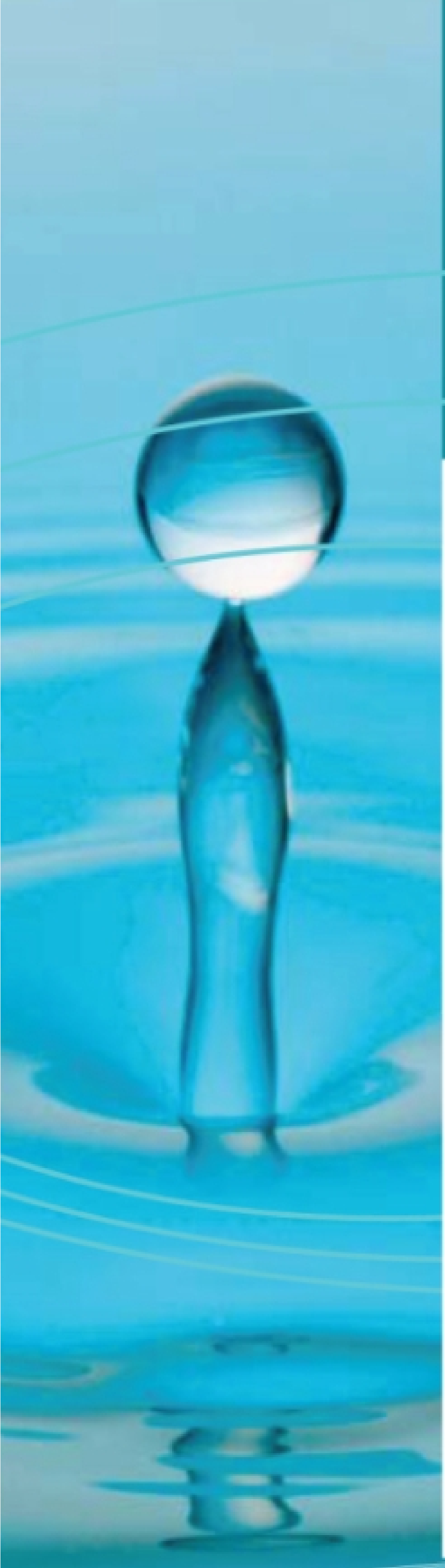

Australian Government
National Water Commission

Australian groundwater modelling guidelines

Companion to the guidelines

Waterlines

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

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Australian groundwater modelling guidelines: companion to the guidelines, July 2013

Author: Sinclair Knight Merz

Published by the National Water Commission
95 Northbourne Avenue
Canberra ACT 2600
Tel: 02 6102 6000
Email: *enquiries@nwc.gov.au*

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Disclaimer

This paper has been prepared by SKM for the National Water Commission and does not necessarily reflect the views or opinions of the Commission.

Australian Government
National Water Commission

SINCLAIR KNIGHT MERZ
SKM

Contents

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Preface

Background

The Australian groundwater modelling guidelines[1] (guidelines) were published by the National Water Commission in June 2012. The guidelines were prepared by Sinclair Knight Merz (SKM) with cooperation of the National Centre for Groundwater Research and Training (NCGRT), NTEC Environmental Technology (now trading as CDM Smith), CSIRO, the US Geological Survey, and the Northern Territory Department of Natural Resources, Environment, the Arts and Sport (NRETAS).

The guidelines are targeted at all stakeholders in modelling projects and provide technical information in a way that can be understood and used by parties with a wide range of educational and technical backgrounds. It has not been possible to write a document that is equally useful to all parties. In general, the guidelines assume a level of a basic understanding of groundwater science (hydrogeology) and modelling methods. Much of the document will be challenging for those without a technical background. The Companion to the Guidelines (the Companion document) provides a summary of the guidelines written in simple non-technical language intended to provide a useful reference for those without formal training or experience in hydrogeology. It is also intended to provide a concise summary of the key points of the guidelines and will be a useful reference for those seeking to gain a quick understanding of the guidelines.

Content

The Companion document presents a summary of the key aspects of the guidelines. It includes a brief description of each of the chapters in the guidelines with a listing of all the Guiding Principles that highlight the key messages of the guidelines. In addition, the Companion document includes a number of clarifications presented as a series of text boxes distributed throughout the document. The clarifications highlight issues that were raised as feedback in a series of workshops in May and June 2013. The clarifications aim at providing further information on specific aspects of the guidelines that will help in their interpretation.

Structure

The Companion document is structured with the same chapter headings and numbers as those of the guidelines. In each chapter there is a brief description or summary of the content of the guidelines followed by a list of the Guiding Principles and then any points of clarification identified from industry feedback.

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[1] Barnett B, Townley LR, Post V, Evans RE, Hunt RJ, Peeters L, Richardson S, Werner AD, Knapton A and Boronkay A 2012. *Australian groundwater modelling guidelines.* Waterlines report No. 82, National Water Commission, Canberra.

1. Introduction

A groundwater model is a mathematical representation (often computer-based) of a groundwater flow system. While groundwater models are, by definition, a simplification of a more complex reality, they have proven to be useful tools for investigating groundwater problems and have provided valuable support for decision-making in groundwater management. Models provide insight on how a groundwater system behaves. Where it can be demonstrated that a model is able to reasonably reproduce past behaviour it can forecast with a degree of confidence a range of responses to changed future conditions (e.g. related to future climatic variations, future changes in land use or future changes in groundwater extraction).

The development of a groundwater model is a complex process that is not free of subjective choices. Guidance on best practice in modelling provides boundaries to these potentially subjective choices.

The National Water Commission initiated the development of the Australian groundwater modelling guidelines (the guidelines) to encourage the incorporation and use of contemporary knowledge and accepted approaches to groundwater model development in settings and for applications commonly encountered in Australia (such as water allocation planning, management of mine water supply and estimation of salinity impacts on river systems).

This Companion to the guidelines (Companion document) seeks to provide a summary of the material in the guidelines to convey the fundamental aspects of sound groundwater modelling practice to an audience that is not necessarily familiar with the scientific disciplines that underpin groundwater modelling (i.e. geology, hydrology and mathematics).

What is a groundwater model?

The term groundwater model can be applied to various tools and techniques used to estimate or predict groundwater (and solute) behaviour. These techniques range from the use of simple mathematical equations through to computer-based models.

The guidelines are focussed on computer-based, mathematical models that simulate groundwater heads and groundwater flow rates. A solute transport model simulates the concentration and movement of substances dissolved in groundwater. Models not only estimate internal flows within the model boundaries, they can also estimate the flows of water and solutes to and from adjoining connected water bodies such as regional aquifers, rivers, lakes or the ocean.

There should be no expectation of a single 'true' model that is able to estimate groundwater heads and flows with absolute certainty. In fact all models are approximations and their outputs will always be uncertain. As such, all model outcomes presented to decision-makers benefit from the inclusion of some estimate of how good or, conversely, how uncertain the modeller considers the results.

The reader is referred to the guidelines for additional background on groundwater processes included in models and for advice on the type of modelling codes and graphical user interfaces that are currently in use in Australia.

The guidelines are a point of reference for best practice (and not a rigid standard) for all those involved in the modelling process, such as:

- those parties responsible for commissioning the development and use of a model
- those people who develop and run models (modellers)
- model reviewers

- those responsible for regulating and managing groundwater resources
- communities that are potentially affected by model outcomes.

There are alternate approaches to modelling that are not covered by the guidelines, and the authors acknowledge that such approaches may be appropriate and justified in many circumstances. The guidelines are not aimed at stifling innovation or the application of new techniques or approaches.

The recommended approach to model development and use is shown diagrammatically in Figure 1. The process is underpinned by a series of interdependent steps with frequent checks and feedback loops to earlier stages. Typically each loop involves modifications and repetition to ensure consistency at all levels. A fundamental concept illustrated in Figure 1 is that the modelling process should include frequent consultation with key stakeholders and reviewers, and that consultation should commence at the model planning stage.

Clarification

The guidelines describe a basic framework within which models can be developed. The framework can be considered as industry best practice and is the authors' best attempt to define approaches that have proven, through experience, to be successful. The guidelines are not regulation or law. They are not aimed at defining an approach or recipe that should be used in all groundwater modelling investigations. They should not be considered as de facto standards because the concept of best industry practice is likely to evolve as new methods are introduced and as software becomes more sophisticated and computers more powerful.

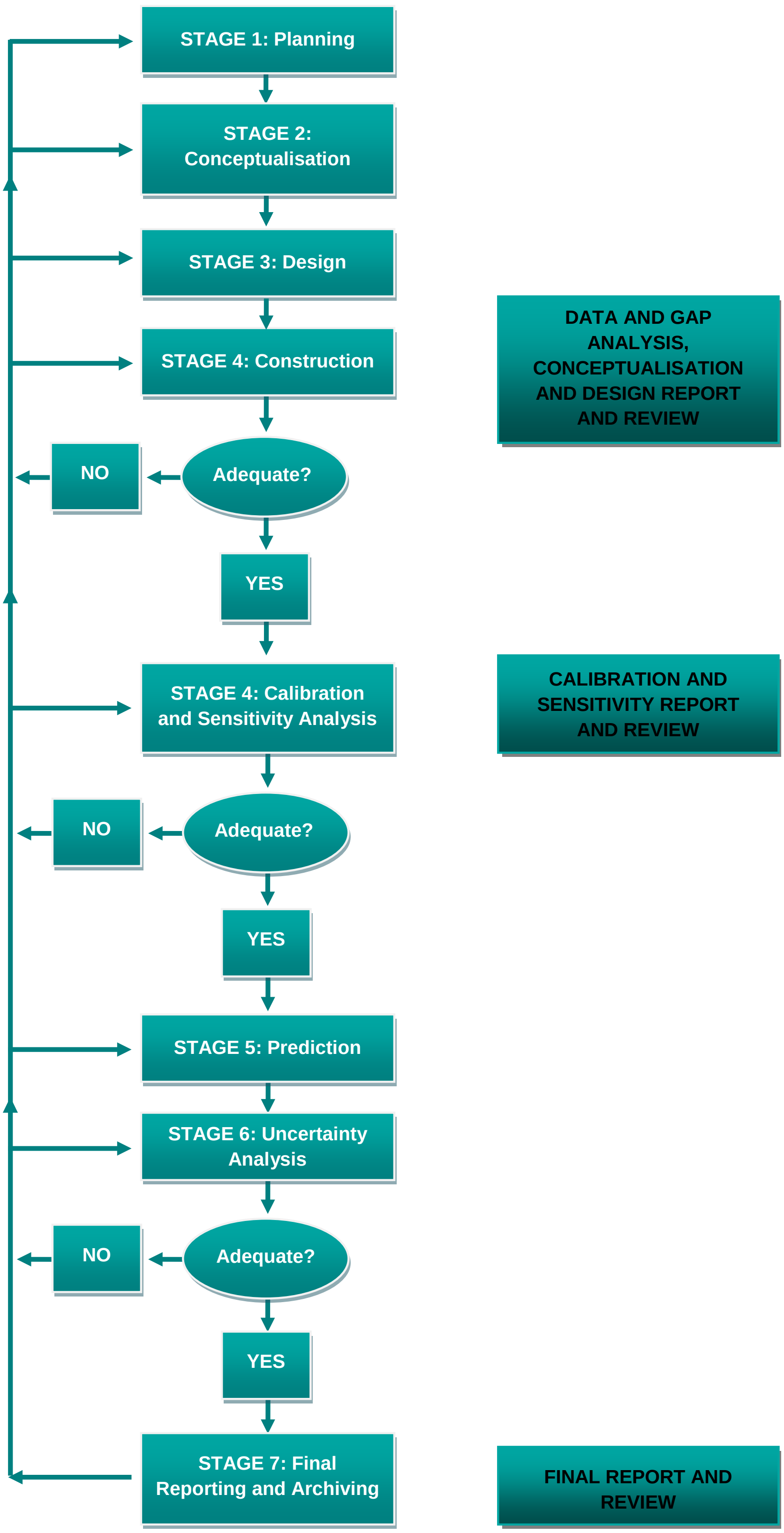


Figure 1 Groundwater modelling process (modified after Middlemis et al. (2001)[2] and Yan et al. (2010)[3]).

[2] Middlemis H, Merrick N and Ross J 2001. *Murray Darling Basin Commission groundwater flow modelling guideline.* Project No.125. Final Guideline Issue 1. 16 January 2001.

[3] Yan W, Alcoe D, Morgan L, Li C and Howles S 2010, *Protocol for development of numerical groundwater model, version 1*, report prepared for the Government of South Australia, Department For Water.

2. Planning

Initial model planning typically involves consultation between the model owner (the party seeking to develop a model), the modeller and other stakeholders with the objective of aligning expectations on what is needed from the modelling project and what can be achieved with the available resources and data. It should involve a dialogue between the interested parties on a range of issues including modelling objectives, the extent of the area of interest, the required level of model confidence, likely limitations, the review process and model ownership.

The modelling objectives provide the context for model development by making clear what model outputs are required and how these contribute to the larger project for which the model is to be developed. The objectives can be used during the review process as criteria to judge whether the model is fit for purpose and is able to answer the questions posed.

The confidence level classification is a system used to indicate the relative confidence with which model predictions can be made. It can be used to determine whether a particular model provides an appropriate level of accuracy or reliability required to meet the modelling objectives. At the planning stage, it is the task of the modeller to provide advice on realistic expectations of the model based on the available data and the time and resources allocated to its development. The level of model confidence required by the model owner may simply reflect the level of confidence that is needed to assess the question at hand. In other words, a model with a lower class of confidence may be appropriate when the modelling objectives are relatively modest.

The guidelines propose three classes of model (Class 1, 2 and 3 in order of increasing confidence; refer to the guidelines Table 2-1). The classification largely depends on the amount of groundwater data on which the model is based, whether its reliability can be demonstrated through consideration of historic groundwater behaviour (calibration) and the manner in which it is used for predictions. The classification of confidence level is particularly useful for the model reviewer as a measure on which to assess whether or not the model has met the agreed requirements.

Models are designed to answer specific questions (as indicated by the modelling objectives). There will be features or aspects of any given model that are not reliable and the modeller is encouraged to identify and document those parts of the model that will not provide reliable or reasonable results. A statement of limitations or exclusions can help to ensure that the model is used only for the purpose for which it was designed.

All parties should agree on who will own the model and who will retain and maintain the model once the project is completed.

Guiding Principles

2.1 The modelling objectives should be a statement of how the model will specifically contribute to the successful completion or progress of the overall project.

2.2 The model confidence level classification provides a benchmark by which to evaluate a groundwater model. It provides an indication of the confidence with which the model can be used to provide the outcomes for which it is designed.

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 an 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.

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.

Clarification

The guidelines provide a number of quantitative and qualitative criteria for assessing model confidence level classification (refer to Table 2-1 in the guidelines). Any particular model will most likely exhibit characteristics of more than one class. It is therefore not necessary for a model to attain or meet all the characteristics of a particular classification. It is suggested that the key aspects of the classification be discussed and agreed between the modelling proponent, reviewer, regulators and modellers so that agreement can be reached on a classification that best reflects those aspects of the model that are of particular relevance to the modelling objectives, the project risks and the environment.

Clarification

The guidelines refer to model "*stresses*" and there are specific quantitative criteria used to assess confidence level class based on the level of stress in predictive scenarios compared to those in calibration. In this context, stress is defined as any addition or extraction of water to or from the groundwater system through climate related factors such as rainfall recharge and evapotranspiration, and through human activity such as groundwater pumping or injection.

Clarification

The guidelines refer to "*high value*" aquifers and "*high value*" environmental assets at risk. There are no definitions for these terms in the guidelines and the various stakeholders in a modelling project may have different understandings of what constitutes a high (and low) value aquifer and a high (and low) value environmental asset. It is recommended that the issue be discussed and resolved at the outset of the project. The appropriate definitions will likely vary with the jurisdiction as many states and territories will have relevant legislation that will provide a useful basis for this determination. Figure 2 shows an example of a potentially high value environmental asset in the Millstream Aquifer in Western Australia.

Figure 2 Cinderwarriner Pool in the Millstream Aquifer in the Pilbara, WA – an example of a high value environmental asset.

3. Conceptualisation

Conceptualisation is a process of creating a conceptual model, which provides the basis for model design and communicates the physical processes that control groundwater occurrence and movement at the study site. The conceptual model should be developed collaboratively across multiple scientific disciplines often involving engagement with project stakeholders. The agreed conceptualisation is often required to be communicated to a wide range of audiences.

The conceptual model is a descriptive representation of the groundwater system and processes operating across the model area. In particular, it identifies those features that influence groundwater behaviour in the pre- and post-development stages (e.g. geology, links to surface water systems, groundwater abstraction and recharge mechanisms) and hence identifies specific aspects of the physical environment that must be represented in the groundwater model. The conceptual model can be presented as a series of two and three dimensional diagrams supported by a narrative of the important groundwater processes and how the system may respond to stresses.

Conceptualisation is always based on measurements and observations. Accordingly, the conceptualisation stage invariably includes data collection, review and analysis, and the data itself should always be critically reviewed to ensure that there are no obvious errors. It is a key point in the project when a decision to progress further in the modelling process is required. It may be that there is insufficient knowledge or data to support development of the conceptual model as planned, which may trigger further collection of data, analysis or re-evaluation of the modelling objectives.

The conceptual model should seek to explain all observed groundwater behaviour in the region. The guidelines encourage regular re-assessment of the conceptualisation at all stages of the project with refinements made as subsequent work suggests that these may be appropriate or indeed necessary. In many cases, the conceptualisation may not be unique (i.e. different conceptualisations can explain all observations). In such cases, alternative conceptualisations should be proposed and maintained as long as possible through the modelling project. At some stage, some of the alternative conceptualisations may be rejected. Whenever alternative conceptualisations cannot be discounted it may be necessary to develop alternative groundwater models.

Guiding Principles

3.1 The level of detail of the conceptual model is dependent on the modelling objectives, the availability of data and the complexity of the groundwater system.

3.2 Alternative conceptualisations are developed when some aspects of the groundwater system or its environment are uncertain.

3.3 The conceptual model is based on observation, measurement and interpretation wherever possible. This requires quality assured data.

3.4 The area of the conceptualisation should be large enough to cover all groundwater stresses (such as extraction, both current and in the foreseeable future) and the impacts that arise from these stresses. It should also be large enough to capture all of the groundwater flow processes controlling groundwater behaviour in the study area.

3.5 There must be an on-going process of refinement and feedback between model calibration and conceptualisation such that revisions and refinements to the conceptual model can be made over time.

Clarification

The terms "*conceptualisation*" and "*conceptual model*" are commonly used in groundwater modelling. In the guidelines conceptualisation refers to an underlying understanding of the hydrogeology of the groundwater system and any proposed development that may affect the groundwater system. The conceptual model often refers to an illustration or schematic representation of the principal features of the conceptualisation (e.g. refer to Figure 3).

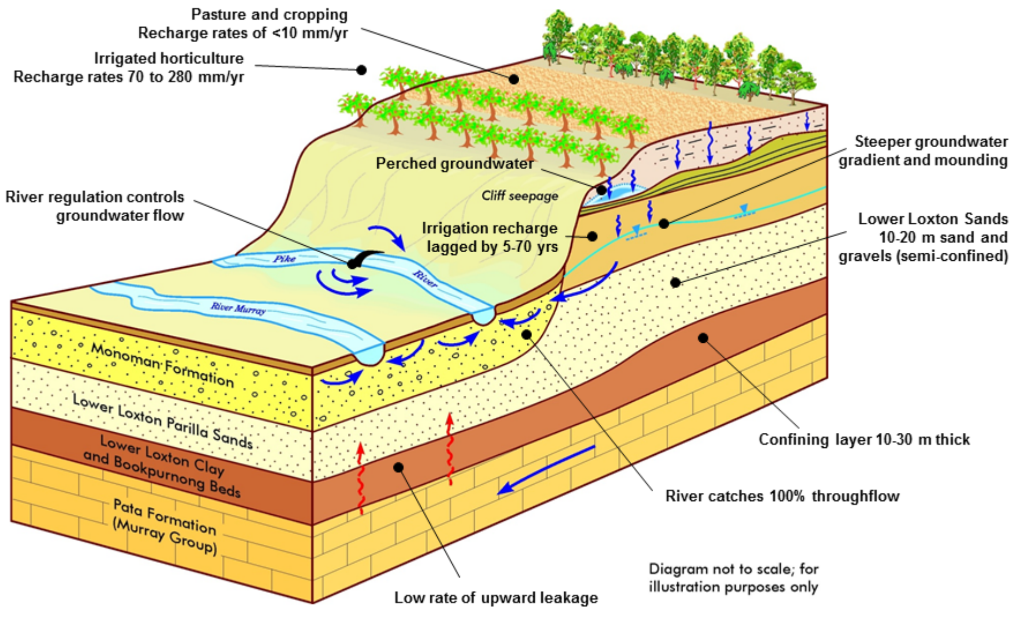


Figure 3 An example conceptual model

4. Design and construction

The design and construction stage involves converting the conceptual model into a numerical or computer model. The design is typically a description of the modelling approach being proposed and how the conceptualisation will be represented. Model construction is the implementation of that approach. It is essential that the design is aimed at ensuring that key features of the conceptual model are correctly represented or included in the groundwater model.

Model design involves a series of decisions on how to best represent the conceptualisation in a computer modelling environment. One of the first considerations is the selection of a suitable software platform in which to construct and run the model. There are a number of commercially available software codes that are commonly used in Australia for groundwater modelling and these are listed in the guidelines (refer to Table 4-1 in the guidelines) with some advice on how to select an appropriate software package (code).

Other issues that need to be addressed in the model design stage include selection of an appropriate model dimension (i.e. whether the model will be developed in one, two or three dimensions), defining the size of the model and how the model can best be divided up into a grid of calculation nodes, and the time frames to be used in the model. Modellers are encouraged to take a pragmatic approach to these issues and to explore simple modelling options where they may be appropriate. For example, consideration of two dimensional rather than three dimensional models is encouraged where a simpler approach may be perfectly adequate to address the modelling objectives (refer to Figure 4 showing a type of two dimensional model design suitable for modelling radial flow towards a central location).

The model design must also consider how to use boundary conditions to represent the interactions between groundwater and adjoining surface water features. It must also consider how climatic conditions (rainfall and evaporation) and groundwater extractions are to be included in the model, and how the variations in hydrogeological properties of the system will be defined.

Guiding Principles

4.1 The model design should reflect the modelling objectives, conceptualisation and target confidence level classification such that appropriate choices are made on the model dimension and size.

4.2 Model run times should be carefully considered to ensure that the model size and complexity will not prevent or hamper the successful calibration and operation of the model within the available project time frame.

4.3 The model arrangement of calculation nodes must provide sufficient detail to be able to adequately represent the problem geometry.

4.4 Steady state or equilibrium models should be considered when the variations in groundwater conditions with time are not important. Where variations over time are important then the model must be run through a series of time stages.

4.5 Initial groundwater levels must be chosen carefully such that they do not result in erroneous model outcomes at early times in the model run.

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

Clarification

Section 4.3.4 of the guidelines provides guidance on the choice of appropriate software packages for various non-standard groundwater modelling applications. That advice includes guidance that modelling fluid flow in coal seam gas projects will usually require the use of a two-phase flow modelling software package. The advice refers specifically to modelling the flow of water and gas in coal seams themselves. Single phase groundwater modelling software packages have been used successfully to model the impacts of coal seam gas production on surrounding groundwater resources. In this case, the groundwater flow model is usually constructed with boundary conditions that represent head changes or fluxes at the interface between the groundwater domain and the two-phase coal seam gas reservoir. The advice provided in this section was current at the time of writing the guidelines. However, significant developments and advances currently being made in various software packages may, in the future, render some of the guidance in this section "*out-of-date*".

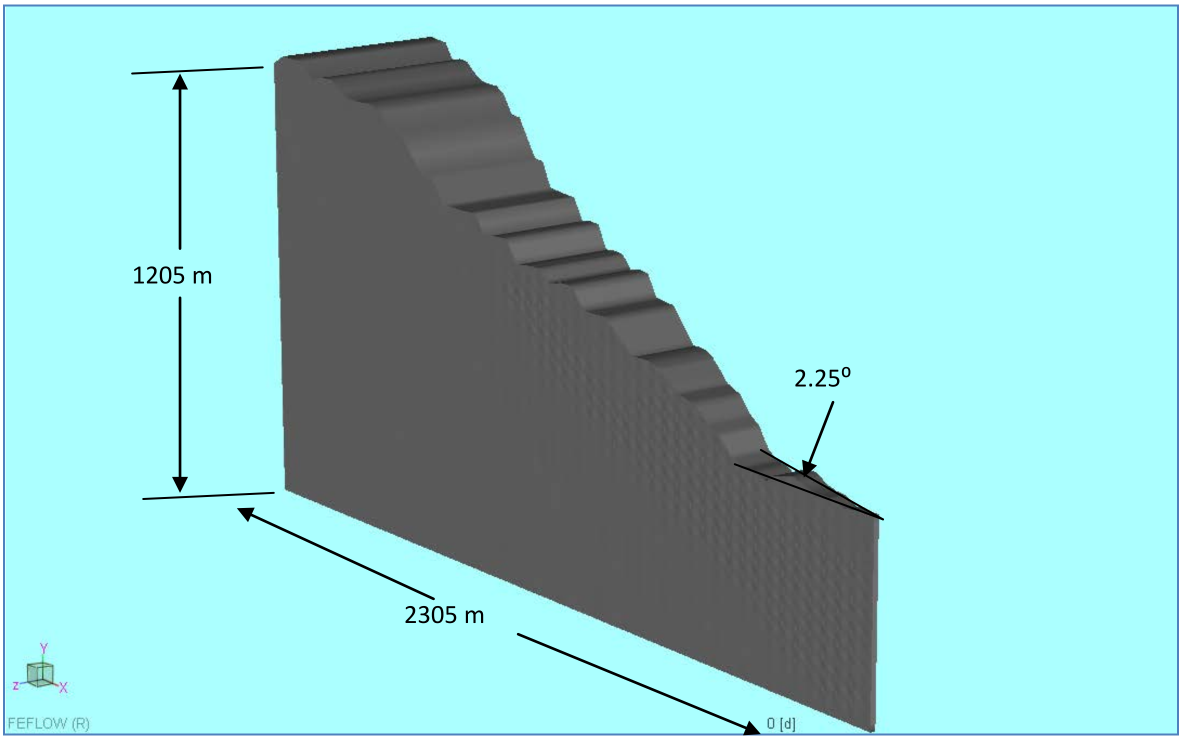


Figure 4 The guidelines suggest consideration of simple model designs. Here a two dimensional radial slice model has been used to simulate inflows to a mine.

5. Calibration

Calibration is the process where the reliability or accuracy of the model is tested by assessing how well it is able to reproduce or match historically observed groundwater behaviour. Typically, calibration is used to refine or modify the key groundwater parameters in the model that control the flow and storage of water. In practice, the model is run many times either in a trial-and-error approach or through an automated procedure until a satisfactory match to observations is attained.

Historically, in Australia, groundwater modellers and model owners have used quantitative measures to illustrate the adequacy of calibration and to judge the reliability of the model as a whole. These measures provide a numerical value that indicates the goodness of fit between the modelled and observed data sets (for example the Scaled Root Mean Square (SRMS) error). Such measures are not necessarily useful as experience has indicated that it is difficult to define rules that are applicable to all models. Experience has shown that efforts solely aimed at achieving a target calibration indicator can lead to poorly structured models where unnecessary complexity is used simply to meet the calibration target. In such cases a model with simpler structure and poorer calibration statistics may well be a better tool for prediction.

As part of the calibration process it is advisable to undertake a sensitivity analysis. This process is aimed at illustrating the sensitivity of calibration to variation in key model parameters and assumptions. The analysis usually involves making small changes to one model parameter or assumption, re-running the calibration model and displaying a model result that can be compared to similar results obtained from the best calibration model and from other sensitivity model runs. The analysis can help identify those model parameters and assumptions that exert a strong influence on model results.

Guiding Principles

5.1 All available information should be used to guide the choice of model parameters and model calibration. All parameters should initially be considered to be uncertain.

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.

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.

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.

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).

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.

Clarification

The guidelines adopt the following definitions:

"Validation" is the process of comparing a groundwater model result to simple, but exact, mathematical solutions (analytical solutions) that include various simplifying assumptions.

"Verification" is a process of reserving a subset of the calibration data set (observed historic data) and testing the calibrated model against this data.

"Post-audit" (refer to Chapter 11) is the process where predictive scenario results are reviewed and compared against actual groundwater behaviour measured during the period within which predictions have been made. The post-audit is undertaken some time after the model is initially developed and allows the original model predictions to be tested against observations.

The guidelines acknowledge that all three methods can be used to good effect in a modelling project. Verification will not always be appropriate as there is often a lack of suitable data for calibration and in many cases it is more efficient to use all available data in calibration. In the event that the model fails to accurately replicate the verification data set, the model will most likely be re-calibrated to rectify this problem. In effect, all of the available data is used in calibration. It is not the intention of the guidelines to discredit the verification or validation approaches.

Clarification

The guidelines promote the use of many different types of data in calibration. Calibration can be improved by increasing the types of observations included in the calibration data set and by using observations of the model features that are of most importance in prediction. While the types of calibration data may be broadly categorised as heads and fluxes, there are many semi-quantitative observations that may be used in calibration. For example, calibration may include targets such as the locations in which springs occur and the locations in which there are artesian aquifer conditions.

6. Prediction

Model predictions (also referred to as predictive scenarios) are run in order to address the key issues identified in the statement of modelling objectives. The calibrated model is modified in a manner required to introduce the future developments and changes to the system that are under investigation. For example, models are often developed to consider changes to the location and rate of groundwater extraction or the introduction of a drained mining pit or excavation. The model is then run for future conditions to determine how the applied changes will impact on groundwater levels and flows. In many cases, these changes will be compared against current conditions and, to facilitate this comparison, a no-change or *null case* model (with current levels of extraction or no future development) is run over the same future time frame.

Predictive models can be run to equilibrium in which case the model results illustrate the final groundwater condition that occurs after a long time, when all changes to the system have stabilised. Alternatively, the model can be run in time stages (calculations are made in a sequence of time steps) into the future so the progressive change in groundwater conditions can be investigated.

Predictive models usually estimate future groundwater behaviour and it is necessary to provide or include assumptions on future climate. For example, most groundwater models include an allowance for groundwater recharge that results from rainfall infiltration. Predictive scenarios must therefore incorporate an appropriate allowance for future recharge that may well differ from current or historic recharge due to the impacts of climate change. The guidelines provide some advice on how best to implement assumptions regarding climatic change in predictive models.

A key feature in many predictive models is the implementation of an assumed change to groundwater extraction. In this case, the modeller must assume the location and rate at which groundwater is pumped from individual wells in the future. There are a number of alternative assumptions that can be made. One assumption that may be appropriate for water resource management models is that the future extraction will be limited to existing licensed wells. Different outcomes will be generated if future extraction is assumed to be from bores that have not yet been constructed or licensed.

Predictive models always include uncertainties and modellers are encouraged to consider material presented in Chapter 7 Uncertainty Analysis.

Guiding Principles

6.1 All model predictions are uncertain and the modeller must acknowledge and address uncertainty through an appropriate uncertainty analysis (refer to Chapter 7).

6.2 Prediction models should be designed in a manner that will yield the results required to meet the modelling objectives and at the same time reduce predictive uncertainty.

6.3 Steady state or equilibrium predictions can often yield useful results particularly when the model is required to provide estimates of long term behaviour where seasonal fluctuations and trends with time can be ignored. Where such factors are important, predictions should be run over a series of consecutive time stages.

6.4 The net impacts of future climate change are best obtained as the difference between predictions that include climate change assumptions and a null case scenario that includes historic or current climate assumptions.

7. Uncertainty

Management decisions will often be directly informed by model predictions, but model results will always be uncertain. Understandable reporting of underlying uncertainty provides necessary context to decision-makers and forms a mechanism by which groundwater models inform a risk management framework. For events with a low impact, a qualitative, limited uncertainty analysis may be sufficient for informing a decision. For events with a high impact, the risks might be better assessed using a more comprehensive uncertainty analysis.

In general, uncertainty associated with predictions made by models results from two components: 1) effects of error in field measurements, and 2) failure to capture complexity of the natural world salient to a prediction. The ability of model calibration to reduce prediction uncertainty can vary from good, when data greatly inform the system needed to make this prediction, to poor, if the prediction is sufficiently dissimilar in type, time, or condition to the data used for calibration. Moreover, in many ways model uncertainty directly results from the stated objective for building the model. Some types of model predictions (contaminant breakthrough, travel time) are directly dependent on system detail, thus inherently carry more uncertainty than predictions that depend on bulk system properties (water balance, capture zones). 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 and the most cost-effective strategy to reduce uncertainty.

Regardless of method(s) used to estimate it, the presentation of uncertainty to a decision-maker is one of the most important aspects of model uncertainty. The goal is to clearly present the modeller's estimate of the representative uncertainty given what is known about the system, the type of prediction(s), and their experience with the model.

Guiding Principles

7.1 Because we cannot construct a single "true" model, simulated results are always uncertain. Model results presented to decision-makers benefit from inclusion of the modeller's estimate of uncertainty associated with simulated results.

7.2 Models are constructed to address specific objectives, often well-defined predictions of interest. Uncertainty associated with a model is therefore always directly related to its objectives.

7.3 Model predictions that depend on a high degree of knowledge of small-scale system detail will always be relatively more uncertain than those that do not. Model predictions that integrate larger areas are often less uncertain because characterisation methods are well suited to discern bulk properties and field observations often directly reflect bulk system properties.

7.4 There is more uncertainty when reporting confidence interval around an absolute model output and less uncertainty when a prediction can be formulated as a subtraction of two model results.

7.5 Linear methods for calculating uncertainty are less computationally intensive than non-linear methods. For many decisions, linear methods are sufficient to convey the modeller's expectation of uncertainty.

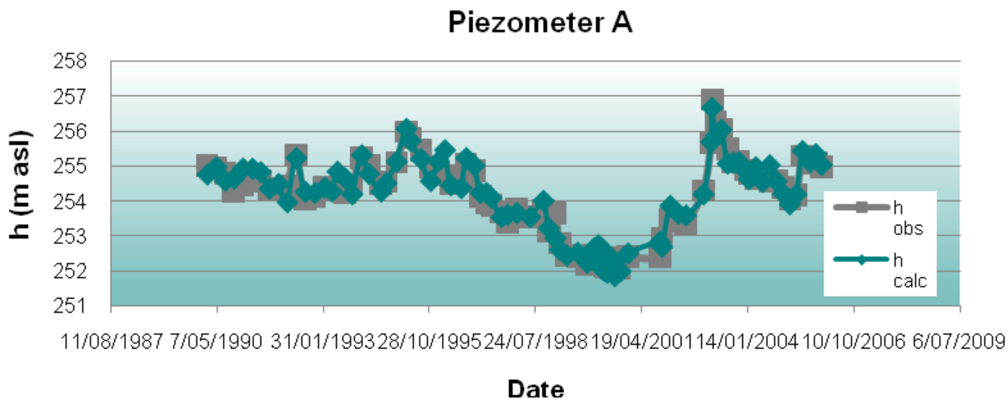
7.6 The presentation of the uncertainty to a decision-maker is likely the most important aspect of model uncertainty. Presentations are most helpful when they contain visual depictions that closely conform to the decision of interest.

8. Reporting

Model reporting encompasses all communication of the conceptualisation, the model design, its calibration and outputs from predictions. This is traditionally achieved through a written technical document, often supported by a number of presentations at workshops. Typically, the report is the final product used by the model owner, groundwater regulators and other key stakeholders. Accordingly, it is recommended that appropriate effort and attention be given to producing reports of a high standard in a staged manner. As a minimum, the following three staged reports should be prepared:

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

The model, all data collected and information created through the modelling process needs to be described in the report. At the same time, an archive of all the model files and all supporting data should be created so the results presented in the report can, if necessary, be reproduced and the model can be used in future studies. It is recommended that appropriate care be taken to present outcomes in a clear and unambiguous manner because the quality of the model is usually judged on the basis of the information presented in the technical report.



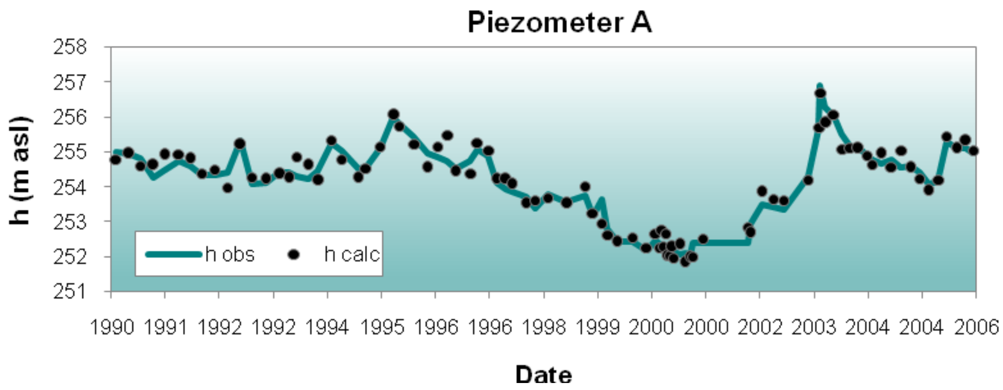


Figure 5 Keep the graph simple by using appropriate density of ink and symbol styles

As an example, Figure 5 shows two versions of the same data; each presents an imaginary observed hydrograph and the calculated equivalent. The upper graph is created using the default settings of mainstream spread sheet software. The lower graph minimises the data-ink ratio. Reducing this ratio will simplify the graph and focus attention on the data.

Guiding Principles

8.1 Prepare individual reports after conceptualisation and design, after calibration, and after predictive modelling.

8.2 Tailor reporting to its target audience, so a report can consist of a section with an executive style summary for a non-technical audience and a detailed section for a technical audience.

8.3 Aim for an objective and clear visualisation of model data and results using appropriate graphs, maps and colour scheme.

8.4 A model archive must reproduce the reported results exactly, while at the same time act as a repository for data and knowledge of the system. For the latter it is recommended that GUI-independent standard file formats be used.

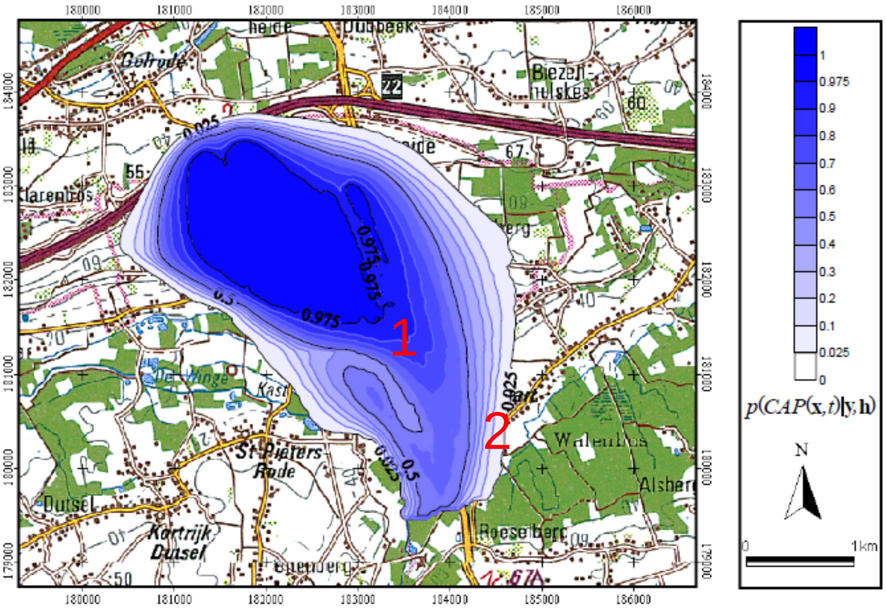


Figure 6 Predictive results of bore field capture zone presented as a probability map to help address uncertainty (From Feyen L, Dessalegn M, De Smedt F, Batelaan O and Gebremeskel S 2002. Stochastic determination of capture zones for the well field "Het Rot" (Belgium) *Aardkundige Mededelingen, 12*, 199-202)

9. Reviews

The aim of the review process is to provide an objective assessment of whether the model has been developed and used in a manner that is appropriate for the stated modelling objectives and the target model confidence level classification.

The reviewer will typically be required to assess whether the model is fit for purpose. This term relates to the model's ability to answer the questions posed by the modelling objectives. The assessment will be based on whether or not each stage of the modelling process has been undertaken in an appropriate manner and whether it has resulted in a predictive tool that can be used with the agreed level of confidence.

The guidelines include a compliance checklist (as shown below as Table 2) and a more extensive model review checklist which is included at Appendix A.

Table 2: Compliance checklist

Question	*Yes/No*
Are the model objectives and model confidence level classification clearly stated?	
Are the objectives satisfied?	
Is the conceptual model consistent with objectives and confidence level classification?	
Is the conceptual model based on all available data, presented clearly and reviewed by an appropriate reviewer?	
Does the model design conform to best practice?	
Is the model calibration satisfactory?	
Are the calibrated parameter values and estimated fluxes plausible?	
Do the model predictions conform to best practice?	
Is the uncertainty associated with the predictions reported?	
Is the model fit for purpose?	

Guiding Principles

9.1 A review should take place after each reporting milestone.

9.2 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
- a post-audit, which is a critical re-examination of the model when new data is available or when the model objectives change.

10. Solute transport models

Solute transport models calculate the concentration and movement of dissolved salts (solutes) in groundwater. The groundwater flow component of solute transport calculations is based on a groundwater flow model, and the further migration of solutes (through dispersion and diffusion) is determined through an additional solute transport equation. Solute transport models are, in all respects, more complicated than groundwater flow models, and are more time consuming to develop and run. This is not only because of the additional solute transport calculations, but also because solute transport models often require more closely spaced calculation nodes and shorter time steps to be able to successfully solve the underlying equations. This often results in the need to limit the size of solute transport models. For example, Figure 7 illustrates the use of planes of symmetry to reduce the number of calculation nodes in a solute transport model.

The density of water is dependent on the concentration of salts that it contains. In situations where there is a substantial difference in concentration, for example, at the location of a saltwater-freshwater interface in a coastal aquifer, density effects have a significant influence on groundwater movement. In these cases, the solute transport model must also calculate water density and its variation caused by both groundwater flow and solute transport.

For some problems, the movement of solutes can be approximated without the need to develop a complex solute transport model. In particular, a groundwater flow model can sometimes provide useful information on solute movement when it is primarily controlled by groundwater flow. For example, calculations that trace individual particles of water in a groundwater model can provide useful information on the maximum likely travel of solutes within a given time frame.

Guiding Principles

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.

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. Solute transport model outcomes are more strongly controlled by heterogeneity (variability in aquifer properties) than groundwater flow models, and this needs to be considered and recognised during all stages of modelling.

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

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.

10.5 Analytical models and/or particle tracking in a groundwater flow model should be used before the development of a comprehensive numerical solute transport model to assess the relevant spatial extent and model timescales.

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.

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.

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 a sensitivity analysis undertaken at the start of solute transport modelling.

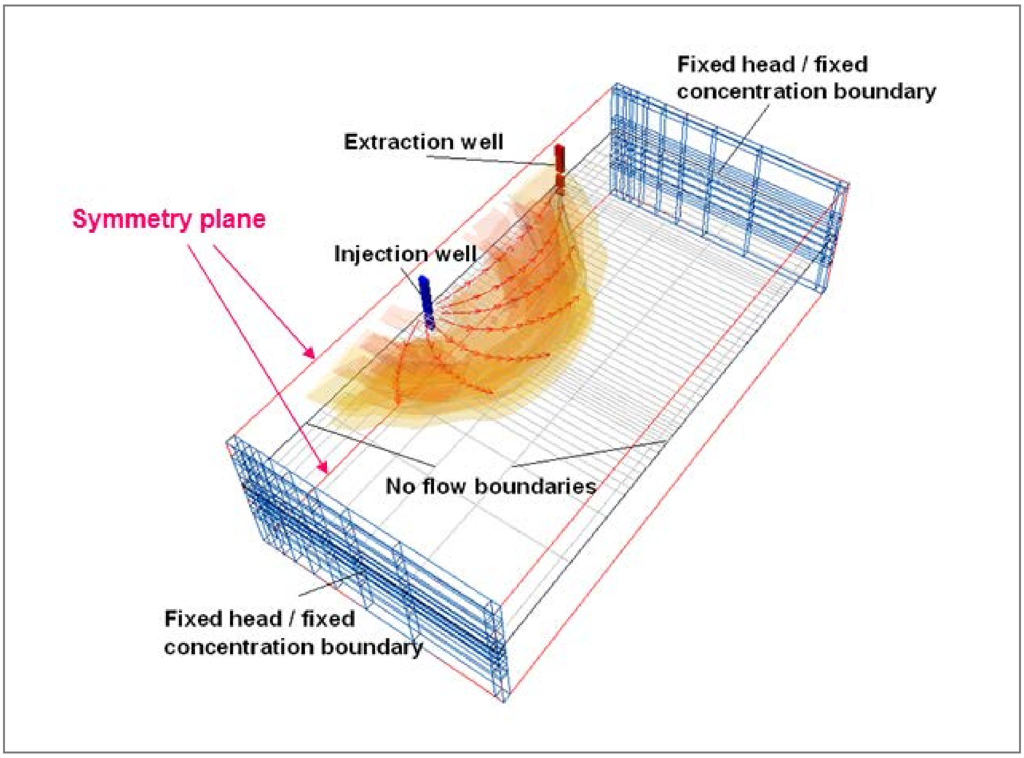


Figure 7 Salinity plume predicted by a solute transport model of an Aquifer Storage and Recovery project. Note how the model makes use of symmetry to limit the size of the model domain. From H Prommer and P Stuyfzan, *Environmental Science and Technology*, Vol. 39, No. 7, 2005.

11. Surface Water–Groundwater Interaction

Surface water-groundwater interaction is the term used to describe the flow of water between a surface water body and groundwater. In a groundwater modelling sense the term indicates an exchange of water (i.e. water flowing into or out of the model) between the groundwater model and a surface water body

There are many ways of incorporating flows to and from surface waters in a groundwater model. The simplest of these is to assign a specified head in the groundwater model that represents the average elevation of the water surface in the surface water body. The groundwater model will estimate a flow of water into, or out of, the surface water body in order to maintain the specified head.

A more accurate approach is to link a groundwater model to a surface water model so that both models include similar flows at their interface. The simplest approach to linking or coupling a surface water model and a groundwater model is to run one model and to use the predicted interface conditions (flows and heads where the two models meet) to control the interface conditions in the other model.

Where the timing of the interaction process is important then more sophisticated approaches to linking groundwater and surface water models may be required and this may lead to difficulties in synchronising the two models. Groundwater models developed for water management purposes are typically run over a period of decades with calculations made on a monthly time step. This timing is appropriate for a groundwater model as the response of an aquifer to changes in inputs or outputs is generally slow. It can take several months or even years for the full impacts of a flooding event to be fully expressed in a groundwater system. On the other hand, response times in surface water bodies such as rivers or lakes is much faster and a short calculation time step (at times less than hourly) may be required to fully represent a flooding event. To fully account for the different response times in the surface water and groundwater models it may sometimes be necessary to run both models concurrently and exchange data between models at every time step (dynamic coupling of the models). This approach requires the groundwater model to be run on a short time step to match the requirements of the surface water model. As a result the computational effort, model run times and the amount of data generated by the groundwater model can become excessive.

Guiding Principles

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.

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.

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. Features that are unlikely to affect model predictions should be left out.

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.

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.

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.

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.

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.

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.

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.

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.

Appendix A – Model Review Checklist

Review Questions	*Yes/No*	*Comment*
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 Water table 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		

Review Questions	*Yes/No*	*Comment*
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?		
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?		
3.6.3 How is the initial concentration of solutes obtained (when relevant)?		
3.7 Is the numerical solution of the model adequate?		

Review Questions	*Yes/No*	*Comment*
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?		
5.5.1 Are the pumping stresses similar in magnitude to those of the calibrated model? If not is there reference made 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 made to		

Review Questions	*Yes/No*	*Comment*
the associated reduction in model confidence?		
5.5.4 Are the assumed stresses and time scale 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 Have 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?		
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		

Review Questions	*Yes/No*	*Comment*
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?		