.9 Is the initial solute concentration distribution sufficiently well-known for transient problems and consistent with the initial conditions for head/pressure?		
7.10 Is the initial solute concentration distribution stable and in equilibrium with the solute boundary conditions and stresses?		
7.11 Is the calibration based on meaningful metrics?		
7.12 Has the effect of spatial and temporal discretisation and solution method taken into account in the sensitivity analysis?		
7.13 Has the effect of flow parameters on solute concentration predictions been evaluated, or have solute concentrations been used to constrain flow parameters?		
7.14 Does the uncertainty analysis consider the effect of solute transport parameter uncertainty, grid design and solver selection/settings?		
7.15 Does the report address the role of geologic heterogeneity on solute concentration distributions?		
8. Surface water–groundwater interaction		
8.1 Is the conceptualisation of surface water–groundwater interaction in accordance with the model objectives?		
8.2 Is the implementation of surface water–groundwater interaction appropriate?		
8.3 Is the groundwater model coupled with a surface water model?		
8.3.1 Is the adopted approach appropriate?		
8.3.2 Have appropriate time steps and stress periods been adopted?		
8.3.3 Are the interface fluxes consistent between the groundwater and surface water models?		

10 Focus topic: Solute transport

In this chapter:

- Introduction
- When to use a solute transport model
- Fundamental concepts
- Conceptualisation
- Design and construction
- Calibration and sensitivity analysis
- Prediction and uncertainty
- Reporting.

Guiding principles for solute transport modelling

Guiding Principle 10.1: 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.

Guiding Principle 10.2: 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.

Guiding Principle 10.3 The importance of variable-density flow should be assessed with a quantitative analysis using all available head and concentration data.

Guiding Principle 10.4: The size of the solute transport-model domain may not be the same as the groundwater flow model domain. Consideration should be given to whether a groundwater flow model should be constructed with a model domain that is greater than the region of interest of the solute transport model.

Guiding Principle 10.5: Analytical models should be used before the development of a comprehensive numerical solute transport model to assess the relevant spatial and timescales.

Guiding Principle 10.6: The grid or mesh for a solute transport model should be constructed with sufficient spatial resolution, both horizontally and vertically, to resolve concentration gradients and to meet the criteria imposed by the numerical solution method. Aquifers and aquitards should be subdivided into multiple layers when vertical variations of solute concentrations need to be resolved.

Guiding Principle 10.7: A stepwise approach to solute transport-model construction should be used to minimise potential errors that may arise due to the high level of complexity of solute transport models.

Guiding Principle 10.8: The effects of the spatial and temporal discretisation and the methods used to solve the solute transport equations should be assessed as part of the sensitivity analysis.

Guiding Principle 10.9: Uncertainty analysis and reporting should reflect the parameter uncertainty and the uncertainty stemming from the adaptation of a particular conceptual model and numerical aspects.

10.1 Introduction

This chapter provides guidance to the modeller on approaches to the simulation of common non-reactive solute transport problems. Similarly to the evaluation of problems relating only to groundwater flow and storage, the investigation of issues involving the transport of solutes requires special considerations. There are additional limitations and requirements that apply to solute transport models, and therefore analysing and predicting solute movement can be substantially more challenging than the quantification of groundwater flow only.

There is a focus in this chapter on the simulation of seawater intrusion, that is, the displacement of freshwater by seawater incursion in coastal aquifers where density differences influence groundwater flow patterns. The modelling of heat in groundwater systems is, for the purposes of these guidelines, considered to be largely analogous to conservative solute transport modelling, and therefore most of what is covered in this chapter applies to the simulation of heat in groundwater, where temperatures do not affect fluid properties (density, viscosity etc) or the properties of the aquifer matrix.

Solute transport situations that are not covered within this chapter include those involving hydrogeochemical reactions, multiphase flow (e.g. non-aqueous phase liquids, gas production and transport), volatilisation, unsaturated zone processes, transport in surface water systems and colloid transport.

10.2 When to use a solute transport model

Figure 10-1 shows some typical application of solute transport models. Successful development and application of a solute model requires that a sufficiently detailed description of the system's key features is obtained (through field measurement and aquifer testing) that matches both the modelling objectives and the required predictive capability of the model. A clear understanding of modelling objectives, including desired model confidence level and the precise nature of solute transport predictions, is needed during the planning stages of investigations, when project timelines and resource requirements need to be estimated. The feasibility and capabilities of solute transport models will be highly dependent on the specific field conditions, available data and the nature of predictive scenarios, and these will have important repercussions for the required budget and timing.

A solute transport model is not always needed to address a solute transport problem. In some cases, the answer can be obtained by using a groundwater flow model. The calculation of the salt load to a river, for example, can be done by multiplying the water flux from the groundwater into the river (calculated using a groundwater flow model) by the salt concentrations in aquifers adjacent to the river. This approach is adequate if the salt concentrations can be estimated or measured with a reasonable degree of accuracy. If, however, the salt concentrations were to vary significantly with time, the model would need to consider these temporal variations, in which case a solute transport model may be warranted. A variable-density flow and transport model may even be needed if salinity differences in the groundwater are so high that buoyancy effects influence flow patterns. Solute transport modelling is fundamentally reliant on a reasonable representation of groundwater flow. It involves stages of development that are similar to and interdependent with the construction of groundwater flow models; namely, conceptualisation, design and construction, calibration and sensitivity analysis, prediction, uncertainty analysis, and reporting. In this chapter, each of these modelling elements is discussed with a focus on the specific requirements of solute transport models beyond those of groundwater flow models. These sections therefore must be read in conjunction with the other chapters in this document.

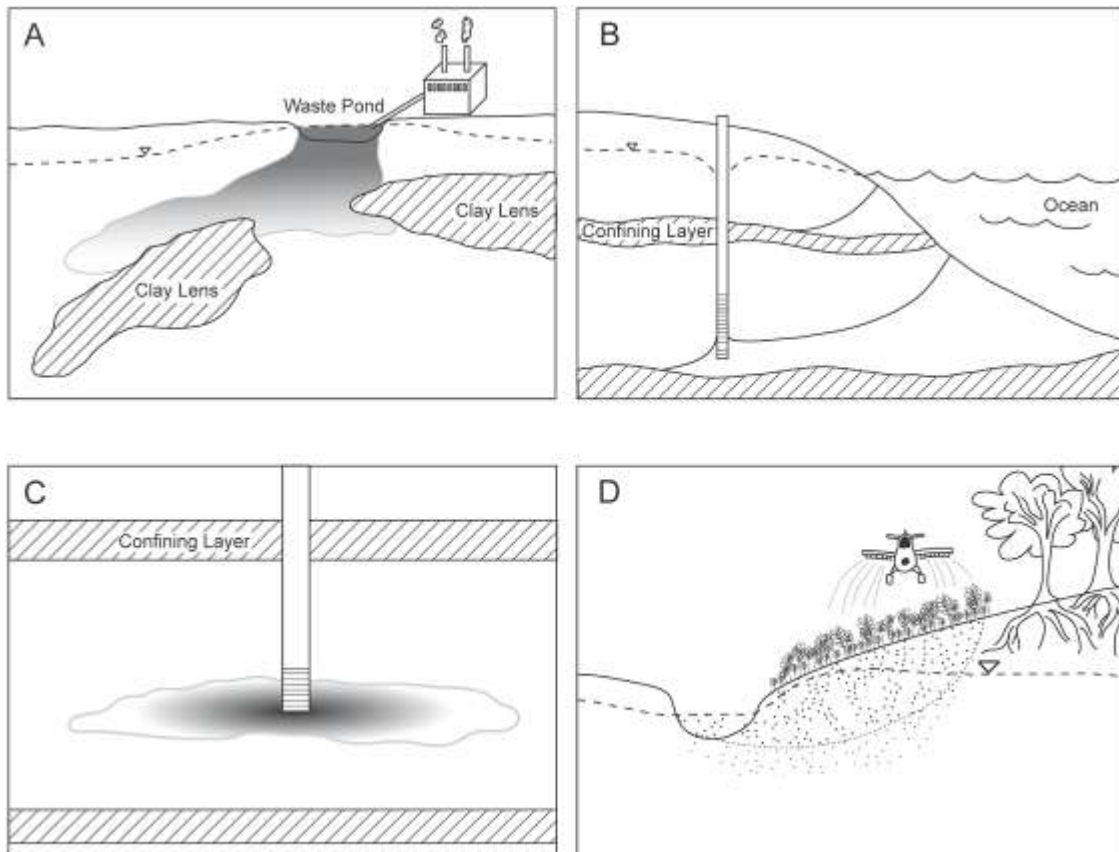


Figure 10-1: Four common solute transport problems: (a) leachate plume emanating from a waste pond; (b) seawater intrusion in a multi-layer aquifer system and upconing of interface due to pumping; (c) injected plume in an aquifer storage scheme; and (d) contamination associated with agricultural practices

Figure by Peta Jacobsen (Flinders University).

10.3 Fundamental concepts

10.3.1 Solute transport processes

The fate of solutes is controlled by both physical and chemical processes. Physical processes include:

- **advection:** the entrainment of solutes with the flowing groundwater in which they are dissolved. The term 'advection' is sometimes used interchangeably with 'convection'
- **molecular diffusion:** the spreading of solutes from zones of high to low solute concentrations by the random (Brownian) motion of molecules. This process occurs whether or not there is groundwater flow
- **hydrodynamic dispersion:** the spreading of solutes that occurs during groundwater flow due to differences in groundwater flow speeds, which are caused by the presence of physical heterogeneities in the porous medium and by variations of the groundwater flow velocity at the pore scale.

Chemical processes can be manifold and may include transformation of solutes in the aqueous phase, but may also extend to transitions of solutes between non-aqueous and gaseous or solid phases. The guidance in this chapter is restricted to solutes that behave conservatively (chemically inert). The decision of whether it is appropriate to treat solutes as conservative is an important one, and the extent to which this is applicable needs to be established by the modeller during the conceptualisation stage of the groundwater modelling process. The simulation of chemical processes is the realm of reactive transport modelling, and is not considered here. Guidance on many of these types of transport problems can be found in the following references: Zheng and Bennett (2002), Appelo and Postma (2005), and Bethke (2008).

Example 10.1: A reactive transport model

The simulation of the fate of metalloids during aquifer storage and recovery calls for a reactive transport modelling approach that considers interactions and transformations of chemical species. This is because the local redox conditions in the target aquifer, which will be affected by the injection of foreign water, control the chemical reactions that can increase or decrease the concentrations of the species of interest. For example, the mobilisation of arsenic (As) is frequently observed during the injection of oxygenated water into a reduced aquifer due to the oxidation of As-containing pyrite. At the same time, iron hydroxides may precipitate and adsorb the released As, resulting in a complex, spatiotemporally variable interplay between aqueous solutes and mineral phases.

Where salinity levels influence the water density, the groundwater flow regime and the transport pathways of solutes may be significantly affected by the density effect. In some cases, the density effects arising from temperature variations may also be significant, but these situations are less common. The characterisation and management of coastal aquifers in particular require consideration of the influence of density effects to properly identify the location and movement of the seawater zone within the aquifer, and its potential to adversely impact freshwater availability.

10.3.2 Solute transport modelling approaches

Solute transport models typically solve two equations, one for groundwater flow and one for solute transport. The governing equation for solute transport is commonly referred to as the advection-dispersion equation (ADE), which is based on the principle of mass conservation for solutes. The modeller needs a thorough understanding of the processes and parameters represented in the solute transport ADE to be able to properly construct and apply solute transport models. Zheng and Bennet (2002) provide an excellent treatment of the subject.

Most approaches to solute transport modelling assume that mixing due to dispersion is analogous to the diffusion process. Diffusion (and by analogy dispersion) is described using Fick's law, in which the concentration gradient multiplied by a diffusion/dispersion coefficient yields the solute flux. The resultant concentration distribution due to advection and diffusion/dispersion is one that, for a homogeneous medium and a constant flow velocity, is normally distributed around a midpoint, which is located at a distance from the source equal to the product of the advective flow velocity and time.

The parameter that quantifies the degree of mixing by hydrodynamic dispersion is a characteristic length, referred to as the **dispersivity**. As with hydraulic conductivity (refer section 1.5.1), dispersivity can be anisotropic (i.e. varying with direction). While it is theoretically possible to decompose the dispersivity into its directional components to capture its anisotropic nature (referred to as the full dispersion tensor), in practice these cannot be measured. Instead, a simplification is applied in which the dispersion in the direction of the flow is controlled by the longitudinal dispersivity, and the dispersion perpendicular to the flow in both the horizontal and vertical directions is controlled by the horizontal and vertical transverse dispersivities, respectively. The hydrodynamic dispersion coefficient is the product of dispersivity and the local groundwater flow velocity, taking into account its direction. The sum of the hydrodynamic dispersion coefficient and molecular diffusion controls the spreading of solutes in transport models.

Box 10A: CAUTION Dispersion in heterogeneous systems

Studies within the international literature have shown that modelling approaches that describe hydrodynamic dispersion analogously to diffusion have great difficulty reproducing observed concentration distributions in highly heterogeneous environments. It has therefore been suggested that the description of dispersion being analogous to molecular diffusion is too simple a concept, except maybe for homogeneous aquifers. Where practical, modellers should attempt to explicitly simulate heterogeneous features such as fractures (i.e. by using a discrete fracture network) or low-permeability lenses. This approach is applicable for relatively large heterogeneities, but not for heterogeneity that exists at the sub-grid scale, as for example in aquifers consisting of fluvial deposits. For these systems, some success has been obtained by using a dual-porosity or 'dual domain' approach. With this approach the aquifer is conceived as consisting of high-permeability zones of relatively fast flow and low-permeability zones with little or no flow, and the exchange between these is controlled by diffusion. Although there are some promising developments in this field, the dual-porosity approach still suffers from the problem that it requires parameter values that cannot be quantified at the field scale, and can therefore only be obtained through model calibration.

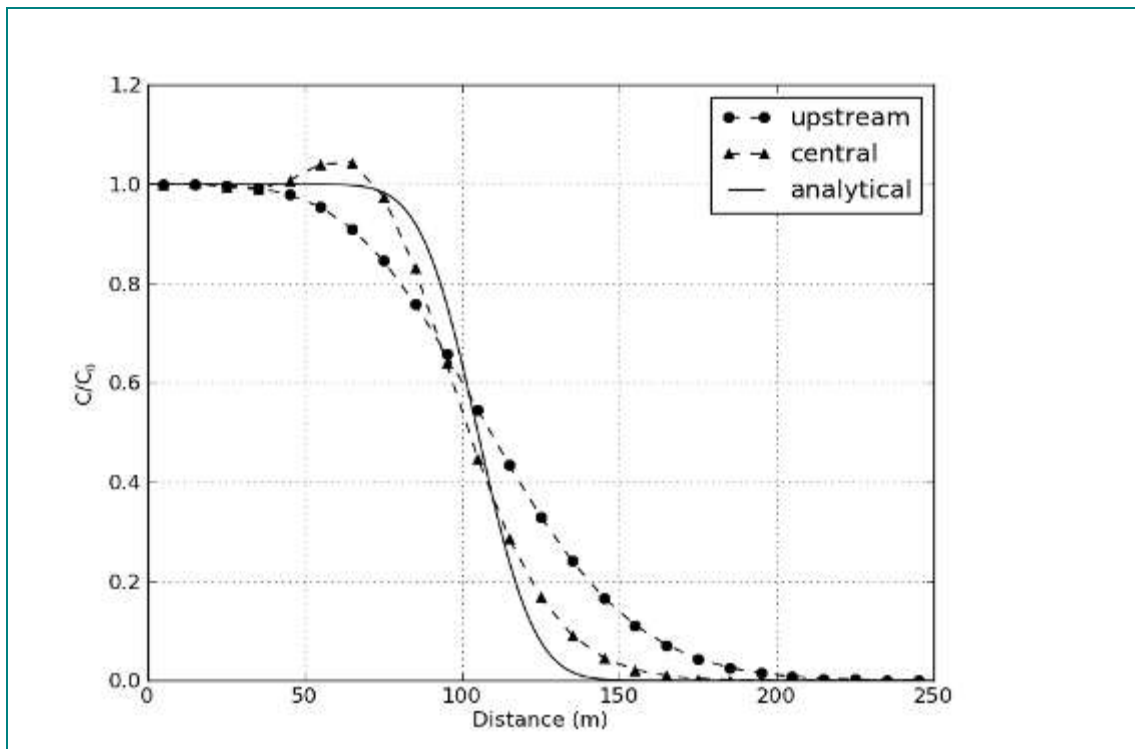
Analytical solutions of the ADE exist, but their applicability is limited to situations where the flow geometry and aquifer transport properties can be simplified considerably. For real-world problems this is rarely the case, and solute transport modelling usually involves a numerical model code. The numerical solution of the ADE suffers from difficulties that can have significant implications on the model outcomes and predictions, and modellers need to be aware of these. The difficulties stem from the mathematical nature of the ADE, which warrants different solution techniques for situations where advection rather than diffusion is dominant. Numerical methods are generally classified in the following manner (Zheng and Bennett 2002):

- **Eulerian:** A fixed spatial grid is used to solve the transport equation. (This also includes the total-variation-diminishing TVD methods.)
- **Lagrangian:** Large numbers of particles are used to approximate transport by advection, dispersion and diffusion.
- **Mixed Eulerian-Lagrangian:** The advection term is solved using a Lagrangian technique and the dispersion/diffusion term is solved using an Eulerian technique.

Example 10.2: The effect of solution techniques

To solve the ADE numerically using Eulerian finite difference techniques, the solute concentration gradient needs to be approximated at each node in the model. There are different ways to do this (Zheng and Bennett 2002). One method uses the solute concentration upstream of the node (upstream weighting) and another uses the average concentration of the node and that of its neighbours (central weighting). The latter technique is more accurate, but tends to create artificial oscillations of the calculated concentrations. This means that calculated concentrations are higher (overshoot) or lower (undershoot) than the maximum and minimum concentrations dictated by the boundary conditions and source terms. This problem is not present with the upstream weighting scheme. This scheme, however, is less accurate and has the effect that the spreading of solutes by dispersion is over-estimated. This phenomenon is an artefact of the numerical method used to solve the ADE and is therefore referred to as numerical dispersion.

These problems are illustrated in the figure below (modified from Zheng and Bennett 2002), which shows the results of a 1D simulation of a continuous injection of a solute after 100 days. The groundwater flow velocity is 1 m/d, and the dispersivity is 1 m. The analytical solution represents the exact solution that the numerical model is supposed to match. The central weighting scheme shows overshoot between 50–70 m, but matches the analytical solution more closely than the upstream weighting scheme, which shows artificial spreading caused by numerical dispersion.



For highly variable flow cases, there may be no single solution technique that is optimal throughout the entire model domain. For example, in highly variable velocity fields such as those involving pumping wells, groundwater flow may range from stagnation points with almost no flow, to well capture zones with very high flow rates. In such cases, diffusion may be the dominant transport mechanism in some parts of the model (i.e. in low-flow regions) and in other parts, advection and dispersion may dominate (i.e. in high-flow regions). Additionally, solute transport predictions often require a sufficiently fine model grid to obtain accurate solutions, especially where plume fronts are sharp (i.e. solute concentration gradients are steep). It is therefore important to assess the nature of errors that arise from both the choice of solution method and the design of the model grid. This is commonly achieved through systematic testing of the solute transport model (see section 10.4.2).

Modelling variable-density groundwater flow is particularly challenging because the groundwater flow equation and the ADE are coupled through the groundwater density, and hence have to be solved within the same simulation. This poses additional challenges to the modelling process, in particular a considerable increase in computational burden, which may impose restrictions on model calibration and sensitivity analyses. The modelling challenges associated with variable-density groundwater problems such as seawater intrusion have given rise to various simplified approaches for obtaining initial approximations, such as the use of non-dispersive, immiscible representations of the seawater-freshwater mixing zone (so-called sharp interface models). Analytical solutions for the steady state position of the seawater-freshwater interface are routinely used to provide first-order approximations of the extent of seawater intrusion in coastal aquifers and for the purposes of designing subsequent numerical modelling efforts.

10.4 Conceptualisation

10.4.1 Overview

Conceptualisation for the purposes of solute transport modelling is essentially an extension of the groundwater flow conceptualisation (refer Chapter 3). However, the conceptual models that underlie solute transport models are often more complex than those for groundwater flow models and hence there is a need for the modeller to factor in those processes related to solute transport at an early stage in the conceptualisation.

The primary aim of the conceptualisation component of a solute transport modelling investigation is to document the processes, parameters and complexities that control solute transport and the simplifications of these that are necessary to develop a computationally tractable mathematical model. The conceptualisation is highly dependent on the questions at hand and the desired model confidence-level classification, in the same manner as for modelling groundwater flow.

Solute transport models can range in complexity from relatively simple analytical solutions, which require a single, spatially and temporally constant value of the groundwater flow velocity, to 3D, regional-scale transient models. The solute transport model will invariably omit significant aspects of the system's complexities (e.g. certain chemical reactions), no matter how complex the model is and therefore a key goal of the solute transport conceptualisation is to describe the main system characteristics beyond the processes represented in the model. That is, the conceptual model should include factors that are excluded from the numerical model to ensure that decision-makers are aware of both the model limitations and the processes that may influence solute transport beyond those used in making predictions.

Example 10.3: A justifiable simplification

In seawater intrusion studies of coastal aquifers, it is common to simulate only a single solutes that represents the total salinity. As intruded seawater migrates through the subsurface, chemical reactions will alter the concentrations of individual solutes, sometimes to a very large extent. But in the majority of cases, the effect of these changes in the concentrations of individual solutes on the total salinity can be neglected. So, if the modelling objectives do not require that concentrations of individual solutes be simulated, the complexities stemming from chemical reactions can be neglected, and the problem can be simplified considerably.

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 timescales
- 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.

10.4.2 Solute concentration data

Guiding Principle 10.1: 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 data that needs to be considered during the conceptualisation stage includes:

- solute concentrations within the model domain, which are used to obtain an overview of the spatial distribution of the solute of interest
- time series data to elucidate important temporal trends, typically ranging over timescales of years to days. For example, concentration time series of contaminant breakthrough at monitoring wells provide critical insight into rates and extent of plume movements, and in coastal aquifers, seasonality in recharge, tidal fluctuations, pumping and agricultural practices will impose controls on seawater intrusion
- information about the source history of contaminant plumes is required to decipher whether source concentrations are constant or varying. This could include information from historic archives, or anecdotal information
- solute concentrations outside of the model domain (including in deeper geological layers), which are required to prescribe model boundary conditions and possibly to establish 'background' conditions.

Monitoring strategies need to be designed such that measurements are sufficient for characterising the migration of solutes (including preferential flow pathways), potential source zones, vertical stratification within aquifers and the position of the interface between fresh and saline groundwater in coastal aquifers. Caution is warranted when wells with long screen lengths are used, as samples obtained from these may represent mixtures of waters with different concentrations, and therefore only provide a rough indication of the flux-averaged mean concentration in the capture zone of the well. Vertical concentration gradients may not be detected if there are only single-depth measurements at a particular location. Seawater intrusion problems are typically characterised by salinity stratification within aquifers. The data collection needs to consider this. If available, indirect measurements of total solute concentrations in groundwater based on geophysical methods should also be considered at this stage.

10.4.3 Solute transport processes

Guiding Principle 10.2: 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.

Guiding Principle 10.3: The importance of variable-density flow should be assessed with a quantitative analysis using all available head and concentration data.

In some cases, especially for regional scale models, advection dominates over diffusion and dispersion, and it may be justified to consider only advective transport. Transport can be approximated using particle tracking (refer section 6.5), which follows an imaginary parcel of water along the flow paths of the model based on the calculated hydraulic head distribution. Particle tracking is appropriate if mixing by dispersion and diffusion can be assumed negligible and if the substance of interest is chemically inert.

In models of coastal aquifers, the model complexity can be significantly reduced if the transition zone between fresh and saline water can be considered as a sharp interface, with no mixing between the two different waters. Sharp interfaces do not exist in reality, but for the purpose of regional seawater intrusion models the transition zone is often sufficiently narrow for this assumption to be justified. The mathematical treatment of the transport problem can be simplified considerably, which means that the computational burden becomes much less compared to models that simulate the mixing of fresh and saline groundwater. A further simplification can be applied when the interface does not move significantly over the length of the model simulation, and where simulation of the flow in the freshwater domain is the objective. In this case the interface can be taken as the impermeable base of the model, and only the flow in the freshwater region is considered. In groundwater systems with wide mixing zones or where interface movements are being considered, however, fully-coupled variable density codes (i.e. codes that solve the flow and transport equations within a single simulation) must be employed.

Assessment of variable density flow conditions

When spatial differences in salinity (and sometimes temperature) exist, the influence they have on the density and hence on the flow dynamics must be evaluated during the conceptualisation stage. This typically involves converting the measured heads obtained from various groundwater salinities to a single reference salinity/density. When this procedure reveals that the correction terms are significant, a variable density modelling approach is warranted. For example, consider the saline part of a 100 m thick coastal aquifer. At the coastline, the head in the aquifer is equal to the mean sea level if hydrostatic conditions prevail and the effect of complicating factors such as tides can be assumed to be negligible. An equivalent freshwater head (see Example 10.4) at a depth of 100 m would be in the order of 2.5 m above mean sea level. Suppose that the heads at the inland boundary in the model are around 3–5 m, and it becomes clear that in this case a variable density model is appropriate.

In general, the importance of density effects increases with the depth of the system and the spatial variability of solute concentrations. Density effects are typically ignored in models of contaminant plumes, although in high-permeability aquifers they may start to become important even for low salinities (TDS ~ 1500 mg/L).

Example 10.4: Assessing the importance of density effects.

To assess the importance of density effects in groundwater systems where salinity is variable, the modeller can convert measured heads to so-called freshwater heads. The freshwater head is an imaginary head that would have been measured if the water in the observation well had been fresh water. By making this assumption, the pressure of the water at the measurement point becomes uniquely related to the height of a water column for all the different observation wells. This is not the case for the field measurements, in which the water in each observation well differs because of salinity differences in the groundwater. The equation that expresses the freshwater head as a function of the measured head is:

$$h_f = z_i + \frac{\rho_i}{\rho_f} (h_i - z_i)$$

[Eqn 10.1]

where h_i and h_f = saline and fresh water heads, respectively, z_i = elevation of the measurement point (centre of the well screen) and ρ_i and ρ_f = saline and fresh water densities, respectively.

Piezometer	Screen elevation (m above reference level) (m)	h_i (m)	ρ (kg/m ³)	h_f (m)
1	-40	1.25	1004	1.42
2	-40	1.20	1006	1.45

Freshwater heads (provided that they are at the same depth) can be compared to infer the horizontal direction of groundwater flow. This example shows that the uncorrected, measured heads indicate that flow is from piezometer 1 to piezometer 2, but the freshwater heads show that the flow is actually in the opposite direction. The conclusion in this case should be that density effects are significant, and that a variable density model is needed. The reversal of the flow direction, as in this example, represents an extreme case, and should not be considered as a general criterion for the need for a variable density model. If flow rates are affected in a more subtle manner, and it is hard to establish the importance of density effects, the modeller has no choice but to run a density variant and a density invariant model. The example presented here is meant to be illustrative only, and is not applicable in all cases. More details and examples can be found in Post et al. (2007), and references therein.

10.4.4 Model extent and simulation time

Guiding Principle 10.4: The size of the solute-transport model domain may not be the same as the groundwater-flow model domain. Consideration should be given to whether a groundwater flow model should be constructed with a model domain that is greater than the region of interest of the solute transport model.

Guiding Principle 10.5: Analytical models should be used before the development of a comprehensive numerical solute transport model to assess the relevant spatial and timescales.

The dimensions and size of the model domain of a solute transport model are not necessarily the same as that of its underlying groundwater flow model. To obtain the flow field required for solute transport simulation, a groundwater flow model may be required that encompasses a much greater area than the region of interest for the solute transport model. This occurs when the solute transport problem is confined to a small region in a groundwater flow system that is driven by regional stresses and boundary conditions. In that case, the modeller may choose to develop a nested flow and transport model for reasons of computational efficiency. A nested flow and transport model has a domain that is only a portion of a larger groundwater flow model, which is used to predict water fluxes through the nested model boundaries. Another approach to limit run times and memory requirements is to model transport along one or more 2D cross-sections. Cross-sectional modelling is typically not appropriate when the flow field is 3D in nature, such as near wells, but if a dominant flow direction can be identified, it may be possible to simplify the solute transport problem to a 2D (or even 1D) problem.

Example 10.5: A nested model

An injection experiment in a multi-aquifer groundwater system was modelled to assess the extent of the injected water and its solutes, and their subsequent fate after the injection was stopped. The injection was into one specific aquifer, but it affected the flow in the adjacent aquifers, and flow in the vicinity of the injection experiment was influenced by regional groundwater flow. The migration of the injected solutes, however, was restricted to the target aquifer only and the concentration patterns in the other aquifers were not part of the modelling objectives. Therefore, in order to simulate the flow, a regional-scale flow model was used, but for the simulation of the solute transport, a nested model was built that was smaller in spatial extent and limited to one aquifer. Appropriate boundary conditions were obtained from the regional model and were used to account for the water and solute exchange across the nested model boundaries.

During the conceptualisation stage, the relevant timescales need to be identified. Solute transport problems can be steady state, but in most cases, a transient model is warranted. For transient solute transport models, the underlying flow model can be steady state or transient. The choice depends on the modelling objectives and the nature of the system. For example, if the long-term average salt load to a river is sought, and there are no stresses that alter the groundwater flow patterns over time, a steady state groundwater flow model and a steady state solute transport model would be adequate. If, however, the seasonal variability of the salt load to a river with a highly variable stage and floodplain width must be determined, both the flow and transport models need to be transient. Example 10.6 gives some additional examples to illustrate when various steady state and transient flow and transport model combinations are warranted.

Example 10.6: Steady state versus transient models

The following examples demonstrate the various combinations of steady state and transient flow and solute transport models, and when they are applicable.

		<i>Flow model</i>	
		<i>Steady state</i>	<i>Transient</i>
<i>Solute transport model</i>	<i>Steady state</i>	Water authorities are interested in the effects of a reduction in long term average recharge on the location of the interface between fresh and saline groundwater in a coastal aquifer. Assuming that the other stresses to the system remain constant, the problem can be addressed with a steady state flow and transport model as only the average conditions are of interest.	This combination never applies: If the flow model is transient, the solute transport model is always also transient.
	<i>Transient</i>	An acid mine drainage plume has developed in an aquifer with a steady flow field. A model is built to predict the development of the plume over the next 25 years. The flow model can be steady state but the transport model must be transient.	A public water supply well is located in an aquifer near a river with a highly variable stage that exerts a strong control on groundwater flow patterns. Concerns exist that pollutants from the river water may eventually reach the supply well, and a model is commissioned to assess how far the pollutants may have migrated into the aquifer. Since the flow field is highly transient, the flow and the transport model both have to be transient.

Analytical solutions to the ADE can be used as low-complexity models to obtain initial estimates of important plume characteristics. For example, a 1D model across the centre of an idealised contaminant plume can be used to produce a rough approximation of the timing, extent and spreading of contaminant migration, by adopting the simplification of a homogeneous aquifer.

Similarly, sharp-interface modelling of idealised coastal aquifer transects provide first-order estimates of the steady state position of the interface between fresh groundwater and seawater (see example box in section 10.10). This will assist in identifying the minimum area of transport simulation.

Example 10.7: The use of a low-complexity model to assess relevant spatial scales

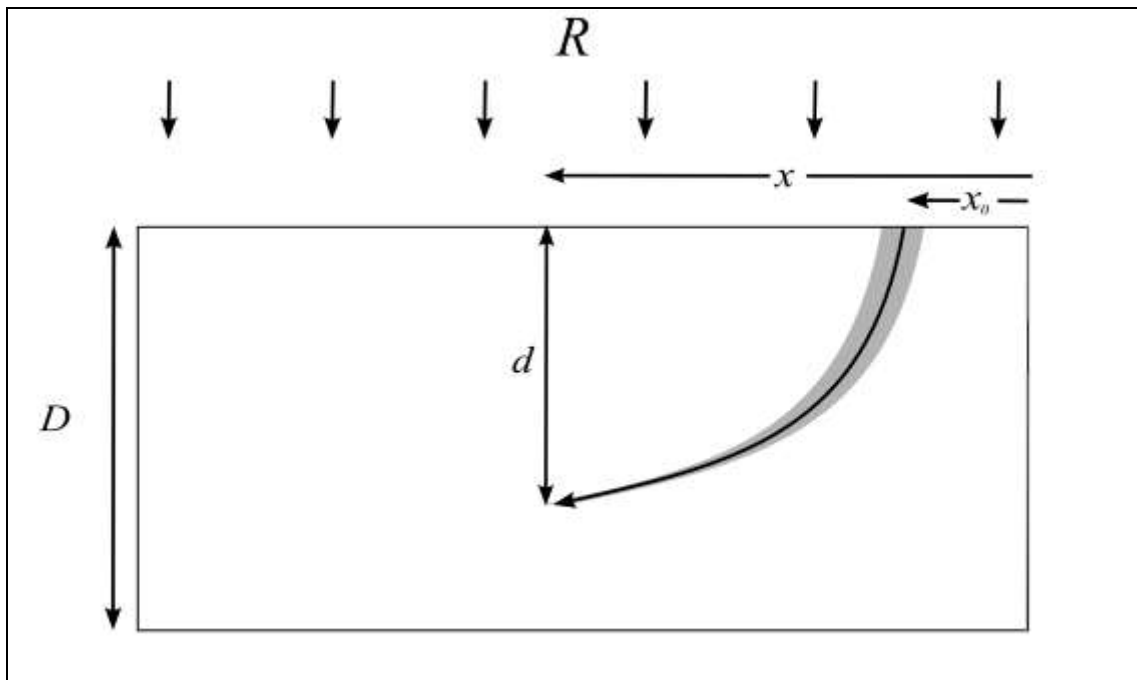
The figure below shows a schematic cross-section of an unconfined aquifer that is recharged by rainfall. The right-hand boundary is a water divide and groundwater flow is from right to left. All groundwater discharges through the left-hand boundary. A leachate plume (indicated by the grey shading) is emanating from a landfill which has its midpoint x_0 located 250 m from the water divide. The recharge is 100 mm/year. The saturated thickness D of the aquifer is 50m and its porosity, ϵ , is 0.3. If it is assumed that the aquifer is homogeneous and that the recharge is uniform across the top of the aquifer, the distance travelled by the plume after time t can be found from using the following equation (Appelo and Postma 2005):

$$x = x_0 \exp\left(\frac{Rt}{D\epsilon}\right) = 250 \cdot \exp\left(\frac{0.1 \cdot t}{50 \cdot 0.3}\right) \quad [\text{Eqn 10.2}]$$

Evaluating this formula with $t = 25$ years gives $x = 295$ m, which means that the centre of the plume has moved 45 m in 25 years. Note that this approach assumes advection only, and that spreading of the solute mass by dispersion and diffusion is neglected. The maximum depth of the plume at time t can be estimated from:

$$d = D\left(1 - \exp\left(\frac{-Rt}{D\epsilon}\right)\right) = 50\left(1 - \exp\left(\frac{0.1 \cdot t}{50 \cdot 0.3}\right)\right) \quad [\text{Eqn 10.3}]$$

which yields $d = 7.7$ m for $t = 25$ years.



10.4.5 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 (refer section 4.5). There are three types of solute concentration boundary conditions (also refer section 4.5):

- **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.

A particular aspect in the spatial delineation of seawater intrusion models is the definition of the boundary condition along the coastline. It should be realised that in many situations, the flow systems that exist on land extend underneath the seafloor (see figure in example 10.10). It may therefore be necessary to include the offshore part of an aquifer system. Given the data scarcity that is typical in these environments, this may introduce considerable uncertainty, and the implications of the choices made during the conceptualisation process may have to be revisited during the uncertainty analysis phase to assess their impact on the modelling outcomes and the formulated objectives.

10.4.6 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, paleoseawater 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. Preliminary modelling may even be undertaken to assess the feasibility of alternative conceptualisations (refer section 3.4), or to guide the data collection, or to prepare an estimate of the initial solute concentration distribution for the model calibration process (noting that the calibration of a seawater intrusion model may be an especially challenging process (see section 10.6)).

10.4.7 Heterogeneity

Groundwater flow conceptualisation usually involves identification and delineation of the primary hydrostratigraphic units (refer section 3.6.2), 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.

Example 10.8: The need to account for heterogeneity

Consider the migration of a contaminant through an unconsolidated aquifer consisting of fluvial deposits comprising sand, silt and clay. Most of the advective transport takes place within preferential pathways made up by the sandy sediments, which are relatively permeable. Hence the timing of the first breakthrough of a contaminant plume into a well is likely to be underestimated because solutes arrive earlier than if an average permeability would be adopted. On the other hand, if this aquifer were to be remediated, flushing of the contaminants will, in reality, be much longer than would be simulated using average properties for the aquifer. This is because solutes that reside in low-permeability clayey or silty sediments, migrate more slowly than for the average-permeability case, and can result in delayed delivery of contaminants for extended periods after the high-permeability regions have been flushed.

An extreme case of this behaviour may be the transport of solutes along preferential flow paths in a fractured-rock aquifer, where the bulk of the solute transport takes place due to rapid flow within the fractures. Transport in the rock matrix is usually dominated by diffusion and hence proceeds very slowly. In that case it is probably more appropriate to model the system as a dual-porosity medium (i.e. flow and storage in the matrix and fractures are assigned different properties) or even using a discrete-fracture model, in which the distributions of fractures within the matrix are explicitly modelled.

Failing to account for heterogeneity where it controls solute transport is likely to result in modelling outcomes that are of limited use. Questions that need to be addressed regarding the role of heterogeneity include:

- How do the hydrostratigraphic units control the solute concentration distribution?
- What aquifer connections exist that may determine the solute migration pathway?
- Are there any faults, other natural subsurface features, or man-made elements such as long-screened wells or open boreholes that can act as conduits for solutes that might need to be considered?
- How does the heterogeneity within aquifers control the spreading of solutes and how will this heterogeneity be represented in the model?

The modeller needs to be aware that a relationship exists between the degree of heterogeneity of the hydraulic conductivity used to simulate flow and the need to account for heterogeneity by means of hydrodynamic dispersion. Hydrodynamic dispersion is, in part, due to the variability of hydraulic conductivity across a range of scales. If, theoretically, all of the variability of the hydraulic conductivity could be captured by the model, spreading of solute mass would be explicitly simulated as a result of a complex flow field. In practice, the variability of the hydraulic conductivity can never be known; neither can the variability at the sub-grid scale be captured in a numerical model. The dispersivity is thus an effective parameter that captures unmodelled features of the system. But as a general guideline, the model should capture as much of the variability of the hydraulic conductivity as possible, so that the complexity of the flow patterns, and the resultant solute spreading, is represented as closely as possible using explicit descriptions of hydraulic conductivity variation rather than dispersivity, consistent with the modelling objectives.

10.4.8 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:

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

Effective porosity

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 (Table 10-1).

Table 10-1: Total porosity values for varying lithological units

<i>Material</i>	<i>Total porosity (%)</i>
Well-sorted coarse sand	31–46
Well-sorted fine sand	26–53
Silt	35–60
Clay	33–60
Sandstone	5–30
Shale	0–10

Source: Domenico and Schwartz (1990)

The problem with assigning a porosity value is that the advective flow may not occur across all of the pore space. At the microscopic scale, the bulk of the flow may occur in the large, connected pores (effective porosity), whereas little or no flow occurs in the small or dead-end pores. Therefore, the porosity that must be used to represent the advective flow correctly is smaller than the total porosity. Clay has a high total porosity, but as much of the water contained in it is bound to the clay particles, it tends to have a low effective porosity. As a general rule, the more uniform or homogeneous the composition of the porous medium, the more closely the effective porosity matches the total porosity. When assigning values to this parameter, a sensible approach would be to start with the value of the total porosity and adjust the parameter to lower values, if needed, during the calibration stage. When the proportion of immobile zones (i.e. pore space with negligible or no advective flow) is large in comparison to the mobile zones, a dual-domain description of the solute transport processes is warranted.

Dispersivity

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 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. It is common practice for models of low-confidence level classification to use values from the literature, but in the absence of model calibration and uncertainty analysis, the applicability of the adopted values to site-specific conditions may be highly questionable. For models targeted at a high confidence level classification where detailed predictions of solute concentrations are part of the objective, tracer tests should be considered as part of the data collection effort.

Box 10B: Values of dispersivity

It has been recognised that there is a correlation between the value of the dispersivity and the spatial scale of the model, at least for local scale (<100 m) problems. Based on a compilation of values published in the literature, it is sometimes suggested that the longitudinal dispersivity is 10% of the distance travelled by a solute from its source (Zheng and Bennett 2002). This is a very rough approximation, but it can be used as an initial estimate in the absence of site-specific data. This relationship breaks down at larger spatial scales (>1 km). 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).

Other than these crude relationships, very little guidance exists on the parameterisation of the hydrodynamic dispersion process, which highlights one of the fundamental weaknesses of the field of solute transport modelling. The dispersivity should always be considered to be a calibration parameter in the model because dispersivity is essentially 'structure imitating', not 'process-imitating' or 'process-based'. The modeller must be aware of this when making predictions.

Diffusion coefficient

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).

As the solute takes a complicated pathway in porous media due to the pore geometry, the actual value of the diffusion coefficient used in models is lower than the values in pure water. The parameter that controls this is the tortuosity, which expresses the actual length of the solute pathway relative to the distance travelled along a straight line. Some codes require the tortuosity as an input parameter, others require an effective diffusion coefficient. If no reasonable estimates of the tortuosity can be made, the effective porous-medium diffusion coefficient can be approximated by multiplying the diffusion coefficient in pure water by the porosity.

Equation of state

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 ADE. 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.

10.5 Design and construction

10.5.1 Model discretisation

Guiding Principle 10.6: The grid or mesh for a solute transport model should be constructed with sufficient spatial resolution, both horizontally and vertically, to resolve concentration gradients and to meet the criteria imposed by the numerical solution method. Aquifers and aquitards should be subdivided into multiple layers when vertical variations of solute concentrations need to be resolved.

Setting the model domain size of a transport model involves trade-offs between computational demands (which increase with domain size) and the need to capture key processes adequately. Solute transport models require a sufficiently fine grid resolution, and this can be a limiting factor in setting the domain size and in the analysis of regional scale transport problems.

The grid resolution must be sufficiently fine to resolve the solute concentration gradients, and the model layer structure must be such that vertical concentration variations within aquifers are captured (e.g. in seawater intrusion models where the transition zone is simulated). This means that in solute transport models, the aquifer is commonly subdivided into several model layers, as opposed to flow modelling where it is often appropriate to represent an aquifer by a single model layer. If the underlying flow model was not originally designed for solute transport purposes, the grid and layer structure may have to be redesigned.

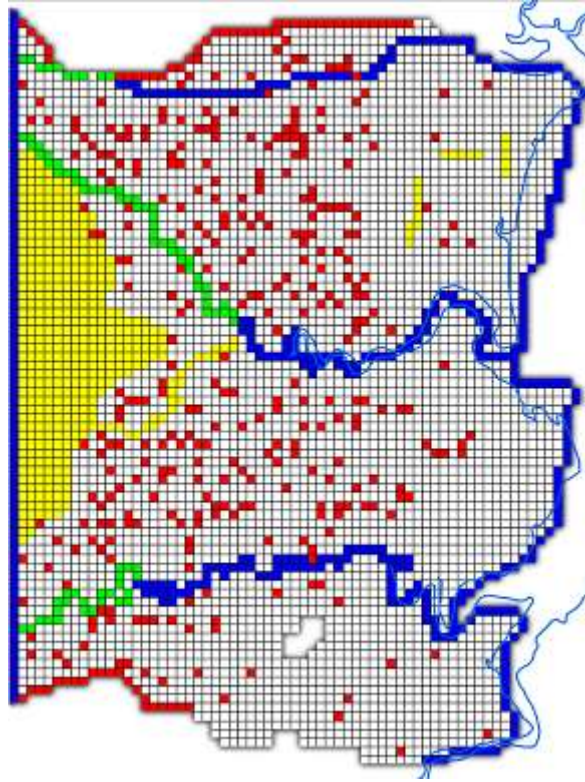
Additional discretisation requirements stem from the nature of the ADE and the difficulties of solving this equation numerically. The numerical difficulties depend in part on the type of solution method that a particular model code uses. Model codes that use an explicit solution method have strict space and time discretisation criteria for reasons of numerical stability. As discussed in section 10.3.1, numerical dispersion and artificial oscillations are problems that are often encountered. Both problems tend to become less severe with decreasing grid size and time steps, which is why the discretisation requirements of solute transport models are stricter than for flow models.

Criteria exist to evaluate whether the chosen grid and time stepping are suitable for the problem at hand. The main criteria are:

- the **grid Peclet number**, which is the ratio of the grid cell size to the dispersivity. It has been found that values of the Peclet number lower than four are usually effective in suppressing artificial oscillations, but values up to 10 have been found to work by some authors. Purely advective problems have a dispersivity of zero and hence a Peclet number of infinity; these require Lagrangian or mixed Eulerian-Lagrangian solution techniques.
- the **Courant number**, which is the ratio of the product of the advective flow velocity and the time step, divided by the grid cell size. The Courant number needs to be less than or equal to unity, which basically states that during a given time step, a solute particle can traverse not more than a single model cell.

Example 10.9: A model grid and boundary conditions for a coastal aquifer

The figure below shows the grid of a seawater intrusion model (Werner 2005). Each cell measures 250 x 250 m. The various colours represent the boundary conditions used. Red cells represent groundwater wells, yellow cells represent drainage features (natural or man-made), green cells represent rivers and blue cells are specified head boundaries. Specified concentration boundaries are applied to specified head cells that coincide with the coastline and estuaries (indicated by the light blue line). The concentration applied at these cells decreases inland to account for the decreasing salinities in the estuaries (not shown).



Dispersion effects and the advective flow rate are spatially and temporally variable, and this makes it challenging to apply the Peclet and Courant constraints in designing the model grid and setting transport parameters. For example, Peclet and Courant requirements may be met in certain parts of the model or during certain periods of the simulation, but not in others, and therefore the discretisation may be suboptimal. A common approach to test if the grid is adequate is to start with a relatively coarse grid to do initial model runs at minimal computational expense. If the modeller decides that the model satisfactorily simulates all transport processes, the grid is refined to test if there is any change in the model outcome, for example by comparing simulated concentration time series at specific locations and/or salinity distributions at different times, as obtained using different grids. If further refinement no longer produces a significant change, grid convergence has been achieved, and the grid size can generally be considered to be adequate.

The computational requirements of a solute transport model may become so large that calibration and sensitivity analysis, or even a single model run, become infeasible. In that case, the modeller has to carefully trade off numerical accuracy versus practical considerations such as memory requirements and computational burden.

10.5.2 Solute concentration distributions

Transient models require a spatially-interpolated field of initial concentrations. As solute concentrations are slower to respond to system stresses than hydraulic heads, the effects of inappropriate initial conditions tend to affect simulation outcomes for longer periods for solutes than for heads. Assigning an appropriate initial concentration to each node in the model is not trivial, especially in 3D models. Two approaches may be chosen:

- A steady state solute transport model is used to determine the initial solute concentrations. This approach is valid if a reasonable assumption of steady state conditions can be made.
- Initial solute concentrations are based on interpolation between measurement points. The main problems that exist with this approach are that (i) this requires a dense network of observation wells, which may not always be available or even feasible and (ii) traditional interpolation techniques, such as inverse-distance weighting, fail to do justice to geological controls on spatial solute variations. Geostatistical techniques such as kriging may be applied such that the interpolation of concentration measurements mimics the geological structure (e.g. using variograms based on aquifer stratigraphy). When concentration data based on water samples is scarce, geophysical measurements may offer an alternative means to interpolate groundwater solute concentrations between point measurements.

10.5.3 Boundary and initial conditions

Fixed concentration boundaries may be appropriate to represent features such as well-mixed and extensive surface water bodies, or salt bodies. Specified mass flux boundaries could include a known advective flux of mass due to groundwater flow across a model boundary such as groundwater recharge. Type 3 boundary conditions are appropriate near model boundaries where outflowing groundwater removes mass from the model domain, but where concentration gradients across the boundary cause dispersive reflux of solutes into the model domain. This may occur, for example, near the boundary between saline surface water into which fresh groundwater flows, such as in models of submarine groundwater discharge.

Solute concentrations of sources in the model are required to simulate the influence of features and processes like injection wells, pond or canal leakage, and river inflow. If these vary over time, information on their temporal variability may also be required if transient conditions are being simulated. Sinks usually are assigned the solute concentration that the water has as it leaves the model across a boundary or into a well. In the case for evapotranspiration, only water, but not solute, is removed from the model, causing solute concentrations to increase.

In variable density models, it is essential that the specified heads or pressures are consistent with the initial density distribution. The increase of the groundwater pressure with depth depends on the vertical distribution of the groundwater density. Some model codes require the heads to be specified as freshwater heads (see section 10.4.3), which increase with depth if the density of groundwater is higher than that of fresh water. The modeller needs to calculate these heads before they are input into the model, which requires the concentrations to be converted to densities using the adopted equation of state. Once the densities at different depths are known, the pressures can be calculated, which can be converted to freshwater head values.

In models that do not explicitly consider the effect of tidal oscillations on groundwater flow, a tidal overheight must be added to the specified head at the model boundary that represents the surface water body (e.g. ocean, estuary). Formulas are available in the literature to calculate the tidal overheight, which is a function of tidal frequency, amplitude and the hydraulic conductivity, among other parameters. These formulas are restricted to specific flow geometries, but can be used as an initial estimate. The value of the tidal overheight can also be measured directly from near-shore or beach piezometers, and can also be considered during the calibration process.

10.5.4 Model code selection

A variety of model codes are available for the simulation of solute transport; these differ in their range of capability, solution techniques for the ADE and the description of the dispersion process. The selection of a model code is an important step in the modelling process and depends on a variety of considerations, primarily dictated by the hydrogeological problem that needs to be simulated, the solute transport modelling objectives and associated conceptual model (refer to 10.4.3).

Particle tracking might be a suitable replacement for more complicated modelling approaches that consider processes other than advection. If this simplification can be made, there is no need to use a model code that solves the ADE, and a conventional groundwater flow model code that has the option to do particle tracking can be used instead. Guidance on the selection of a groundwater flow model code can be found in section 4.3. Particle tracking options may vary among model codes, for example, some model codes can only handle steady state particle tracking.

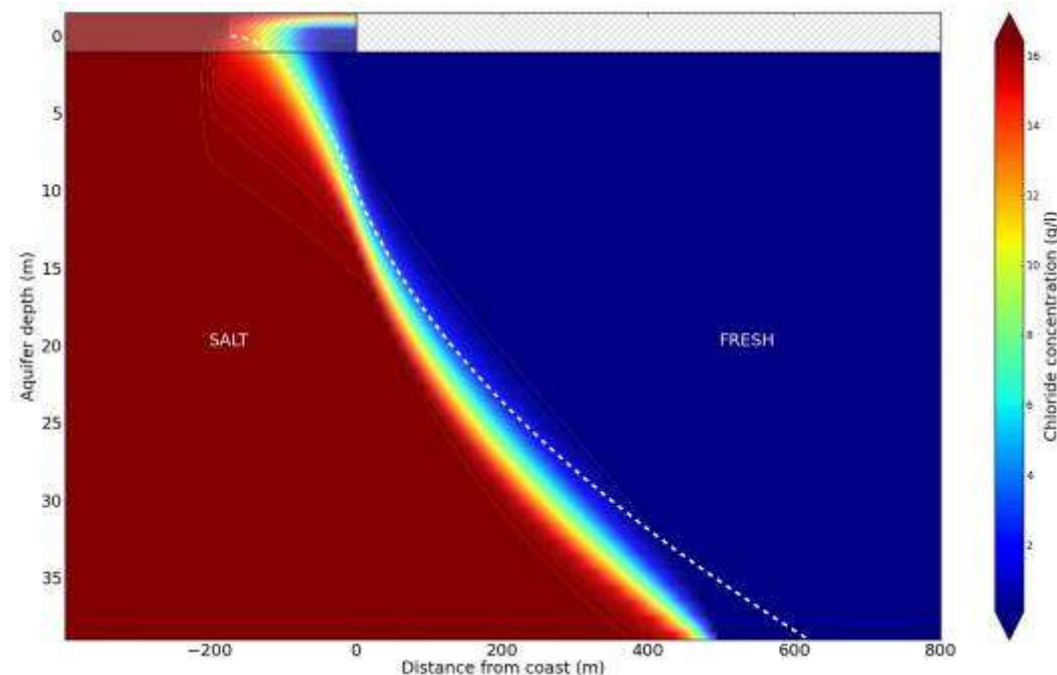
The difficulties related to the numerical solution of the ADE and the simulation of dispersive mixing have led to the development of a variety of model codes and solution methods. Model codes that apply Eulerian solution methods are preferred when a fine spatial and temporal discretisation are required to adequately represent the conceptual model. This is mostly applicable to local-scale problems. In typical regional-scale models, where advection dominates, model codes that apply a Lagrangian or a mixed Eulerian-Lagrangian approach are usually better suited. These methods suffer from other drawbacks such as mass balance errors, large memory requirements and numerical difficulties where stagnation points and irregular concentration patterns exist. Some model codes offer multiple-solution methods, which have the obvious advantage that a single model code can be used for a variety of applications, and also comparisons between solution methods are therefore more easily achieved. The modeller always needs to evaluate during the conceptualisation stage which transport processes need to be simulated and consider this in selecting the most appropriate model code.

There are several model codes in widespread use that are able to simulate the effects of density on groundwater flow arising from the invasion of seawater into aquifers. The capabilities of these model codes differ in the way they handle the interaction between fresh and saline groundwater. The most comprehensive model codes consider the mixing of fresh and saline water, and simulate the change of groundwater salinity in space and time. These should be selected in areas with wide mixing zones, and where the coupling between flow and transport and transient simulation of the migration of solutes is the objective. There are also model codes that assume that a sharp interface exists between fresh and saline groundwater and that mixing between them can be neglected. These are applicable in regional scale problems of seawater intrusion where the transition zone is thin in comparison to the thickness of the fresh groundwater body. Some model codes, finally, take the density effect on the flow calculation into account, but do not simulate the change of solute concentrations over time. These can be appropriate in studies of seawater intrusion where the position of the transition zone does not move during the simulation period, but where density effects are expected to affect the flow.

A list of solute transport codes is provided in Table 4-1.

Example 10.10: A comparison between a coupled variable-density model and an interface approximation

The figure below shows a coloured contour plot of the chloride concentrations calculated using a cross-sectional variable density model. Freshwater inflow occurs through the right-hand boundary, the landward side of the aquifer is confined (the confining layer is shown as the hatched area) and the model domain extends below the seafloor. A semi-confining unit (dashed area) separates the aquifer from the ocean. The sharp interface approximation is also shown and it can be seen that the position of the toe of the intruded seawater is over-predicted by the sharp-interface approximation. Still, for regional-scale modelling purposes, the sharp-interface approach appears to be a suitable alternative. The run times of the numerical variable density model could be in the order of hours, whereas the sharp-interface approximation can be programmed in a spreadsheet for immediate evaluation.



Picture kindly provided by Amy Roach (Flinders University).

10.5.5 Model construction

Guiding Principle 10.7: A stepwise approach to solute transport model construction should be used to minimise potential errors that may arise due to the high level of complexity of solute transport models.

In general the construction of a solute transport model involves the following steps, assuming that a flow model already exists:

- model grid construction (for sub-models) or refinement (for existing models), including further vertical discretisation (refinement) of flow model layers of individual aquifers
- specification of the boundary conditions for solute concentrations
- specification of the stress periods, time steps and transport time step size/geometric increment
- definition of the initial concentrations
- definition of the distribution of the transport parameters (dispersivities, diffusion coefficients, and effective porosities)
- for variable-density models, specification of the parameters for the equation/s of state
- selection of the solution method for the ADE, and its associated parameters and convergence criteria.

It is recommended that a step-by-step approach be taken to the construction of a solute transport model. It is better to add model components sequentially to allow progressive testing as the complexity of the model is increased.

Box 10C: CAUTION Consistent use of model parameters

The modeller must ensure that the parameter values that are entered into the model are consistent with the definition of the parameters in the ADE employed by the model code. For example, in some model codes the diffusion coefficient in pure water is the input parameter, but in other model codes, the effective porous medium diffusion coefficient needs to be entered into the model.

The inconsistency of units is a common pitfall. Consider, for example, the parameters required for the equation of state, which are commonly the density of fresh groundwater and the density change per unit concentration change. The modeller needs to ascertain that these parameters are consistent with the units of length, solute mass, water mass and time that are being used. Inconsistent units are often the cause of unexpected model behaviour, which may be more easily diagnosed if simple ('by hand') calculations of such aspects as the magnitude of density effects, timing and extent of concentration movements, and steady state and/or sharp-interface conditions are first estimated using simpler approaches (e.g. analytical solutions).

Once a model has been constructed it is advised to conduct a preliminary model run using the estimated hydrogeological and transport parameters as a first check to see if the simulated concentrations are reasonable. Reasonable in this context typically means that they are not smaller or larger than the minimum or maximum concentrations of any of the sources or the initial concentrations, and not smaller than the initial concentrations. Where the initial concentrations are zero, the modeller should check for negative concentrations. Where evapotranspiration is simulated, solute concentrations may reasonably be expected to increase above the maximum concentrations in any of the model sources.

10.6 Calibration and sensitivity analysis

10.6.1 Calibration

As with calibration of groundwater flow models (refer Chapter 5), the calibration of solute transport models involves establishing that the model is able to simulate observed conditions. Calibration criteria are typically concentrations, or derived measures, such as the plume mass or the time to reach peak concentrations. Concentration patterns are much more sensitive to local-scale geological heterogeneity than are heads, and models may have difficulty reproducing the concentrations or their temporal variability of single observation wells. If that is the case, an aggregate quantity like the plume mass is a more suitable calibration criterion. First and second moments (i.e. average and spread) make good 'targets', and lead to more stable calibrations to actual concentrations as well. Alternatively, a large acceptance criterion may have to be adopted, as long as it can be ascertained that the model is capable of simulating the main features of the system. As advection is the dominant transport process in many modelling studies, the parameters that control groundwater flow, such as hydraulic conductivity and aquifer geometry, will also be affecting the calculated solute concentration patterns. In fact, simulated concentrations are often more sensitive to the values of the hydraulic conductivity than are the heads. The modeller could exploit this during the calibration process, as the solute transport model is likely to provide additional constraints on the flow patterns that could aid in the optimisation of the flow model parameters. Calibration of the flow model and transport model parameters simultaneously is often referred to as 'coupled flow-and-transport calibration' in the literature.

Besides the flow model parameters, parameters that can be adjusted during the calibration of the solute transport model include:

- effective porosity
- dispersivity
- diffusion coefficient
- source history and locations.

This contains only parameters that, unless the model is a variable density model, have no effect on the simulated head distribution.

The difficulty associated with measuring dispersivity values, and their scale dependence, means that the dispersivity is almost always a calibration parameter. It is rather common to see spatially uniform dispersivities and diffusion coefficients, even in regional-scale models, due to a general lack of information about their spatial variability. If parameters are not appropriately constrained during model calibration, the resulting dispersivity may reach values that are physically unrealistic (tens of metres or more). If there is no evidence for physical processes causing such high dispersivity values, it is more likely that in these cases, calibrated dispersivity values are compensating for processes that are otherwise misrepresented in the model. Therefore, when such high values have to be adopted to fit the data, it is likely that the conceptual model is flawed and needs to be revisited. The dispersivity should also not be increased beyond physically reasonable values in an attempt to meet the grid Peclet number requirements. For contaminant transport, the locations of contaminant sources and their mass loading history is often highly uncertain and is therefore often considered to be a calibration parameter.

10.6.2 Sensitivity analysis

Guiding Principle 10.8: The effects of the spatial and temporal discretisation and the methods used to solve the solute transport equations should be assessed as part of the sensitivity analysis.

Sensitivity analysis in solute transport modelling has the same objective as in groundwater flow modelling and the discussion of this topic (refer section 5.4) equally applies to solute transport modelling. As the outcomes of solute transport models are highly dependent on the selected solution method and its parameters, as well as the transport step length, the sensitivity of the results to these should also be evaluated during this stage. This is not common in groundwater flow modelling, but it is advisable to do so in solute transport modelling to get a better quantitative estimate of the effect of the selection of a particular solution method, its parameters, and the grid-cell size resolution and time-step size on the outcomes.

10.7 Prediction and uncertainty

Guiding Principle 10.9: Uncertainty analysis and reporting should reflect the parameter uncertainty and the uncertainty stemming from the adaptation of a particular conceptual model and numerical aspects.

Within the context of solute transport modelling, model prediction involves running the (calibrated) model with anticipated stresses, with the objective of establishing the future development of solute concentrations. Any stresses that have an effect on groundwater flow can be expected to have an effect on solute concentration patterns as well. However, solute concentrations may change even if the future groundwater flow pattern remains the same. This may occur when the solute concentrations of water sources in the model change, or when a solute source is removed, such as in the clean-up of contaminated sites. Also, solute transport may occur for considerable timescales after the head conditions have stabilised following a change in the system state, and solute disequilibrium (i.e. exhibiting transient conditions) is often encountered in systems where flow appears to have stabilised (i.e. reaching steady state conditions). In the case of seawater intrusion, the position of the interface may depend on earlier sea levels or other pre-historical events, despite head conditions that reflect modern-day conditions.

Predictive uncertainty can stem from uncertainty relating to model parameters, conceptualisation and future scenarios. Parameter uncertainty pertains to both the solute transport parameters and the parameters of the groundwater flow model that underlie the transport model. The lack of data on solute transport parameters frequently forces modellers to use literature values for the dispersivities, diffusion coefficient and porosity, and this places a greater responsibility on the modeller to evaluate the implications (in terms of predictive uncertainty) of adopting values that are not site-specific.

Uncertainty relating to transport parameters like dispersivity is introduced through the fact that they can only be calibrated using measured concentrations in the region where the plume has become established. If in future scenarios the plume migrates and expands, it may enter regions of the model where other dispersivity values apply, for example, as a result of a different degree of heterogeneity. In that case, the spreading of the plume by hydrodynamic dispersion will be under- or overestimated. An assessment of the potential for this to occur should be made, which involves an evaluation of the degree of geologic heterogeneity.

Given that solute transport parameters are usually poorly constrained and highly uncertain, it is common practice to define the values of the dispersivity, diffusion coefficient and effective porosity as constant, at least within individual hydrostratigraphic units.

When site-specific data is scarce or unreliable the modeller can choose to:

- decide that the lack of information prohibits the desired modelling approach or level of complexity and either (i) opt for a simpler model (and redefine the objectives) or (ii) collect additional field data
- decide to optimise the most uncertain values during the calibration and sensitivity analysis stage
- consider worst-case prediction scenarios, especially in contamination studies
- run multiple models assuming a probabilistic parameter distribution, which acknowledges the uncertainty and assigns a spread around the most reasonable value.

In deploying solute transport models it is advisable to consider more than one realisation of the aquifer geology. This arises from the importance of aquifer heterogeneities in controlling solute transport, combined with the difficulties in obtaining accurate representations of aquifer hydraulic property distributions. Stochastic approaches are often adopted whereby numerous different heterogeneous hydraulic distributions are devised that are consistent with field observations of geological characteristics and that accommodate the hydraulic parameters obtained from aquifer testing. In this way, it may be possible to approximate elements of contamination risk and provide estimates of uncertainty arising from certain aspects of the model construction.

The greater complexity of conceptual models associated with solute transport models compared to groundwater flow models results in a greater risk of the modeller overlooking essential features of the system, or making decisions during the conceptualisation stage that lead to an oversimplified model representation of the real-world system. Such unmodelled features may be identified during the calibration stage, for example, when they result in the need to adopt unrealistic parameter values. But when they go unnoticed, unrepresentative transport parameters will be specified in the model predictions, and a great degree of prediction uncertainty may be expected. It is essential that the conceptual model and numerical simulations are interlinked and co-dependent, such that unrealistic parameter values arising through modelling (e.g. calibration) allow for adjustment of the conceptual model and diagnosis for where characteristics of the system may not have been adequately conceptualised, or where aspects of the conceptualisation and associated transport processes have been overly simplified.

Example 10.11: The effect of an unmodelled feature on model predictions

The modelling of contaminant migration relies on knowledge of the number and locations of sources, as well as the solute loading history. More often than not this information is not available. The gradual increase in solute loading from a landfill may result in a disperse leachate plume. If this information is unknown to the modeller, the observed concentration distribution may be erroneously interpreted as being due to spreading caused by aquifer heterogeneity. Hence, the adopted dispersivity values in the calibrated model will be too high, and future predictions will overestimate the spreading of the plume.

Care must also be taken when the mixing zone between fresh and saline groundwater in coastal aquifers is simulated. Tidal fluctuations tend to cause the transition zone to widen. In a steady state groundwater model, this process cannot be explicitly represented, and the adopted value of the dispersivity is likely to be overestimated as a result. Mixing may therefore be overestimated if these values are subsequently used without modification in a transient model.

As mentioned previously, the choice of solution method and its parameters can have a profound effect on the predicted solute concentrations. Hence, predictive uncertainty analyses in solute transport modelling need to include evaluations of their effect on solute transport simulations. This is relatively straightforward to do if a model code is used that implements multiple solution methods.

10.8 Reporting

The reporting requirements of solute transport models are largely the same as for groundwater flow models, with the provision that more information needs to be provided as a result of the greater complexity of solute transport models. The assessment of the role of geological heterogeneity during the conceptualisation stage needs to be carefully examined. Moreover, given the difficulty associated with the quantification of solute transport model parameters, and the fact that they are often based on literature values, the motivation for the selection of the chosen values must be discussed, and literature sources cited.

It is common practice in groundwater flow modelling to include hydraulic head maps in a report or a presentation. Such maps, however, have limited value in modelling studies of variable-density systems, because, in contrast to uniform density systems under isotropic conditions, the hydraulic head gradient does not indicate the direction of groundwater flow. Therefore, rather than presenting the head contours with the aim of depicting groundwater flow directions, reports on the results of variable-density models should present flow vectors or streamlines to visualise groundwater flow patterns.

If normalised concentrations are presented (e.g. as is sometimes done to compare simulations with variable concentration ranges), it should always be clear what concentration was used to normalise the values. Visualisation of 3D contaminant plumes can be difficult, and typically requires specialised visualisation software that allows slicing and extrusion of contours. A colour legend to indicate the concentration contour values is required when filled contours are presented, with the red shades preferably referring to the high concentrations, and blue shades to low concentrations (see Example 10.5.5).

Analogous to the water mass balance of flow models, solute transport models report a solute mass balance. The error in the mass balance needs to be small (<1% for mass conservative schemes), and the report should always provide this information. It should be kept in mind that Lagrangian-solution techniques are not mass-conservative and larger mass balance acceptance criteria may apply than in flow models or in solute transport models that employ an Eulerian approach.

11 Focus topic: Surface water–groundwater interaction

In this chapter:

- Introduction
- Fundamental concepts
- Conceptualisation
- Design and construction
- Calibration and sensitivity
- Prediction and uncertainty
- Reporting and review.

Guiding principles for surface water–groundwater interaction

Guiding Principle 11.1: The conceptual model should account for the range of types of surface water bodies within the region of interest and the flow regimes and types of connection that would be expected to occur, under natural, current and future conditions.

Guiding Principle 11.2: Collection and analysis of data, especially of data related to surface water bodies, should be planned and coordinated by all stakeholders working together to ensure that data is collected at compatible locations and scales to allow development of robust conceptual models.

Guiding Principle 11.3: A conceptual model involving surface water–groundwater interaction should be developed to achieve a balance between real-world complexity and simplicity, such that the model includes all those features essential to the representation of the system, and enable predictions to meet objectives. Those features that are unlikely to affect model predictions should be left out.

Guiding Principle 11.4: The domains of surface hydrological and hydrogeological systems should be conceptualised based on an understanding of how these systems function independently and together as a coupled system. If surface run-off enters the hydrogeological domain and acts as a source of recharge, surface hydrological modelling may be required beyond the boundary of the hydrogeological domain.

Guiding Principle 11.5: The conceptual model should include consideration of the time required for the full impacts of changes in groundwater systems to be observed in surface water systems, and vice versa. The time to a new dynamic equilibrium will influence model design, as well as the assignment of climatic and other stresses during predictive runs.

Guiding Principle 11.6: A modelling approach based on linking or coupling surface water models to groundwater flow models should be used when surface water dynamics are significantly affected by exchange flows. When surface water dynamics are likely to be unaffected, or only slightly affected, an approach based on groundwater flow modelling with standard boundary conditions may be adequate.

Guiding Principle 11.7: If a decision is made to link or couple surface water and groundwater models, the choice between hydrological, hydraulic and hydrodynamic surface water models should be made based on the spatial and temporal scales of interest, and on whether surface water dynamics based on conservation of energy and momentum are likely to be needed relative to simpler approaches based on water balance alone.

Guiding Principle 11.8: Analytical solutions should be used to develop an understanding of the nature of surface water–groundwater interaction prior to regional scale numerical modelling, or in parallel with such modelling as a way of checking the numerical modelling.

Guiding Principle 11.9: The level of spatial discretisation should be chosen based on conceptualisation of exchange flows and an understanding of the relationship between the size of surface water bodies and cell or element sizes. The level of temporal discretisation (time steps) should be chosen based on the temporal variability of surface water levels or fluxes and on requirements for stability and accuracy.

Guiding Principle 11.10: Models that include surface water–groundwater interaction should be calibrated using a variety of different metrics that measure the behaviour of the surface water system. This may imply a need to calibrate by trial and error, because more formal automated methods may not be easily adapted to some of the performance measures of interest.

Guiding Principle 11.11: Sensitivity analysis of models that include surface water–groundwater interaction should test the sensitivity of spatial and temporal discretisation, as a way of demonstrating model robustness.

11.1 Introduction

Surface water–groundwater interaction is a term used to describe the exchange of water between a surface water body (such as a river or a lake) and groundwater. Modelling of surface water–groundwater interaction requires knowledge of groundwater modelling, but also special understanding of the exchange processes that occur between surface water and groundwater. In some cases it becomes necessary to simulate the dynamics of both surface flows and groundwater flows, using techniques and software that are appropriate to the timescales of all flow processes.

This chapter provides an overview of the way interaction between surface water and groundwater is conceptualised, and the approaches to design and construction of models that include surface water–groundwater interaction. Modelling of surface water–groundwater interaction requires all the same stages of development as modelling of groundwater flow; conceptualisation, design and construction, calibration and sensitivity analysis, prediction, uncertainty analysis, and reporting. Each of these is discussed in this chapter with a focus on the specific requirements of surface water–groundwater interaction, beyond those of groundwater flow models. Chapter 11 must therefore be read in conjunction with all other chapters in these guidelines.

11.2 Fundamental concepts

11.2.1 What is surface water–groundwater interaction?

Surface water–groundwater interaction⁵ includes any situation where water above the land surface interacts with groundwater below the land surface. Examples include:

- lake–aquifer interaction and stream–aquifer interaction
- interaction between groundwater and water in oceans, seas, estuaries, lakes, salt lakes, ponds, swamps, marshes, wetlands, rivers and streams
- interaction between groundwater and water contained in or behind man-made structures such as dams, tailings dams, evaporation ponds, dredge ponds, flooded excavations, mine pit lakes, canals (including irrigation canals), drains, ditches and buried pipelines
- groundwater discharge to the land surface at springs (whether at a break in slope on a hillslope or in an ephemeral drainage line, or structurally controlled by faults such as mound springs near the southern edge of the Great Artesian Basin)
- groundwater discharge from the walls or floor of open-cut and underground mines, from road cuttings, from the toe of embankments, from horizontal drains, or into tunnels and underground caverns.

Diffuse or distributed recharge at a regional scale is not always considered to be surface water–groundwater interaction, because recharge can occur without ponding of water at the surface. But diffuse recharge is part of a continuum of processes at different spatial and temporal scales. If a dry streambed floods in response to rainfall and surface run-off, infiltration into the unsaturated zone can cause the watertable to rise until there is direct connection between surface water and groundwater. Diffuse recharge can also cause the watertable to rise to the land surface, such that a surface water body is formed.

Unsaturated flow includes the processes of infiltration and exfiltration, driven by rainfall, evaporation and transpiration (the latter two being collectively referred as evapotranspiration). Including these processes as part of a general definition of surface water–groundwater interaction emphasises the importance of exchange of water and solutes through the upper boundary of the groundwater flow domain, that is, with the atmosphere. The land-surface boundary condition has been described as the key to hydrology, because it controls the exchange of water between the atmosphere and the enormous volume of groundwater stored in the unsaturated and saturated zones beneath the earth's surface.

Groundwater modellers and reservoir engineers (who simulate oil, gas and geothermal reservoirs) share the challenges caused by a lack of certainty about the detailed structure and properties of the subsurface medium through which fluids flow. In many respects, it is the complexity of the land-surface boundary condition, including surface water–groundwater interaction, which creates unique challenges for groundwater modellers.

⁵ It is because of the long history of studies of lake–aquifer interaction and stream–aquifer interaction that interaction between surface water and groundwater is often described as surface water–groundwater interaction, rather than groundwater–surface water interaction. These terms are increasingly used interchangeably.

11.2.2 Types of impacts that can be modelled

Modelling should be undertaken with a clear understanding of purpose. Types of situations that may require modelling of surface water–groundwater interaction include:

- Proposals to develop or expand borefields for water supply, irrigation systems in alluvial floodplain aquifers or mining operations (either open cut or underground) may require an assessment of the extent to which a cone of depression at the watertable will extend to nearby rivers and streams, inducing leakage from those surface water bodies, with potential impacts on surface water supplies. Deep mines may lead to a cone of depressurisation in a confined aquifer that induces leakage through overlying aquitards, and ultimately from rivers and streams. The rivers and streams can sometimes be represented simply, with assumed water levels, and the impact of leakage on streamflow can sometimes be assessed independently using a surface water simulation model. In other cases a more sophisticated representation of surface water may be required.
- Water sharing and allocation at a regional scale may require tighter integration of models, since a significant issue is determination of long term yield in rivers and streams (see Example 11.1). In this case, it may be necessary to simulate exchange flows between surface water and groundwater, and also to simulate surface run-off, using a hydrological catchment model to estimate run-off to rivers and streams and possibly diffuse recharge to the watertable.
- Flood studies tend to be focused on shorter timescales, with flooding caused by extreme rainfall events, and the subsequent rise and fall of a flood wave. Any rise in surface water levels increases the flow of surface water towards groundwater, whether as temporary bank storage or as recharge to a lower watertable. Flooding may require simulation of flooding over extensive flood plains, rather than within the channels of rivers and streams. It may be necessary to predict surface water levels as well as rates of discharge, taking into account exchange flows to and from groundwater.
- Studies of the evolution of mine-pit lakes after closure of mines relate mostly to long-term discharge or recharge of groundwater through mine pits, until a new dynamic equilibrium is attained. A mine-pit lake can be treated simply, for example, as a lumped fully mixed water body characterised only by its surface elevation, or with sophisticated hydrodynamic models that predict the evolution of stratification, in temperature and water quality.

Example 11.1: Surface water–groundwater interaction modelling studies.

A typical situation where the quantification of surface water–groundwater interaction is necessary is in the planning and management of water resources and assessment of the impact of groundwater and stream abstractions on the reliability of water supplies and environmental flows. Double accounting and double allocation of water resources can occur when surface water and groundwater are considered to be separate resources. Quantification of the interaction between surface water and groundwater is essential in order to examine the security of total water allocations (Evans 2007a,b).

11.2.3 Flow regimes and types of connection

It is not possible to model surface water–groundwater interaction without a good understanding of the physical processes that occur. In essence, exchange flows between surface water and groundwater are driven by differences between surface water level or stage and heads in adjacent groundwater.

The understanding of surface water–groundwater interaction has evolved significantly in recent years, especially in terms of how to simulate surface water–groundwater interaction with simulation models. Much of the early research was undertaken in the USA (e.g. Winter 1976, 1978, 1983, 1986; Winter et al. 1998). Sophocleous (2002) provides additional background information in a review paper. An Australian Government website, <www.connectedwater.gov.au>, provides information about connected waters and includes an extensive reference list.

Significant research has been undertaken on surface water–groundwater interaction processes that are relevant and important in an Australian context. In most cases the research combines field investigations with modelling, sometimes using existing modelling techniques, sometimes developing new modelling techniques, and sometimes using models to explore and explain the nature of the interaction. Examples include research on:

- lakes and wetlands on the Swan Coastal Plain near Perth, Western Australia (e.g. Townley and Davidson 1988; Townley et al. 1992, 1993; Nield et al. 1994; Townley and Trefry 2000; Smith and Townley 2002; Turner and Townley 2006)
- floodplain–groundwater interactions in the lower River Murray in South Australia (e.g. Narayan et al. 1993; Jolly et al. 1994; Jolly et al. 1998)
- stream–aquifer interaction in the Murray–Darling Basin (e.g. Reid et al 2009; Brunner et al. 2009a, 2009b, 2010, 2011; Brownbill et al. 2011; Heritage Computing 2009, 2010).
- coastal and estuarine dynamics at a range of timescales (e.g. Smith and Turner 2001; Nielsen 2009, Chapter 8; Lenkopane et al. 2009; Xin et al. 2011)
- representation of groundwater processes in river operation and planning models (e.g. Rassam 2011; Rassam et al. 2011).

Five fundamentally different types of connection have been identified in freshwater environments, and many variations exist within these five. The five main types of connection are shown in Figure 11-1, together with terminology commonly used by surface water and groundwater hydrologists. While some terms are not widely used, surface hydrologists recognise the possibility of flow-through regimes, and groundwater hydrologists recognise that shallow lakes and wetlands can be perched above the watertable, possibly supporting a localised groundwater mound.

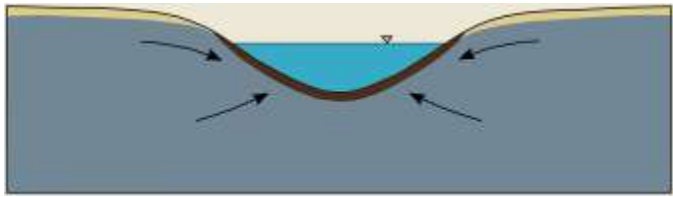
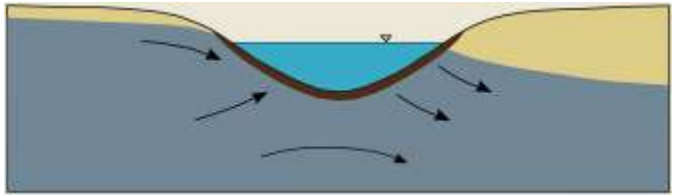
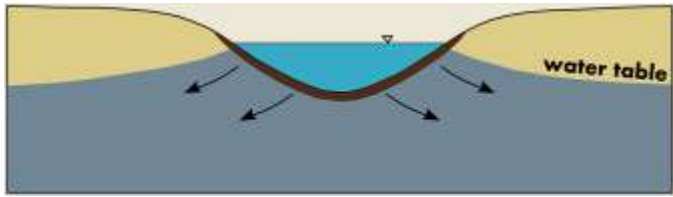
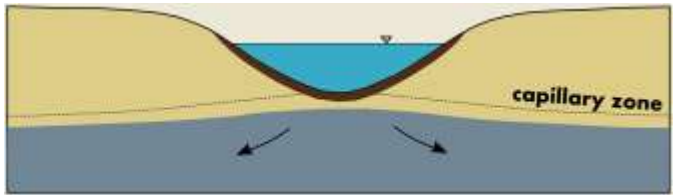
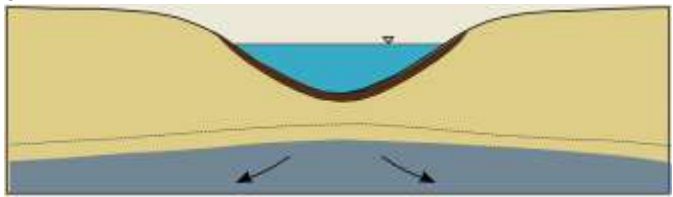
<i>Flow regime</i>	<i>In surface hydrology</i>	<i>In groundwater hydrology</i>
a 	Gaining stream	Discharge water body
b 	-	Flow-through water body
c 	Losing stream, connected	Recharge water body
d 	Losing stream, in transition	Perched recharge water body
e 	Losing stream, disconnected	Perched recharge water body

Figure 11-1 Flow regimes and types of connection

Figure 11-1 combines the results obtained by many researchers into one diagram. Figures 11-1a,b,c are well-known to those who work on lake–aquifer interaction, while figures 11-1c,d,e are well-known to those who work on stream–aquifer interaction, particularly in the context of losing streams.

Research on large surface water bodies, such as lakes and wetlands (see references above), led to recognition of a fundamental distinction between three types of surface water bodies:

- discharge water bodies (Figure 11-1a) (which receive groundwater discharge over the whole of the bed)
- recharge water bodies (Figure 11-1c) (which lose water by recharge to groundwater over the whole of the bed)
- flow-through water bodies (Figure 11-1b) (which receive groundwater discharge over part of the bed and lose water as recharge to groundwater over the remainder).

This classification evolved from the point of view of groundwater, thinking of discharge from and recharge to unconfined aquifers in direct connection with surface water bodies.

In fact the groundwater flow patterns near each of these types of water bodies can be further subdivided. Nield et al. (1994) used software developed by Townley et al. (1992) to show that there are 11 variants on each of Figure 11-1a and Figure 11-1c and 17 variants on Figure 11-1b. All 39 flow regimes are subtly different. Townley and Trefry (2000) showed that the same 39 flow regimes also occur in 3D, for example, beneath circular lakes and wetlands.

A gaining stream (from the stream's point of view) is a discharge water body (from the underlying aquifer's point of view). A losing stream (from the stream's point of view) is a recharge water body (from the underlying aquifer's point of view).

Rivers and streams act as flow-through water bodies (Figure 11-1b) at a variety of scales. In any system of meanders, water can short-circuit across a meander, albeit slowly, via the intervening aquifer. Some surface water flows beneath each riffle as groundwater. Local-scale flows in the hyporheic zone for water quality and for maintaining ecological function are extremely important (Winter et al. 1998).

Losing streams have been shown to operate in three modes (Brunner et al. 2009a, 2009b, 2010, 2011; Brownbill et al. 2011):

- as a connected system (Figure 11-1c), with a watertable continuous with the water level in the stream
- as a disconnected system (Figure 11-1e), with a watertable sufficiently deep that the capillary fringe is below the base of stream sediments
- in transition (Figure 11-1d), with a watertable below the base of stream sediments but with the capillary fringe still in contact with these sediments.

The rate at which losing streams lose water to groundwater varies as the conditions beneath the streambed change from saturated to unsaturated to almost dry (moisture content at field capacity).

Any of these flow regimes can exist in steady state, but natural systems are dynamic. Some urban wetlands in Perth cycle seasonally from a recharge regime following road run-off after winter rainfall, to a flow-through regime as the wetland level declines, to a discharge regime when evaporation dominates wetland water balance in summer, to a flow-through regime as evaporation declines and the wetland level recovers, and again to a recharge regime in winter. Rivers in the Murray–Darling Basin flood following rainfall, with the watertable rising until some reaches become gaining reaches, and some have the characteristics of flow-through regimes. As flooding recedes and the watertable declines, the same reaches become losing connected reaches, and ultimately losing disconnected reaches, but only after passing through a transition period with increased losses due to suction in the capillary fringe.

Proposed projects can cause a flow regime to change from one to another. If a pumping well is installed near a gaining stream, a flow-through regime may develop, with regional groundwater discharge on one side of the river, while the river recharges the aquifer on the other.

Surface water–groundwater interaction is also influenced by solute concentrations, especially where concentrations are sufficiently high to cause density-driven flow. Seawater intrusion along the coast is a special case of surface water–groundwater interaction, where exchange flow is caused by a combination of regional groundwater discharge from a coastal aquifer and density-driven convection at depth (see Chapter 10). Salt lakes may have evolved from discharge lakes to flow-through lakes, with net discharge of groundwater over geologic time leading to an accumulation of salt that now drives density-driven exchange flows.

Box 11A: CAUTION Challenges associated with differences in characteristics between surface water and groundwater

The interface between surface water and groundwater separates regions in which hydrological processes are fundamentally different. Table 11-1 describes key differences between surface water and groundwater.

Table 11-1: Differences between surface water and groundwater

<i>Characteristic</i>	<i>Surface water</i>	<i>Groundwater</i>
Resistance to flow	Small, caused by friction as water flows over a rough surface.	Large, caused by friction on a very large surface area, as flow occurs through narrow tortuous pathways in porous or fractured soil and rock.
Speed of flow	Fast, leading to almost horizontal water surfaces in large water bodies and slowly varying levels in rivers and streams.	Very slow, mainly because of high resistance, and generally with very small gradients in piezometric head.
Storage	In the absence of flow, e.g. in a lake, an additional 1 m of water raises the water level (a measure of potential energy) by 1 m.	In the absence of flow, an additional 1 m of water can raise the watertable (a measure of potential energy) by many metres, from 10 m to 100 m or more in materials with very small porosity (specific yield).
Response times	Short, caused by dynamic variations in rainfall.	Longer, because of the combined effects of specific yield and transmissivity, and because recharge, pumping and exchange flows vary more smoothly over longer periods of time.

The interface between groundwater and surface water is a boundary to both domains. From a modelling point of view, if each domain is modelled independently, the interface must be represented by a boundary condition.

One challenge in modelling surface water–groundwater interaction is caused by the fundamental difference in timescales between flow processes in surface water and groundwater. These are a direct result of the differences described in Table 11-1.

Surface water in rivers and streams moves quickly relative to groundwater, and the equations describing the movement of surface water must be solved with very small time steps. In some situations, for example, with networks of one-dimensional streams, the equations can be solved relatively quickly in each time step, but the number of time steps may be very large. When modelling flood plains or estuaries, the 2D and 3D surface water models have many cells and still need very small time steps.

Groundwater moves slowly, and the equations can sometimes be solved with relatively large time steps. However the nature of the 3D groundwater flow equations requires the solution of large systems of simultaneous equations, often approaching 1 million equations at every time step⁶. As a result the groundwater flow equations can be slow to solve in each time step.

Full coupling of surface water and groundwater flow models must meet the requirements of both types of flow calculation. This implies a need to solve very large systems of equations a large number of times, because of the small time steps required to resolve surface flows. This dilemma often leads to the need for simplifications to the conceptual model, based on the experience of the modeller. Simplifications are also driven by lack of data and lack of budget.

11.3 Conceptualisation

11.3.1 Overview

Guiding Principle 11.1: The conceptual model should account for the range of types of surface water bodies within the region of interest and the flow regimes and types of connection that would be expected to occur, under natural, current and future conditions.

There is no single correct way to represent surface water–groundwater interaction in a groundwater flow model. How a modeller proceeds depends on:

- the purpose of modelling (the questions to be answered)
- consideration of the nature of surface water–groundwater interaction and the level of detail required
- practical matters related to available modelling tools (such as the ability of software to represent the conceptual model with an appropriate level of detail)
- the availability of data, the budget for the project, the skill and experience of the modeller etc.

Just as conceptualisation of regional-scale groundwater flow relies on a hydrogeologist's ability to conceptualise the structure of the hydrostratigraphic system (see Chapter 3), conceptualisation of surface water–groundwater interaction relies on the modeller's ability to imagine or infer how exchange flows occur between surface water and groundwater. The conceptual model provides the framework for all the stages of modelling that follow.

11.3.2 Data collection and analysis

Guiding Principle 11.2: Collection and analysis of data, especially of data related to surface water bodies, should be planned and coordinated by all stakeholders working together to ensure that data is collected at compatible locations and scales to allow development of robust conceptual models.

It is important that collaboration occurs between those responsible for collection of surface water data, those responsible for collection of groundwater data, and the modelling team. Conceptualisation requires data to be collected at compatible locations and scales. Failure to coordinate can result in an inability to understand types of connection and conceptual process with the required level of confidence.

⁶ Thirty years ago, it was good practice to set up models with up to 1000 unknowns. Twenty years ago, it was common to solve for 10 000 unknowns. By 10 years ago, it was common to solve for 100 000 unknowns. It is now relatively easy to solve for 1 million or more unknowns.

In addition to all types of data used in typical groundwater modelling studies (refer section 3.5), data that may be useful in the context of surface water–groundwater interaction includes:

- hydrographic data, i.e. measurements of water levels and discharge rates at gauging stations within the study area. The process of converting water level data to hourly or daily discharge relies on stage-discharge or rating curves that in turn rely on measurements of velocity at different river levels
- digital elevation data, which are needed in the form of a digital terrain model (DTM). Surface topography is generally needed for development of regional groundwater flow models. For surface water–groundwater interaction, more accuracy may be required to define the geometry of the interface between surface and groundwater. Studying a DTM in the context of available measurements of watertable elevations and water levels in rivers and streams may help the development of a conceptual model, leading ultimately to design and construction of a model. The accuracy of data needed for the model cannot be determined until the type of model is known. Sometimes an accurate survey along the centreline of channels is required. When 1D models are used along rivers and streams, surveys of cross-sections are also required, within the main channel and also to quantify overbank storage. In the case of deep water bodies, and shallow water bodies when studied at a local scale, bathymetric data may also be needed to define the interface between surface water and groundwater
- photographs along rivers and streams, which are a good way of recording the type and condition of vegetation, or any other surfaces that affect surface roughness. Surface roughness is a key parameter of hydraulic and hydrodynamic models, so any previous estimates of Manning’s roughness coefficient n , Chezy’s roughness coefficient or Darcy-Weisbach friction factor may be useful
- mapping of a stream–aquifer connectivity index. See www.connectedwater.gov.au.
- previous studies of surface hydrology or flooding, with or without modelling
- anecdotal evidence, in the form of qualitative observations of flow or presence of water, which is often valuable. Observations of when and where flows are observed to increase or decrease can be important, especially when interpreting contribution of groundwater to a lake or river. For example, persistence of wet or moist conditions in low rainfall periods can indicate groundwater discharge
- water quality data, including salinity and temperature, and sometimes including the results of specific tracer studies designed to enhance understanding of surface water–groundwater interaction. Tracer studies can be passive, for example, based on stable isotopes, or on atmospheric deposition of tritium or chlorofluorocarbons (CFCs), or active, based on injection and measurement of a wide range of substances. Any data that provides indications of directions or rates of flow, or even of connectivity when this is in doubt may be useful
- measurements or estimates of riparian vegetation water use, or evapotranspiration elsewhere on the land surface.

Issues relating to data quality are relevant and some discussion on this issue is provided in section 3.5.

11.3.3 Developing the conceptual model

Guiding Principle 11.3: A conceptual model involving surface water–groundwater interaction should be developed to achieve a balance between real-world complexity and simplicity, such that the model includes all those features essential to the representation of the system, and enable predictions to meet objectives. Those features that are unlikely to affect model predictions should be left out.

Perhaps the most important stage of conceptualisation is when decisions are made about what will be included in a model and what will be left out (refer section 3.2). The decision about how to balance complexity and simplicity, about what to include and what not to include in a model, depends on the questions being asked, and also on the skill and experience of the modeller.

Because surface water–groundwater interaction occurs at a wide range of spatial and temporal scales (refer section 11.2), the challenge is to incorporate details about those parts of the system that really matter.

- It is generally not necessary to include depressions in the land surface that fill during intense rainfall, or ripples in a lakebed caused by wave action, but if the questions being asked are at either of these scales, these details would be important, and the spatial extent and simulation time for the model would be defined relative to these needs.
- It is neither necessary nor practical to include sophisticated models of net recharge at the land surface in every regional-scale groundwater flow model. A proposed mine in a desert region, for example, may draw water from storage over a mine life of tens of years, and in that time the total net recharge may be negligible relative to cumulative mine inflows. But if the purpose of modelling is to predict the effect of changes in land use on regional aquifers due to alterations to the recharge regime, this may be necessary. Recharge models can be run independently, with the results applied to the surface of groundwater flow models. It is also possible to simulate unsaturated flow in detail, as part of regional groundwater flow calculations.
- In simulating any catchment, it will never be possible to include all tributaries in a stream network. Using Strahler's stream order, the streams at the top of a catchment are considered to be first-order streams. So in a catchment whose largest stream (or river) is fourth order, it would be reasonable to include third- and fourth-order streams, and to ignore first- and second-order streams. Simulation of ephemeral streams that are sometimes dry is more difficult than simulation of streams that are always flowing.
- Rivers, streams, drains and irrigation canals may be smaller than the cells or elements in a regional scale model. The same may be true of lakes and wetlands, especially in situations where there are hundreds or thousands of small surface water bodies within a model domain. In such cases, these surface water bodies are considered to be sub-grid scale, and must be represented in an approximate way, with some kind of average effect, rather than individually.
- If individual lakes or wetlands need to be simulated, and if their shorelines are gently sloping, so that the size of the water surface varies significantly as the watertable rises and falls, the question of grid or mesh design is important. If an individual lake is about the same size as one cell or element, it is not possible to use the same methods that could be used if each lake was represented by tens of cells or elements.

Box 11B: CAUTION Scale of modelling

Surface water–groundwater interaction can be predicted in detail using local scale models of a single wetland or one reach of a river. However, it is not possible for every wetland and every reach of every river to be simulated in detail in a regional scale model. All stakeholders, including proponents, regulators (acting on behalf of the community) and modellers, need to discuss expectations before and during modelling to ensure that expectations can be met.

Chapter 3 of these guidelines focuses on conceptualisation of groundwater flow models, with an assumption that groundwater flow is governed by Darcy's Law. A key part of conceptualisation involves consideration of all relevant physical processes, so it is important to consider the nature of surface water flows, and what influences or controls the rate of flow.

Sometimes the flow in surface water bodies is so slow that it does not need to be taken into account. When flow does need to be considered, there are at least three distinct approaches. There is a distinction between processes and approaches to assessments of those processes in a model environment. In the following, reference is made to the approaches that should be considered while developing a conceptual model:

- **Hydrological approaches** are used at a regional scale, over periods of years, and perhaps with a focus on long-term yield and water supply. These approaches are based on conservation of volume (i.e. water balance equations, based on conservation of mass, assuming that water is incompressible with constant density). Rainfall run-off is simulated at the land surface and discharge is computed in networks of rivers and streams. The level in a river or stream is estimated from discharge using a stage-discharge or rating curve, and this level is used to compute exchange flows between surface water and groundwater.
- **Hydraulic approaches** are used at a more local scale, over periods of days and weeks, and perhaps with a focus on flood management. These approaches are based not only on conservation of volume (mass) but also on conservation of energy or momentum, either in 2D in plan or in 1D. They assume a single layer of surface water, with constant head and velocity throughout the water column in 2D or throughout the cross-sectional area in 1D. Hydraulic approaches are often used to simulate flow in river and stream channels and also on flood plains.
- **Hydrodynamic approaches** are used in deep or density-stratified water bodies, like mine-pit lakes or tidal estuaries. These approaches are also based on conservation of mass, energy and momentum. They are applied in 3D or in 2D in vertical section, and take into account vertical gradients in head and velocity.

If it appears necessary to simulate surface water flows, because of a belief that surface water–groundwater interaction will be such that changes in the groundwater system may modify surface water flows, a choice must be made as to which type of surface water modelling will be used.

11.3.4 Model extent in space and time

Guiding Principle 11.4: The domains of surface hydrological and hydrogeological systems should be conceptualised based on an understanding of how these systems function independently and together, as a coupled system. If surface run-off enters the hydrogeological domain and acts as a source of recharge, surface hydrological modelling may be required beyond the boundary of the hydrogeological domain.

Guiding Principle 11.5: The conceptual model should include consideration of the time required for the full impacts of changes in groundwater systems to be observed in surface water systems, and vice versa. The time to a new dynamic equilibrium will influence model design, as well as the assignment of climatic and other stresses during predictive runs.

Surface hydrological catchment boundaries rarely coincide with hydrogeological boundaries.

A common situation is that a surface hydrological catchment or river basin is larger than or smaller than a hydrogeological domain of interest. The surface and subsurface hydrological boundaries do not coincide. A decision must be made about the size and shape of the domain in which groundwater flow is to be simulated. If surface run-off entering a groundwater model domain provides a significant source of recharge, it may be reasonable to simulate surface run-off in surface catchments that extend beyond the groundwater model domain.

It is often stated that the watertable is a subdued reflection of the surface topography. Even subtle variations in watertable elevation, controlled by shallow hydrogeological properties and surface hydrological processes, can drive regional directions of groundwater flow at the basin scale.

In mountainous terrain, it is possible for a groundwater divide (effectively a no-flow boundary) to exist approximately beneath a topographical divide, but the impact of a proposed project, for example, a mine, on one side of the divide may cause the divide to move. In this sense the natural groundwater divide is not and should probably not be represented as a no-flow boundary (refer to section 4.5).

The duration of predictive modelling needs to be chosen in relation to the timescales over which the surface water and groundwater systems respond. In the case of recovery after mining, and evolution of a mine-pit lake, the time taken for a new dynamic equilibrium to evolve may be much longer than the period of mining. There are also lag times associated with impacts on river baseflows due to groundwater abstraction that can be decadal compared to sub-day event-based variations in surface water flows (Sophocleous 2002). The duration of modelling must be considered at the time of conceptualisation, and prior to model design, because it will influence data collection, and generation of synthetic climate data for long runs in the future.

Surface water–groundwater interaction plays an important role in determining the time to a new dynamic equilibrium. An assumption of constant recharge will fail to represent induced recharge, a phenomenon in which evapotranspiration is reduced when the watertable falls, such that net recharge to the watertable actually increases. Coupling of rivers and streams to aquifers can lead to increased recharge when the watertable falls. Induced leakage tends to reduce the time until a new dynamic equilibrium is reached.

It is not uncommon for a conceptual model to become relatively complex, including so many details that if a model could indeed be set up, the simulation time would be prohibitively long. Conceptualisation requires a balance between the desire to simulate all surface water–groundwater interactions and the practical need to keep simulation times to hours, or at most days.

11.3.5 Additional physical properties

Just as aquifer properties must be considered during conceptualisation (refer section 3.6.2), it is important to consider the physical properties that influence surface water–groundwater interaction and the dynamics of surface water.

Conductance is a parameter required in many modelling approaches. Conductance is used in many of MODFLOW packages (refer Table 11-2), and the same term is used in many other software packages. Conductance can have two interpretations:

- Conductance is usually considered to be a physical property of a layer of sediment at the base of a surface water body, sometimes called a sealing, clogging or colmation layer. Such a layer is caused by deposition of fine clay or silt particles that tend to clog the pore space in sands and gravels that make up the bed of many active rivers and streams. Clogging can also be caused by deposition of organic matter, for example, caused by algal populations in lakes and wetlands. As a property of a physical layer, conductance is equal to the hydraulic conductivity in the direction of flow (usually considered to be vertical) divided by the thickness of the layer, or sometimes the product of this and the length and width of a reach of river or of a cell or element beneath a large surface water body).
- Conductance is sometimes considered to be a non-physical model parameter that represents the effects of convergence or divergence of flow near a surface water body that only partly penetrates an aquifer. Convergence and divergence are especially important in anisotropic media, because the rate of groundwater flow upwards towards or downwards away from shallow surface water bodies is affected by low values of vertical hydraulic conductivity. Conductance may be used in this way with or without a physical layer of sediment being present. Conductance as a model parameter cannot be measured directly. It is a surrogate for the combination of hydraulic conductivities and geometries that occur in the near field of the water body. A number of analytical solutions give guidance for this kind of conductance, but values are generally either assumed or chosen during model calibration.

Conductance can change with time. Scouring (associated with floods) and sediment deposition (associated with periods of low flow) can change the thickness of bottom sediments whose properties may influence surface water–groundwater interaction. Time variations in converging and diverging flow patterns could also cause effective conductance to change in time. However, it is unusual for surface water–groundwater interaction models to include time variations in streambed conductance.

Surface water models need a number of model parameters, depending on the nature of the models.

- Hydrologic models need descriptions of land-use characteristics, run-off coefficients or infiltration coefficients, and capacities of soil moisture stores, all of which are used to convert rainfall and evaporation to estimates of long-term catchment yield, or run-off during extreme rainfall events.
- Hydraulic and hydrodynamic models need roughness coefficients or friction factors that explain how energy is lost through turbulence in rapidly flowing rivers and streams. They also require an accurate DTM such as LiDAR (refer section 11.3.2).

11.4 Design and construction

11.4.1 Choosing a modelling method

Guiding Principle 11.6: A modelling approach based on linking or coupling surface water models to groundwater flow models should be used when surface water dynamics are significantly affected by exchange flows. When surface water dynamics are likely to be unaffected, or only slightly affected, an approach based on groundwater flow modelling with standard boundary conditions may be adequate.

Guiding Principle 11.7: If a decision is made to link or couple surface water and groundwater models, the choice between hydrological, hydraulic and hydrodynamic surface water models should be made based on the spatial and temporal scales of interest, and on whether surface water dynamics based on conservation of energy and momentum are likely to be needed relative to simpler approaches based on water balance alone.

As described in Chapter 4, design and construction starts with the selection of a method for representing the conceptual model and preparing the model for predictive runs. Section 4.2 focuses on the choice of a numerical method, for example, between finite difference and finite element methods. But surface water–groundwater interaction involves many more choices, because the behaviour of surface water bodies can be represented and simulated in many ways.

Sometimes the nature of surface water–groundwater interaction can be represented in a groundwater flow model with normal boundary conditions (as described in section 4.5); in other words, no special modelling techniques are required, other than awareness of the nature of the interaction and an understanding of how a particular boundary condition can represent that interaction.

Sometimes the surface hydrological system depends so much on the dynamics of groundwater, or vice versa, that linked or coupled surface water–groundwater flow modelling is required.

In linked and coupled models, the conditions at the interface between surface water and groundwater are known as *matching conditions* or *interface conditions* rather than boundary conditions. Water balance equations are solved in each domain, subject to the following requirements at the interface:

- Piezometric head (hence pressure) within groundwater must be equal to piezometric head (hence pressure) in the surface water body, at every point on the interface, at all times.
- The flux across the interface must be continuous, ensuring conservation of mass, that is, a loss from one region is a gain in the other, at every point on the interface, at all times.

It is also possible for linked and coupled models to account for transport of solutes such as salt.

Useful reviews of approaches to modelling surface water–groundwater interactions are provided by Rassam and Werner (2008) and Furman (2008). The latter describes more rigorous interface conditions, based on conservation of momentum, that are needed in special circumstances.

A brief introduction is provided in this section on options for:

- representing surface water–groundwater interaction standard boundary conditions in groundwater flow models
- using analytical solutions
- linking and coupling surface water and groundwater models.

The choice between these approaches depends on those aspects described in section 11.3.1. Of most importance, perhaps, is the conceptualisation of surface water–groundwater interaction flow processes, and the extent to which it is believed that surface water dynamics will be influenced by the exchange flows with groundwater. If surface water flows are likely to be unaffected, or only slightly affected, the use of standard boundary conditions is reasonable. However, if surface flows are likely to be affected, such that they cannot be predicted without modelling, some form of linked or coupled modelling may be required.

When including the effects of surface water–groundwater interaction in a regional groundwater flow model, the modeller must know, or assume, whether exchange flows are sufficiently large to modify the water balance of surface water bodies or the dynamics of surface flows. Where a flooded river loses surface water to bank storage and regains it during the receding limb of the flood hydrograph, the dynamics of surface water flow may need to be simulated in detail. Where the surface water body is a large lake or reservoir, it may be reasonable to approximate the behaviour of the surface water, or to simulate it very simply, for example, with a lumped water balance model.

Representing surface water using boundary conditions

When groundwater modellers know or assume simplified representations of surface water systems, the interface between surface water and groundwater can be represented using any of the three types of boundary conditions that are used in groundwater flow modelling (refer section 4.5).

- Type 1 (Dirichlet, or prescribed head) boundary conditions can be used to represent large water bodies such as lakes, rivers and streams, when the spatial and temporal variation of surface water levels is known or assumed. They can be used to represent excavations such as mine pits, and springs, including mound springs. Often a seepage-face condition is applied, such that the boundary condition is only applied if the flow at that location is computed to be discharge, that is, flux out of the groundwater model domain. Head can be constant or varying in space and time.
- Type 2 (Neumann, or prescribed flux) boundary conditions can be used to represent flows to or from surface water, if such flows can be estimated. In 3D modelling, recharge and evapotranspiration are examples of fluxes across the upper surface of the model domain.
- Type 3 (Cauchy, or mixed) boundary conditions can be used to represent exchange between surface water and groundwater, when neither piezometric heads nor flows are known, but surface water levels can be prescribed, and a relationship, generally based on Darcy's Law, can be defined between heads and exchange flows.

Use of standard boundary conditions is probably the most common way to represent surface water–groundwater interaction, but is limited to situations where the modeller is confident that the assumed boundary conditions are correct and will not be affected by changes that occur during predictive runs.

Analytical solutions

Guiding Principle 11.8: Analytical solutions should be used to develop an understanding of the nature of surface water–groundwater interaction prior to regional scale numerical modelling, or in parallel with such modelling as a way of checking the numerical modelling.

A number of analytical solutions exist for groundwater flow with boundary conditions that represent steady or transient behaviour of adjacent surface water bodies. A smaller number of analytical solutions exist for situations where surface water and groundwater are fully coupled, with interface conditions.

Analytical solutions are useful because they provide a means of obtaining estimates of the extent and impact of surface water–groundwater interaction very quickly. An analytical solution for flow into and out of bank storage during a flood event may be very useful, and may provide a method of quickly estimating aquifer properties based on measurements of levels and heads during the event. They are useful for simple sensitivity analysis, for example, to see how exchange fluxes would vary if water levels or material properties were different

Analytical solutions can be closed-form solutions, where the solution can be evaluated using a formula, but sometimes analytical solutions need to be evaluated numerically, using software. They are sometimes considered to be approximate, because it is often necessary to make simplifying assumptions, like homogeneity and isotropy of aquifer properties, in order to find a solution. However, analytical solutions are very accurate, subject to those assumptions, that is, the assumptions may be inaccurate, rather than the model.

Analytical solutions are more likely to be useful for assessing the behaviour of a single surface water body, such as a lake or a reach of a river, rather than many surface water bodies in a regional context. They could be used to simulate a small part of a region in parallel with numerical modelling at regional scale in order to check the behaviour of the numerical model.

Numerical linking and coupling of models

Surface water models and groundwater models can be linked or coupled in several ways with varying levels of sophistication (refer Example 11.2). Models can be classified as follows:

- Loosely linked. One model is run to completion, and its outputs are used as inputs to the other model. For example, a groundwater model could be run to predict discharge to streams, and a surface water model could subsequently use these results as estimates of contributions to baseflow. This kind of linking is mainly undertaken manually.
- Dynamically linked. A special-purpose computer code provides outputs from one model as inputs to a second model, and outputs from the second model as inputs to the first model. The most common approach is for a surface water model to compute exchange fluxes based on heads, and for a groundwater model to compute heads based on fluxes. The models execute in parallel, with information passing between models after each stress period or time step. This can be accomplished, for example, via batch scripting. Virtually any surface water model, from the simplest hydrological model to 3D hydrodynamic models of lakes, estuaries or the near-shore coastal zone, can in principle be dynamically linked to any groundwater model
- Loosely coupled. The two models are closely interrelated, in terms of their input/output and possibly equation solvers etc., and they may appear to the user to be a single model. However, the equations of surface water flow and groundwater flow are still solved separately, with the results are passed between two models. For the user, looking at model input and output, the coupling may appear to be complete, but it is simply managed by another software code.
- Fully coupled. There is a single code that simulates everything. Matrix equations are formed and solved via a single-formulation and equation-solving procedure. A single global balance is achieved at each time step via solution of a single matrix equation.

A number of commercial software packages support the solution of surface water–groundwater interaction (refer section 11.4.2). Examples include:

- options for representing lakes, wetlands, rivers and streams using normal boundary conditions in finite difference, finite element and finite volume models

- options for representing rivers and streams using coupled one-dimensional hydrologic or hydraulic models capable of dynamically routing continuous flows or flood waves down rivers and streams
- options for computing two-dimensional overland flow at the surface using kinematic or diffusion wave models of shallow surface flows
- options for computing infiltration and exfiltration, using one-dimensional vertical or three-dimensional unsaturated flow equations to represent the movement of water through the unsaturated zone between the surface and groundwater.

A special case of numerical modelling involves the use of analytic elements. A number of analytic element models allow rapid assessment of the effect of pumping wells on rivers, streams or lakes. Analytic element methods allow simple analytical representations of individual components of a hydrological system to be superimposed. While initially developed for homogeneous conditions and steady state, analytic element models are now available for multi-layer systems and transient conditions.

Example 11.2: Three examples of linked and coupled models

Murray–Darling Basin Sustainable Yields Project (MDBSY) (Rassam et al. 2008).

Prior to the MDBSY there had been few studies in Australia on surface water–groundwater interaction at a regional basin scale. The MDBSY project used both analytical and numerical modelling approaches for the assessment of surface water–groundwater interaction and the impacts of groundwater abstraction and surface water management on long-term reliability of total water allocation. Modelling allowed estimates of the changes from the original or historical net flux, under various scenarios.

Numerical groundwater models were generally based on finite difference methods using Type 3 boundary conditions to represent the rivers. The Type 3 boundary conditions used heads imported from the surface water model(s). Evapotranspiration was found to be a significant component of the water budget and was incorporated as an areal flux controlled by the depth to watertable below the surface.

The MDBSY ran surface water and groundwater models iteratively, in a loosely linked fashion, until a dynamic equilibrium or quasi-steady state was achieved. A limitation with this approach is the need for transfer of large amounts of data between groundwater and surface water models.

Daly River Catchment, Northern Territory (URS 2008; Knapton 2010).

The Daly River project used a two-layered 3D finite element groundwater model, with the upper layer coupled to a 1D river model that uses an implicit finite difference scheme for the computation of unsteady flows in the rivers. Rainfall-run-off modelling was used to generate the overland flow component for the river. Coupling of the surface water model and the groundwater model was accomplished using an interface module that transfers fluxes between the river and the aquifer.

The scale of the study area (>52 000 km²) required a finite element groundwater model due to the greater flexibility in the mesh design compared to rectilinear grids used by finite difference codes. This enabled refinement of the mesh around points such as bores and linear features such as rivers. Finer discretisation along the boundaries enabled better representation of the curvature of the groundwater table near the discharge zones. It also enabled accurate mapping of the surface water computation grid points to the groundwater model boundary condition nodes.

Groundwater exchange with the river was simulated using Type 3 boundary conditions with variable transfer rates. The groundwater model was calibrated to groundwater levels and dry season baseflow, which was assumed to represent groundwater discharge. The surface water model was calibrated to available gauging station flows and stage heights.

Sandy Creek in the Pioneer Valley, Queensland (Werner et al. 2006).

This integrated model was constructed using a finite difference code calibrated to near-stream observations of watertable behaviour and multiple components of gauged streamflow.

Streamflow in Sandy Creek is represented using a channel-flow package, which solves the diffusion wave approximation of the 1D Saint Venant equations. The channel-flow package is implicitly coupled to the Richards equation for 3D variably saturated flow via stream leakage, with both the groundwater and surface water conditions computed simultaneously. Dual stress period capacity allows boundary conditions and system stresses to be assigned in the stream model at different time intervals from those of the groundwater flow model.

Although this coupled model can generate overland flows, the calibrated rainfall run-off model was used instead of the data- and computationally intensive overland flow package. The rainfall run-off modelling and hydrograph modelling generated tributary inflows and stream pumping in the Sandy Creek. Consistency between the groundwater model and the rainfall run-off model, in terms of streamflow, stream–aquifer interaction and stream pumping, was enforced through a process of repetitive inter-model data exchange followed by recalibration of both.

The use of the river management package allowed for the simulation of stream pumping management rules, that is, the estimation of stream-pumping rates as they relate to climate, stream flow, cropping patterns, irrigation practices, soil type, entitlement volumes and licence conditions. However, the coarseness of spatial discretisation, which is required for practical reasons of computational efficiency, limits the model's capacity to simulate small-scale processes (e.g. near-stream groundwater pumping, bank storage effects).

11.4.2 Software selection

As discussed in section 4.3, it is not the purpose of these guidelines to recommend specific modelling software, whether open source or commercial. However, a decision was made to identify a number of software packages that are commonly used in Australia, and some of those listed in Table 4-1 are capable of simulating surface water–groundwater interaction in some way.

Given the extent to which MODFLOW is used, it seems reasonable to list a number of MODFLOW packages that have some relevance to surface water–groundwater interaction (see Table 11-2). Only the first version of each package is listed, without any indication of compatibility with any versions of MODFLOW or any GUI.

Since MODFLOW-2000, the concept of modular software has been extended to include the notion of different 'processes'. Whereas MODFLOW was originally written only for groundwater flow, without solute transport, a new groundwater flow (GFW) 'process' in MODFLOW is now complemented by a Variably-Saturated Flow (VZF) 'process', which has more functionality than the UZF package listed in Table 11-2. In other words, as MODFLOW evolves, it may include capabilities which surpass the packages currently used to simulate surface water–groundwater interaction.

MODFLOW is not the only option for simulating surface water–groundwater interaction. FEFLOW also has a wide range of capabilities for representing boundary conditions, but it uses a more generic approach, based on the use of standard boundary conditions. In particular, FEFLOW allows all boundary conditions to be applied subject to time-varying constraints. A specified head can be set subject to the direction of flow through the specified boundary, or even based on concentrations and mass flux.

Both MODFLOW and FEFLOW can be coupled to MIKE 11, with sophisticated flood-routing capabilities, and MIKE SHE and HydroGeoSphere are integrated surface water–groundwater modelling packages, also capable of representing the unsaturated zone.

Box 11C: CAUTION regarding selection of modelling software

In principle, selection of software should not precede development of a conceptual model. However, conceptualisation is likely to be influenced by the skill and experience of modellers with surface water–groundwater interaction and by their knowledge of the capabilities of specific software packages at their disposal. This leads to a risk of choosing software because it is available and has been used before and a risk of developing a conceptual model that is constrained by that choice.

Table 11-2: MODFLOW packages relevant to surface water–groundwater interaction

<i>Package</i>	<i>Name</i>	<i>Description</i>
BAS	Basic	Supports specified head boundary conditions.
WEL	Well	Supports specified flux boundary conditions.
MNW	Multi-Node Well	Supports wells or specified flux boundary conditions that apply in multiple layers.
RCH	Recharge	Allows constant recharge (specified flux per unit area) to be applied at the land surface, or to the highest active layer.
CHD	Time-Variant Specified-Head	Allows specified heads to vary in each time step.
FHB	Flow and Head Boundary	Allows specified flow and head boundary conditions to vary at times other than the beginning and end of stress periods and associated time steps.
EVT	Evapotranspiration	Computes evapotranspiration decreasing from a maximum at the surface to zero at some extinction depth.
ETS	Evapotranspiration Segments	Allows a piecewise linear approximation to evapotranspiration from its maximum to the extinction depth.
DRN	Drain	Assumes that discharge via a drain is linearly proportional to the difference between head and drain elevation, as long as the head is above that drain elevation, with the coefficient of proportionality being a conductance.
GHB	General-Head Boundary	Assumes that flow into or out of an aquifer is linearly proportional to the difference between head and some defined elevation, with the coefficient of proportionality being a conductance.
DRT	Drain with Return	Allows a proportion of water leaving the aquifer via a drain cell to be returned to another cell.
RIV	River	Allows exchange flow between an aquifer and a river, as in the GHB package, except that when the watertable falls below the bottom of the streambed, leakage from the river no longer depends on watertable elevation, but rather on the elevation of the bottom of the streambed, based on an assumption of zero pressure at that location. Conductance depends on the length and width of river reaches.
SFR	Streamflow-Routing	Supports interaction between streams and aquifers, limiting recharge (leakage from streams) to the available streamflow at any location. Also computes unsaturated flow beneath streams, using a kinematic wave approximation to Richards' equation.
DAF	Diffusion Analogy Surface-Water Flow	Routes flows through a system of interconnected one-dimensional channels (branches and reaches) with the amount of flow from the stream to groundwater being limited to the available streamflow. Exchange flow is computed based on head difference, streambed thickness, streambed hydraulic conductivity and stream width.
RES	Reservoir	Allows lakes to grow and shrink in size, horizontally across many cells and vertically over many layers, without taking surface water balance into account.
LAK	Lake	Allows lakes to grow and shrink in size, horizontally across many cells and vertically over many layers, including a dynamic lake water balance based on rainfall, evaporation, surface runoff and exchange flows with groundwater.
UZF	Unsaturated-Zone Flow	Simulates percolation through an unsaturated zone between land surface and the watertable.

11.4.3 Discretisation in space and time

Guiding Principle 11.9: The level of spatial discretisation should be chosen based on conceptualisation of exchange flows and an understanding of the relationship between the size of surface water bodies and cell or element sizes. The level of temporal discretisation (time steps) should be chosen based on the temporal variability of surface water levels or fluxes and on requirements for stability and accuracy.

This section should be read in conjunction with sections 4.4.2 to 4.4.5 on discretisation of groundwater flow models.

Surface water–groundwater interaction occurs at a vast range of spatial and temporal scales. Sometimes, the interaction between a single surface water body and groundwater can be the main focus of a model. At other times, there can be so many instances of surface water–groundwater interaction in a model domain that the detail is sub grid scale, and important processes can only be represented approximately, by applying average conditions across many cells or elements. Examples of various model scales are provided in Example 11.3.

Successful representation of the interaction depends on the skill and experience of the modeller. Choosing the right level of detail depends on the purpose of modelling and the conceptual model for the interaction. These affect the choice of modelling tools, grid design and parameterisation.

Sometimes the implications for model and grid design are counter-intuitive:

- It is tempting to think that a large lake would need to be represented by many cells or elements. However, because the water level in a large lake is horizontal, the gradient in piezometric head along the bed of a large lake is zero, so, close to the bed, there is almost no horizontal flow. Fine resolution is needed near the margins of the lake, where the majority of exchange flows occur, and where there is curvature in the distribution of head. The challenge is getting sufficient resolution where it is needed, without refining a grid or mesh where resolution is not needed.
- It may seem reasonable to represent a river or stream in a regional scale model as a network of cells, but there are many reasons why more resolution may be needed. Sometimes fine resolution is needed because surface water–groundwater exchange occurs in an area where a gently dipping hydrostratigraphic layer subcrops alluvial sediments, to represent precisely that part of the model domain that is critical to calculation of exchange flows. Fine resolution may be needed to capture subtle changes in streambed elevation, especially if the watertable in some losing reaches is in transition from connected to disconnected (see Figure 11-1 c,d,e). Furthermore, exchange flows may be so sensitive to the existence or absence of an unsaturated zone that unsaturated flow needs to be explicitly represented, with many layers in the vertical direction (Brunner et al. 2010).

In general, if more resolution is required in the spatial and temporal distributions of exchange flows, it may be necessary to represent the geometry of the interface between surface water and groundwater in more detail. This applies to the shape of the interface in plan, and in some cases to the shape of the interface in vertical section, for example, the bed of a river.

Discretisation in time in linked or coupled models must depend on the temporal variability of water levels in surface water bodies, which in turn depends on the nature of the problem being addressed, for example, the distinction between long-term yield studies and flood studies. Time stepping must also depend on the minimum time steps needed for stability and accuracy, especially when hydraulic or hydrodynamic models are used.

Table 11-3: Examples of different levels of detail

<i>Type of model</i>	<i>Possible level of detail</i>
Rivers and streams meandering across regional scale aquifers, with direct connection between surface water and alluvial aquifers whose watertables are continuous with surface water levels in times of flow, or below the bed at times of no flow	Rivers and streams can be represented by lines of connected nodes or cells, representing one-dimensional channels. Bed elevation is prescribed, and the thickness, width and hydraulic conductivity of the bed (especially if it is less permeable than the underlying hydrostratigraphic units) are defined. Water levels in the rivers and streams are either prescribed, as a function of space and time, or computed using a coupled model.
Network of leaky irrigation channels	Individual channels can be represented by several nodes or cells across the width of each channel, possibly with narrow elements or cells along each side of the channel.
Coastal environments, such as tidal mangrove marshes	The design of a finite element mesh can reflect the high-tide line, and contours of equal elevation above and below that line. Some surface water models allow curvilinear finite difference grids that also follow contours of topography and bathymetry. Tidal boundary conditions are defined over a large number of nodes or cells at the top of the model. Models of this kind often include transport of salt with density coupling.
Lakes and wetlands that grow and shrink in size as the regional watertable rises and falls.	Elements or cells inside each lake can be represented using effective properties (e.g. very large hydraulic conductivity and specific yield equal to 1), or coupled to lumped water balance models that represent the water balance of a lake, while ensuring that the head above all flooded elements or cells is equal to the elevation of water in the lake.
Mine-pit lakes, where lakes gradually form in abandoned open-cut mine pits	Cells inside the volume of a mine pit are assigned effective properties that allow water to accumulate due to a combination of groundwater inflows and direct rainfall, less evaporation.
Flow in a stream, in pools and riffles, such that the distribution of head along the centreline of the stream causes water to flow through the bed of the riffles, into and out of the hyporheic zone	The model mesh or grid needs sufficient resolution along the stream, so that bed elevations and heads can reflect the subtle gradients that drive exchange flows.
Unidirectional or oscillating (wave-induced) flow-over ripples on the ocean floor, causing flow through the ripples, thereby influencing hydrochemical exchange processes	A detailed finite element mesh or finite difference grid is needed inside each ripple, to capture the detail of periodic flows.

11.4.4 Boundary and initial conditions

The principles described in section 4.5 and 4.6 still apply to models that involve surface water–groundwater interaction, but a key difference is that the whole issue of surface water–groundwater interaction is in essence related to the representation of important boundary conditions, that is, the boundary of the hydrogeological domain that is connected, directly or indirectly, with surface water.

Any surface water model that is linked or coupled to a groundwater model must have well-defined boundary and initial conditions, but formal discussion of hydrological, hydraulic and hydrodynamic models is beyond the scope of these guidelines.

11.4.5 Model construction

As described in section 4.7, and also in section 5.2.3, decisions need to be made at the time of model construction, or earlier during design, about how all model parameters vary in space. Conductances and roughness coefficients, for example, may be assumed to be constant along the length of a river, or may be assigned reach by reach.

This concept of parameterisation applies to all the properties of surface water models that might be linked or coupled to groundwater models. Careful and systematic parameterisation leads to a clear understanding of how many coefficients or model parameters influence the behaviour of the model, and therefore of the number of model parameters that could potentially be adjusted during model calibration.

Selection of solution methods is important during setup of linked and coupled models. Most equation solvers have parameters that influence rates of convergence and ultimately the accuracy of solutions. A good understanding of the behaviour of surface water models is required.

11.5 Calibration and sensitivity analysis

Guiding Principle 11.10: Models that include surface water–groundwater interaction should be calibrated using a variety of different metrics that measure the behaviour of the surface water system. This may imply a need to calibrate by trial and error, because more formal automated methods may not be easily adapted to some of the performance measures of interest.

Guiding Principle 11.11: Sensitivity analysis of models that include surface water–groundwater interaction should test the sensitivity of spatial and temporal discretisation as a way of demonstrating model robustness.

The fundamentals of calibration remain the same (refer Chapter 5). The objective is to find values of model parameters that cause a model to fit historical measurements as well as possible, subject to a range of constraints, including the water balance embodied in the model itself.

It is well-known that calibration of groundwater flow models is more effective when there are at least some measurements of flow between the surface water and groundwater domains. This is because flow measurements help to alleviate non-uniqueness issues, as described in section 5.4.1. Calibration of linked and coupled models is equally valuable in the sense of improving the level of confidence in predictions.

Baseflow separation and quantification can be difficult, nevertheless it is sometimes successful. In the case of linked and coupled models, it is sometimes useful to develop and calibrate a surface water model independently, prior to removing the baseflow component and linking or coupling the surface water model to a groundwater model.

Model calibration can be used to estimate all those parameters that are typically estimated for a groundwater flow model, as well as (refer section 11.3.5):

- conductances
- roughness coefficients or friction factors in rivers and streams
- all other parameters of hydrologic, hydraulic and hydrodynamic models.

As well as calibrating on watertable elevations and piezometric heads, calibration of models that involve surface water–groundwater interaction can attempt to match a wide variety of predictions that relate to surface water. These include:

- hydrographs of surface water levels and flows at different locations
- cumulative discharge along a river or stream, which can be compared with streamflow records at gauging stations. Cumulative flow is a useful measure of the integrated behaviour of a catchment and helps to put bounds on estimates of regional scale average hydraulic conductivities
- baseflow, including the gradual decline or recession in baseflow after significant rainfall and run-off events
- the locations of gaining and losing reaches, and changes in their locations
- a wide range of statistics of streamflow, including means, medians, variances and correlations in space and time, based on instantaneous flows or aggregated on a seasonal or annual basis
- flow-duration curves which show the probability of exceedance of discharge as a measure of the frequency of extreme run-off events, and as an indication of how often baseflow is occurring.

Trial-and-error calibration based on visual comparisons is the most common approach to calibration. However, calibration by automated methods is possible, but more difficult, because of the range of types of parameters that need to be estimated. The choice of objective function is more difficult, because if the objective of calibration is to match observations of both heads (or levels) and flows, there is no longer a single-weighted least squares objective function (e.g. seeking to minimise SRMS). There are at least two least squares components in the objective function, involving measurements in different units, and weights are needed to balance the importance placed on measurements of heads versus the importance placed on measurements of flows.

Calibration of regional-scale models remains difficult. Rassam et al. (2008) discuss their use of dynamic equilibrium calibration methods (refer Example 11.3) and have made recommendations for how could be improved in the future. This reference is particularly useful as an example of critical examination of a number of modelling studies, with insights into what worked and what did not.

Sensitivity analysis with linked or coupled models is likely to involve a number of model predictions into the future, with a number of important model parameters varied one at a time from their best estimates (refer section 5.5).

Given the sensitivity of surface water–groundwater interaction to spatial discretisation near the connections between surface water and groundwater, as well as to temporal discretisation, an important part of sensitivity analysis may be the testing of sensitivity to spatial and temporal discretisation. This may include sensitivity to bed elevations, or to the geometry of cross-sections.

11.6 Prediction and uncertainty

Predictive modelling and uncertainty analysis using models that involve surface water–groundwater interaction is conceptually no different from approaches used in flow modelling (refer Chapter 6 and 7).

Special care is needed to ensure that assumptions made in relation to surface hydrology are consistent with those made in relation to groundwater. If the purpose of a model is to assess the impacts of a proposed new mine, of a new irrigation scheme or of climate change on a coupled surface water–groundwater system, the implications of the proposed changes must be carefully considered (refer Example 11.4).

Example 11.4: Consistency in assumptions

A mine may cause the watertable to fall (due to seepage into the mine), a new irrigation scheme may cause the watertable to rise (due to irrigation return flow) and climate change may cause either (due to decreases or increases in rainfall recharge). If standard groundwater modelling boundary conditions are used to impose river levels, for example, the levels cannot be assumed to be unchanged during predictive scenarios. They must be consistent with the changes that are being assessed. In situations such as these, there may be a greater need for linked or coupled models, and for surface hydrological models that predict recharge and evapotranspiration as a function of depth to watertable and exchange flows via connected or disconnected forms of surface water–groundwater interaction.

Sometimes it is difficult to calibrate models that include surface water–groundwater interaction, yet at the same time there is reasonable confidence in a model to predict the right trends. In these situations, it is not common practice for one set of predictions to be made using the best possible model, and for further predictions to be presented not in absolute terms, but rather as differences relative to this base case.

11.7 Reporting

The reporting requirements of models that include surface water–groundwater interaction are largely the same as for groundwater flow models (refer Chapter 8), except that more information needs to be provided to describe the behaviour of surface water systems.

Special attention should be paid to describing the conceptual model, especially in relation to the spatial and temporal scales at which surface water–groundwater interaction is occurring, and justifying the modelling approach.

Since different types of data are used in calibration, different graphical representations are also possible. For example, a measure of model performance may be presented as a comparison of observed and simulated flow-duration curves that show the probability of exceedance of discharge as a measure of the frequency of extreme run-off events and as an indication of how often baseflow is occurring.

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Appendix A—Summary of existing groundwater flow modelling texts, standards and guidelines

Overview

A number of existing modelling guidelines and associated literature were gathered and reviewed to identify current international best practice. There are many textbooks and scientific papers that focus in detail on specific techniques or aspects of groundwater modelling. Such texts are not covered in this review. The following sections on Australian and international guidelines provide a brief context of where the *National groundwater modelling guidelines* sit among the limited number of guidelines currently in existence. The annotated bibliography is intended to point readers to additional useful information.

Australian guidelines

Until now there has been no national standard or guideline for groundwater modelling in Australia. The *Groundwater flow modelling guideline* (prepared for the Murray–Darling Basin Commission (MDBC) in 2001) became broadly accepted in the Australian groundwater modelling community as a de facto national guideline, although it was not developed as such. This was the first document of its type in Australia and, while not a standard, has been used as such in many cases. The MDBC guideline was developed to provide both an overview of the modelling process for non-modellers and guidance on best-practice techniques for modellers. While much of the content is applicable more broadly, the MDBC guideline targeted the types of practical applications and physical settings encountered in the Murray–Darling Basin and is focused on resource management models commonly undertaken in the Basin for the MDBC and other government agencies. It provides guidance on the modelling process, from conceptualisation through to reporting and model reviews. The model review checklist provided as an appendix has been used widely.

The scope of the MDBC guideline is limited to groundwater flow modelling and, since its publication, there have been significant advances in groundwater modelling. Areas of particular advancement are those of calibration, sensitivity and uncertainty analyses and surface water–groundwater interaction. Solute transport modelling is being implemented more widely and the need has arisen for a national guideline to provide current best practice guidance on a broader scope of groundwater modelling applications than was covered in the MDBC document.

On a more localised scale, in 2010 the SA Department for Water (DFW) developed a draft *Protocol for development of numerical groundwater model*. The protocol provides brief specifications of how DFW models are to be constructed and run, with frequent reference to the MDBC guideline. Detailed specifications of DFW reporting and archiving requirements are provided and the model review checklist from the MDBC guideline is provided as an appendix. The WA Department of Water (DOW) is currently developing a ‘Groundwater modelling guideline for urban drainage in areas of high water table’. This aims to provide more prescriptive guidance on DOW requirements of groundwater models used to support applications for urban development projects than that provided by the MDBC guideline. Much of the guideline is based on information from the MDBC guideline and the ASTM International standard guides.

International guidelines

Internationally, several national and regional jurisdictions have produced guidelines for groundwater modelling. Some are restricted to groundwater flow modelling, while others also include guidance on solute transport modelling. Hill et al (2004) present an overview of selected international guidelines.

ASTM International, formerly known as the American Society for Testing and Materials (ASTM), produces a series of 'standard guides' covering different aspects of groundwater modelling. Most of the guides refer specifically to groundwater flow but some include information on broader applications of groundwater modelling. The guides are technical documents that are updated or reapproved regularly, ensuring the content is current. While they are not standards, as a group, they have influenced the development of many of the guidelines internationally.

In 1992 the US Environment Protection Agency USEPA produced a document covering the overall process for groundwater flow and solute transport modelling. Most international guidelines follow, with minor variations, the overall modelling process presented in this paper. The Dutch Department of Public Works released a *Good modelling practice handbook* for hydrologic modelling in 1999, which presented a detailed outline of the modelling process. In 2001 the UK Environment Agency developed a *Guide to good practice for the development of conceptual models and the selection and application of mathematical models of contaminant transport processes in the subsurface*, which provides guidance specific to contaminant transport modelling that is not covered in many of the other groundwater modelling guidelines. This was followed in 2002 by *Groundwater resources modelling: guidance notes and template project brief*, which is more focused on groundwater flow modelling. The New Zealand Ministry for the Environment commissioned *Groundwater model audit guidelines* in 2002, which addresses both groundwater flow and contaminant transport modelling.

Annotated bibliography

Anderson MP and Woessner WW 1992, Applied groundwater modelling. Simulation of flow and advective transport, Academic Press, San Diego, 381 pp.

This widely used text book provides detailed information on groundwater modelling theory combined with guidance on the construction, calibration and use of groundwater flow models. Practical examples are used throughout the text to illustrate the implementation of concepts. A chapter is dedicated to particle tracking and advective transport (i.e. simple cases of solute transport). While not the focus of the book, there is brief discussion of unsaturated flow, multiphase flow, solute transport, approaches to modelling fractured media and density-dependent flow of miscible fluids.

ASTM D5447-04 (2010), Standard guide for application of a ground-water flow model to a site-specific problem.

Outlines a framework of steps to develop, apply and document a groundwater model, but acknowledges that, in practice, there is significant iteration between steps and that some modelling projects may not require all steps. Designed for saturated, isothermal groundwater flow models, the concepts are applicable to broader groundwater modelling projects. The steps outlined are: define study objectives, develop a conceptual model, select a computer code or algorithm, construct a groundwater flow model, calibrate the model and perform sensitivity analysis, make predictive simulations, document the modelling process, and perform a post-audit. An example set of headings for model reporting is provided.

ASTM D5490 (reapproved 2008), Standard guide for comparing ground-water flow model simulations to site-specific information.

Describes a range of quantitative and qualitative means of comparing model results to observations from a site, and emphasises the importance of using both types of comparisons. States that models with different objectives may place different importance on matching one or more type/s of information (e.g. heads, flow directions, vertical gradients, flows).

ASTM D 5610-94 (reapproved 2008), Standard guide for defining initial conditions in ground-water flow modelling.

Provides a very brief overview of approaches to assigning appropriate initial hydraulic heads for a mathematical groundwater flow model.

ASTM D5611-94 (reapproved 2008), Standard guide for conducting a sensitivity analysis for a ground-water flow model application.

Presents an approach to carrying out combined sensitivity analyses of model calibration and model-predicted outcomes to model input parameters. The approach is relatively simple; involving analysis of the effects of varying one or more input parameters above and below their calibrated value/s. Model sensitivity to a given parameter is classified into one of four groups, which are used to define the validity of the model as a predictive tool (for a specific objective). Monte-Carlo and other probability-based approaches to identifying predictive uncertainty are not covered.

ASTM D5718-95 (reapproved 2006) Standard guide for documenting a ground-water flow model application.

Presents a generic set of topics to be covered in model reporting. Model archiving is discussed briefly, and recommendations are given on materials to be archived, such that a model can be reused in the future and that a third party can perform a post-audit.

ASTM D5880-95 (reapproved 2006), Standard guide for subsurface flow and transport modelling.

Provides a broad overview of what a model is and classifies types of subsurface models according to various criteria. Models are grouped into representing four types of processes: fluid flow, solute transport, heat transport and deformation. Models are grouped into three fidelity classes with increasing reliability: screening, engineering calculation and aquifer simulator. Various types of mathematical models and solution methods are described in broad terms. Sources of model error are discussed.

ASTM D 5981-96 (reapproved 2008), Standard guide for calibrating a ground-water flow model application.

Presents techniques for calibrating a groundwater flow model in the following three steps: establish calibration targets and associated acceptable residuals, identify calibration parameters and history matching. The steps and techniques can be applied to manual (i.e. trial and error) or automated calibration processes and to other types of models (e.g. solute transport).

ASTM D6170-97 (reapproved 2010), Standard guide for selecting a ground-water modelling code.

Describes key issues and provides guidance on a process for selecting one or more models for a modelling project, without referring to any specific models or codes. Emphasises that model choice should be linked with modelling objectives and that analytical, semi-analytical and numerical models are each well-suited to different projects. A detailed checklist is provided for characterisation of the groundwater system and potential models to aid identification and ranking of potential models. Areas covered are general model characteristics, flow system characterisation, solute transport and fate characterisation, heat transport characterisation, rock/soil matrix deformation characterisation.

Dutch Department of Public Works 1999, Good modelling practice handbook, Institute for Inland Water Management and Waste Water Treatment report 99.036.

Not written specifically for groundwater modelling, this handbook reads very much like a guideline, written in two parts. The first part documents in considerable detail a recommended modelling process that is applicable to a range of applications. Checklists and templates are provided for use by modellers during the process. The second part outlines application to a range of water-related problem classes.

Environment Agency (United Kingdom) 2001, Guide to good practice for the development of conceptual models and the selection and application of mathematical models of contaminant transport processes in the subsurface, national groundwater and contaminated land centre, report NC/00/38/2.

This provides specific guidance on contaminant transport modelling, with significant discussion of transport theory and analytical modelling that might be found in a textbook. Being dedicated to contaminant transport modelling, much of the technical material presented in this document is not covered in guidelines focusing on groundwater flow modelling alone, although the modelling process is similar.

Environment Agency (United Kingdom) 2002, Groundwater resources modelling: guidance notes and template project brief, R&D technical report W213.

This detailed guideline includes considerable technical detail. While it focuses on groundwater flow models, the use of hydrogeochemical data is mentioned briefly. Numerous demonstrative examples are provided throughout the document.

eWater 2009, Initial review of models in use across Australia.

This review contains an inventory of over 100 hydrologic (not groundwater specific) models in use by Australian government agencies. It contains a short summary of each model's purpose, provider/custodian, strengths and weaknesses.

Hill MC, Middlemis H, Hulme P, Poeter E, Riegger J, Neuman SP, Williams H and Anderson M 2004, Brief overview of selected groundwater modelling guidelines, FEM MODFLOW, Karlovy Vary, Czech Republic.

This short paper presents an overview and comparison of a selected group of international groundwater modelling guidelines. Areas of similarity and conflict are identified.

Hill MC and Tiedeman CR 2007, Effective groundwater model calibration with analysis of data, sensitivities, predictions and uncertainty, John Wiley and Sons, Hoboken, 455 pp.

This detailed text book promotes and covers the topic of inverse (automated) calibration techniques. It provides theory and technical detail as well as a set of *Guidelines for effective modelling*. The techniques outlined in the book aim to quantify calibration quality, data shortcomings and needs, and uncertainty of parameter estimates and predictions.

Murray–Darling Basin Commission 2001, Groundwater flow modelling guideline, report prepared by Aquaterra, January 2001.

This guideline was commissioned by the MDBC to provide clarity of the modelling process to community stakeholders and regulators and is written in relatively simple terms. It focuses on the types of practical applications and physical settings encountered in the Murray–Darling Basin and the scope is limited to groundwater flow modelling, although many of the concepts are applicable more widely. A model review checklist presented as an appendix in this guideline has been used widely within the broader Australian groundwater modelling community.

New Zealand Ministry for the Environment 2002, Groundwater model audit guidelines, report prepared by Pattle Delamore Partners Ltd.

These guidelines are written to inform model auditing but, in effect, act as a set of guidelines for groundwater modelling. Much of the content is similar to that of the MDBC guideline. Analytical and numerical models for both groundwater flow and contaminant transport are addressed.

Reilly TE and Harbaugh AW 2004, Guidelines for evaluating ground-water flow models, US Geological Survey Scientific Investigations Report 2004-5038, 30 pp.

While the title suggests this report provides guidance on evaluating groundwater flow models, in doing so it also provides descriptions of steps in the process of developing a groundwater model and a brief overview of some of the technical aspects to numerical modelling. The document is written using language and at a level that enables non-modellers to understand the concepts and guidance provided. The result is closer to a brief groundwater flow modelling guideline that provides key questions for those evaluating or reviewing models. The report emphasises several times that a model should be evaluated based on the objectives of the study.

Scottish Environment Protection Agency (SEPA) 2009, Modelling methods for groundwater abstractions, regulatory method WAT-RM-27.

This document provides general information on the process for developing simple analytical and numerical models in support of applications for a licence for groundwater abstraction. It covers SEPA's general expectations when assessing a model used to support an application and is written in language easily understood by non-modellers.

US Environmental Protection Agency 1992. Fundamentals of ground-water modelling, Ground Water Issue paper EPA/540/S-92/005.

This technical paper presents an overview of groundwater flow and solute transport modelling in saturated porous media. A diagram of the modelling process is presented, similar to those that have been used in several more recent guidelines. The use of probabilistic approaches to deal with uncertainty in parameter estimation and predictive outcomes are discussed. Despite being highlighted in this early overview there has been a long lag, partially due to computing constraints, in such approaches being adopted in other guidelines and by the majority of the modelling community. A suggested format for groundwater modelling reports is presented.