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Groundwater Model Audit Guidelines

Ministry for the Environment

Groundwater Model Audit Guidelines

Prepared for
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Executive Summary

A mathematical groundwater flow model is created by having a conceptual description of the groundwater system and translating this into a mathematical framework into which existing appropriate data are incorporated. A model cannot completely represent a natural aquifer system, rather it is a simplified version of a groundwater system. A model represents the essential physical features of a groundwater system and allows quantification of its response to changes in system stresses. For groundwater models, examples of system stress include groundwater recharge from rainfall percolation or stream seepage, abstraction from pumping wells, or the discharge of a contaminant into an aquifer.

There is an ever increasing use of groundwater models as there is general recognition and acceptance that an attempt to simulate environmental processes numerically can provide a sound basis for the making of important decisions. However, alongside the growing use of models in environmental management is a growing scepticism regarding the sometimes inappropriate application of these models. There are many cases where the use of models in environmental management has been disappointing at best, and misleading at worst. This scepticism is partially related to poor development and testing of the model concept, inappropriate application, or mistakes in model use.

These guidelines provide a framework within which a model auditor can assess the validity and uncertainty of the predictions of a model. The main tasks of the model auditor are to check through the modelling process and assess the validity of the modelling results, primarily by:

(a) identifying whether there are any modelling errors; and

(b) determining whether the model results are meaningful in the context of the particular question being asked of the model, given the modelling uncertainty. This model uncertainty is related to:

- parameter uncertainties associated with parameter variability and measurement errors and;
- model assumptions.

Use of these guidelines as a model audit framework cannot guarantee that the model is valid, nor do these guidelines describe how models should be utilised. Indeed, the nature of groundwater modelling is so varied that it is not considered desirable to be so prescriptive. Instead this is a report and tool for auditors to provide background details on models and guidelines on some areas where an auditor may want to check the modelling process to help assess its suitability for any particular application. There are so many variables in the approach to any particular modelling project that it is not desirable for the audit process to determine how a modelling project should be undertaken. Rather, the auditor should be aware of the issues that can arise and, with

an improved understanding to the background of modelling, be in a better position to undertake their audit function.

Furthermore, these guidelines are not a substitute for education in modelling, rather, they are a tool to assist and guide those appraising and, or auditing models. Consequently those who are given the task of auditing or appraising models must first decide whether they are qualified to audit or appraise the model, or whether they need assistance from someone with more appropriate modelling expertise.

Groundwater models

A groundwater model is created by translating a conceptual idea of a groundwater system into a mathematical framework into which appropriate data is incorporated. Groundwater models can be distinguished by their solution method, of these the most common are analytical and numerical models. Analytical models incorporate many simplifying assumptions allowing an exact solution to be found, however there is a limited capacity for spatial or temporal variability of the parameters used in the model. In contrast, numerical models allow greater physical complexity to be represented. To do this, the area of interest is subdivided into small areas (referred to as cells or elements) and the flow equation is approximated by algebraic equations for each. These algebraic equations are solved numerically through an iterative process.

The modelling process

The auditing process requires that the auditor goes through the same steps as the modeller (albeit much quicker) and form their own opinion regarding the credibility of the model. The modelling process incorporates the following stages:

- Definition of the modelling problem
- Model conceptualisation
- Model calibration
- Model predictions and predictive uncertainty analysis
- Reporting

Defining the modelling problem

The most important first step in a modelling project is to define the modelling problem for which the modeller must find solutions. Once this has been decided, the complexity of the modelling software and data requirements are appropriately defined. For example if the modelling problem or purpose is to rank the relative stream depletion effects of bores adjacent to a surface waterway, and the absolute magnitude of the stream depletion effect is not important, a simple analytical model is appropriate using regional data. However where it is important to predict the magnitude of a response to a change in hydrogeologic conditions – for example when an irrigation scheme is proposed , then it is

important that site specific data are gathered, and a model complex enough to incorporate the variability of the data is used.

Model conceptualisation

Once the modelling data and software requirements have been defined, the model conceptualisation stage occurs. This comprises four main parts:

- Site characterisation. This involves collecting and compiling all the available data relating to the aquifer system within which the groundwater problem occurs. This is undertaken to a level of detail that is appropriate for the modelling problem.
- Building a conceptual model. The conceptual model describes in words and mathematical equations the key components of the aquifer system. These key components include the boundaries of the model domain area, the hydrogeological framework and flow system components and the interrelationships between these components. At this stage the simplifying assumptions that are appropriate for the model are chosen.
- Parameterisation. Optimisation of parameters used in the model by sensitivity analysis, statistics and geological zonation.
- Choosing the model code. Once appropriate model assumptions have been identified, a model code consistent with these assumptions is selected.
- Discretising the data in time and space. Discretisation choices determine when and where the model solution will be calculated.

Errors at the model conceptualisation stage, such as an overly simple model design, inappropriate selection of physical and hydrogeological boundaries, or lack of information etc, propagate throughout the entire modelling process, compromising model predictions. These guidelines provide checklists for the model auditor and modeller to use in determining whether or not such problems have occurred.

Model calibration

In model calibration, the model parameters are adjusted until model outputs best match the measured field data. The range of possible model predictions is helpfully constrained when a model is calibrated. Both qualitative and quantitative calibration targets are used. Qualitative targets include matching of piezometric contour patterns, or matching to established relationships between data types such as spring-fed stream flows and groundwater levels, or water balance information. Quantitative targets relate to the residuals between modelled and measured points at particular times, and include the mean squared error, the correlation coefficient, etc.

Calibration errors relate to: the uncertainty of the calibration targets; the use of unreasonable model assumptions to force a fit to calibration targets; and solver or

numerical instability. Again the guidelines provide checklists for the model auditor to consider whether these problems have occurred.

Models need also to be verified by matching their output against a set of data independent of the calibration data.

Model predictions and predictive uncertainty analysis

Model predictions are undertaken by running the model with adopted parameters (calibrated or most reasonable uncalibrated), and imposing a predicted stress which represents future conditions.

When a model is calibrated to measured data, there is typically a range of parameter combinations that allow equally good model fits, i.e. calibrated model solutions are not unique. This is partly related to parameter uncertainty and also to the bias imposed by simplifying assumptions on the model. When a model is uncalibrated there is an even larger range of reasonable parameter combinations. Consequently it is important to attempt to determine the range of possible calibrated or uncalibrated models that exist. Model predictions can then be made with the most conservative of possible models.

There is also uncertainty in the predicted future stresses of an aquifer, for example to what extent will the aquifer be developed, what are long term rainfall predictions, etc. Consequently, either a large range of 'reasonable' future stresses need to be defined, or the initial estimates of future stresses should be frequently reassessed as monitoring information becomes available.

Predictive uncertainty is inevitable. The guidelines provide checklists for the model auditor to consider whether predictive uncertainty has been appropriately explored and conveyed in the reporting of model results.

Reporting

Model auditing requires that the model report is detailed enough so that an independent modeller can see sufficient input and output data to confirm the accuracy and assumptions within the model. If necessary, the auditor should have enough data so that they could duplicate the model results.

The information that can be included in a model report is outlined in Section 6 of these guidelines.

Modelling appendices

Many of the model audit issues are specific to the type of model being used. These issues are addressed in the Appendices A to D that have been prepared for analytical flow and contaminant transport models and numerical flow and contaminant transport models. Greater detail is provided in these appendices specific to the particular modelling type. Checks and methods useful for determining the credibility and limitations of the model output are included in these appendices where example case studies are illustrated.

ACKNOWLEDGEMENTS

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1.0 Introduction

To obtain approval for many engineering and agricultural projects, individuals and companies need to predict the quantifiable effects of the development on the environment. Many projects result in some impact on groundwater systems, for example by abstractions from water supply wells, or discharges onto land or water, or changes to the land surface that affect the quality and quantity of infiltrating water. Groundwater modelling provides an invaluable tool both for exploring the potential future impacts of proposed developments and enhancing understanding of the effects of existing projects. There is an ever increasing use of groundwater models as there is general recognition and acceptance that an attempt to simulate environmental processes numerically can provide a sound basis for the making of important decisions.

However, alongside the growing use of models in environmental management is a growing scepticism regarding the application of these models. There are many cases where the use of models in environmental management has been disappointing at best, and misleading at worst. This scepticism is partially related to poor conceptual development of the model, or inappropriate application or mistakes in model use. However, it is also related to the fact that all models are approximate representations of the real world and therefore contain an inherent uncertainty, e.g. when a model is calibrated to measured data, there is always a range of combinations of possible inputs that allow adequate reproduction of these data.

This document provides a guide to assist Regional Council staff auditing or appraising groundwater models. In this situation Council staff must consider whether meaningful assessments of effects on groundwater and associated environments have been reported. It should also assist modellers in developing useful models and anyone using model results. These guidelines are a reference desktop tool for aiding those intending to audit models. They are neither a substitute for model instruction manuals, nor are they to be seen as short course notes for modelling in general.

The guidelines aim to promote a better understanding of the validity of any groundwater model and the uncertainty of its predictions by providing a framework within which validity and uncertainty can be investigated. This in turn serves to facilitate a better understanding of the potential effects on the environment from a proposed or existing activity and consequently allows improved implementation of the Resource Management Act.

Use of the guidelines as a model audit framework cannot guarantee that the model is valid nor do the guidelines describe how models should be utilised. The nature of groundwater modelling is so varied that it is not considered desirable to be so prescriptive. Instead this is a report for auditors and provides background details on models and guidelines on some areas where an auditor may want to check the modelling process to help assess its suitability for any particular application. There are so many

variables in the approach to any particular modelling project that it is not desirable to be prescriptive. Rather, the auditor should be aware of the issues that can arise and, with an improved understanding to the background of modelling, be in a better position to undertake their audit function.

These guidelines are not a substitute for education in modelling, but rather a tool to assist and guide those appraising/auditing models. Consequently those who are given the task of auditing or appraising models must first decide whether they are qualified to audit or appraise the model or whether they need assistance from someone with more appropriate modelling expertise. How the potential auditor makes that decision is not within the purview of this report.

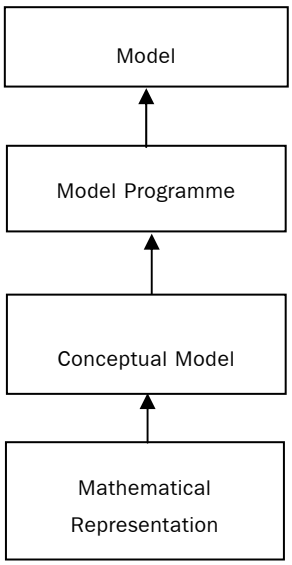
A literature review formed the initial phase for the preparation of these guidelines. A number of references have proved particularly useful. Most notably these are the American Society for Testing and Materials model guidelines (ASTM, 1996), the Murray Darling Basin Commission modelling guidelines (MDBC, 2000), the Michigan State Land and Water Management Hydrologic Studies Unit web page (2000) and the STOWA Good Modelling Practice Handbook (1999).

1.1 Groundwater Models

A groundwater model is created by translating a conceptual idea of a groundwater system into a mathematical framework, into which existing appropriate data are incorporated. Essentially the model is a non-unique and simplified version of a groundwater system. It represents the essential physical features of the groundwater system and allows quantification of the its response to changes in system stresses. For groundwater models, examples of system stress include groundwater recharge from rainfall percolation or stream seepage, or pumping from wells, or the discharge of a contaminant into an aquifer.

Figure 1 below shows the relationship between the various representations of a model.

Figure 1: Model Representations



There are two kinds of groundwater models: those modelling groundwater flow; and those modelling contaminant transport.

Groundwater flow models simulate an aquifer flow system, the questions usually asked of these models include: What is the sustainable yield of an aquifer, its response to aquifer recharge, or to abstraction rates. The answers are defined in terms of groundwater flow direction, water levels, and leakage through confining layers or from streams, or the specific route of a water particle. Typical outputs for groundwater flow models are flow directions and flow rates, both in the aquifer or in hydraulically connected surface water bodies, and last, but not least, predictions of water levels.

Groundwater contaminant transport models predict the movement of solute and or heat in groundwater. Questions typically asked of contaminant transport models include: What is the maximum concentration that may be expected at a particular well, after a proposed discharge into groundwater has occurred? At what time will the maximum concentration occur? How should a groundwater remediation system be best designed for a particular site? Contaminant transport models simulate the behaviour of a contaminant in a groundwater system. These include the advection and diffusion of the contaminant, removal of the contaminant by adsorption or desorption onto or from rock or sediment, the spread or dilution of the contaminant by dispersion, and chemical reactions of contaminants. The outputs from a contaminant transport model usually relate to contaminant concentrations or aquifer temperatures at various distances away from the source, at specified times.

Model creation requires the adoption of a number of simplifying assumptions appropriate for the specific project and to an adequate degree of detail. Whereas models are a simplification of the real world, they need to be sufficiently complex to reproduce field results within an acceptable error tolerance. The appropriate degree of model complexity varies depending on the available data and the question being asked of the model.

Groundwater models are often distinguished by their solution method, which includes physically based analytical or numerical models, and statistical models such as neural network models. Analytical and numerical models are by far the most common and consequently, they are the focus of these guidelines.

In most real-world situations the factors needed for a realistic description are likely to be difficult to quantify, varying in time and/or space. Mathematical models for such problems generally require complex numerical expressions and a considerable amount of data to characterise the problem. However, it is often justifiable to make a number of simplifying assumptions e.g. the aquifer is homogeneous and infinite in extent. When enough simplifying assumptions are used, a simple mathematical equation can be

derived, such that an exact solution to the equation can be found, this is called an analytical model. They can be solved by hand or by using simple computer programs, but they do not allow for complex spatial and temporal variability.

In contrast, numerical models allow greater physical complexity to be represented in the model (i.e. fewer simplifying assumptions), but cannot be solved exactly. They require numerical iteration methods to solve the governing flow equations, i.e. the equations themselves do not give an exact solution, instead the model must iterate to an approximate solution that falls within an accepted band of error tolerance. Numerical models allow spatial and temporal variable data to be represented. These models are used in cases where the essential model features – i.e. those that will affect model predictions – are complex.

Models can also be distinguished and classified in a number of other ways, including:

- *The degree to which our knowledge of physical processes is used, for example many of the processes related to many chemical reactions are typically ignored in a contaminant transport model.*
- *Spatial dimension - 1, 2 or 3 dimensions and discretisation of space – universal, regular grid or irregular elements.*
- *Domain of application – unsaturated or saturated zone models, contaminant and heat transport, or flow models. These guidelines only address saturated zone models, although the general principles can be applied to all models.*
- *Resolution in time – steady state, instantaneous or fixed duration.*
- *Mathematical solution mechanism.*

1.2 Model Auditing and Appraisal, Errors and Uncertainty

1.2.1 Model Auditing and Appraisal

The auditing process requires the auditor to think through the same steps as the modeller (albeit much more quickly). The most efficient method in which to carry out an audit is to review the model report. This requires that the model report is detailed enough such that an independent modeller can see sufficient input data, calibration to field data, and model simulation outputs to confirm the validity of the model. From reading the report, auditors should be able to form their own opinion regarding the credibility of the model. The report should contain enough data so that the auditor would be able to duplicate the model results. As both auditing and modelling progress through the same steps, the framework for model auditing can also be used as a quality assurance tool for groundwater modelling work.

The auditing process can be most useful for a large model, if it is conducted progressively through the modelling project, so that any auditor's feedback can be incorporated into the model development, rather than comments coming at the end of a modelling project which may potentially cast doubt on its usefulness.

The Murray Darling Basin Commission flow modelling guidelines (MDBC, 2000) make a useful distinction between model appraisals and model audits. Model appraisals can be undertaken by non-modellers and allow the general completeness of the modelling work to be assessed. Model audits are generally undertaken by experienced modellers and assess the integrity of the model at every key step (milestone) in the modelling process and assess the impact the model assumptions may have on the resulting model predictions. This distinction between model appraisers and auditors is useful and anyone applying these guidelines should consider which is their most appropriate role given their experience with respect to a specific modelling project.

The guidelines envisage that the model auditor will usually review a model report, although they may request additional model data if something is unclear. Consequently, the guidelines list details that should be included in the model report. However, if these details are omitted from the model report the auditor can then source these details from the model files, journal and raw data if necessary. From the models and model reports reviewed as part of this project, it appears that very few model reports in New Zealand currently contain enough information to allow a model audit without reference being made to the model data and files.

1.2.2 Errors and uncertainty

Model errors occur in both the conceptualisation phase of a model and in the data input, calibration, and predictive simulation stages. One such error is putting model boundaries too close to the area of interest, such that they incorrectly affect the model parameterisation and model predictions. Another may be that the model solution is numerically unstable. There is also a range of errors due to carelessness that are common, such as an incorrect pumping sign being used, or a model stress not being specified over an entire stress period. A model report needs to be relatively detailed to allow the auditor to check for these errors. Alternatively the auditor may need to review the model files and/or journals.

Model uncertainty is related to parameter uncertainty and model assumptions. Parameter uncertainty is related to the fact that aquifers are heterogeneous, so parameters are spatially variable. Yet we are only able to measure the parameters at a few points in the domain of the model. In addition parameter measurements are imperfect, incorporating errors and the measurements themselves are dependent on the volume of the aquifer involved in the measurement, i.e. analysis of a slug test at a well will likely indicate a different hydraulic conductivity than that of a three month pumping test. The parameters known at some discrete points in a model have an error term associated with them whereas the parameters over the remainder of the model domain are unknown and have to be estimated.

Model assumptions are used to simplify the complexity of the real physical world, and allow solutions to the model problem to be determined. However sometimes the model

assumptions made do not accurately represent the physical processes being addressed. For example, if a model is required to match the measured migration of a contaminant to a number of down gradient wells, and the aquifer is heterogeneous, then a model which assumes a homogeneous aquifer will only roughly approximate the real situation. If the purpose of a model is to predict a worst case concentration in a specific down-gradient well, using a model that assumes a constant dispersivity will give a different estimate than one that assumes a scale dependent dispersivity. (NOTE, most contaminant transport models available assume a constant dispersivity, and the model user approximates a scale dependence by altering the dispersivity for each distance being investigated by the modeller).

While checking through the modelling process the **model auditor** must assess the validity of the modelling results, primarily by:

(a) identifying whether there are any modelling errors; and

(b) determining whether the model results are meaningful in the context of the particular question being asked of the model, given the modelling uncertainty.

Model uncertainty is related to:

- parameter uncertainties associated with parameter variability and heterogeneity within the aquifer, measurement errors, interpretation of measurement errors, or lack of measurements;
- model assumptions.

1.3 Document Structure

The guidelines aim to assist with the auditing process by providing a general lay-out of the various parts of the modelling process, explaining how they should be carried out, and identifying the errors that have been encountered.

The main focus within each section of these guidelines is on the following:

- *A clear description of each stage of the modelling process;*
- *The effects of data and model assumptions at each modelling stage on the model validity and uncertainty;*
- *Potential errors at each modelling stage that may compromise the validity of the model.*

There are four detailed appendices attached to the main document, relating to: analytical flow models, analytical contaminant transport models, numerical flow models, and numerical contaminant transport models. Greater detail is provided in these appendices specific to the particular model type. The appendices also incorporate case studies illustrating various aspects of the modelling process. Checks and methods necessary to

determine both the validity and significance of the model output are included in these appendices.

The general layout of the document is consistent with the consecutive steps undertaken in a modelling exercise. These are defined as follows:

Setting up of the modelling process (section 2.0)

Start a model journal

Defining the problem and determining the model objectives

Model requirements

- **Model Conceptualisation (section 3.0)**

  Site characterisation

  Conceptual model

  Choice of model code

  Discretisation in time and space

  What can go wrong in model conceptualisation

  The importance of groundwater monitoring

- **Model calibration (section 4.0)**

  Parameterisation

  Calibration techniques

  Model verification

  Analysing the calibration

  The non-uniqueness problem and what can be done about it?

  Calibration errors

- **Predictions and predictive uncertainty (section 5.0)**

  What methods are currently available to address predictive uncertainty?

  Simulation results errors

  Interpretation and reporting model predictions and results

- **Documentation and model report (section 6.0)**

This process is shown in Figure 2. The modelling process has feedback to previous modelling steps as deficiencies in early modelling steps often only become clear when

working through the modelling process. The presence of such feedback makes the modelling process an iterative procedure.

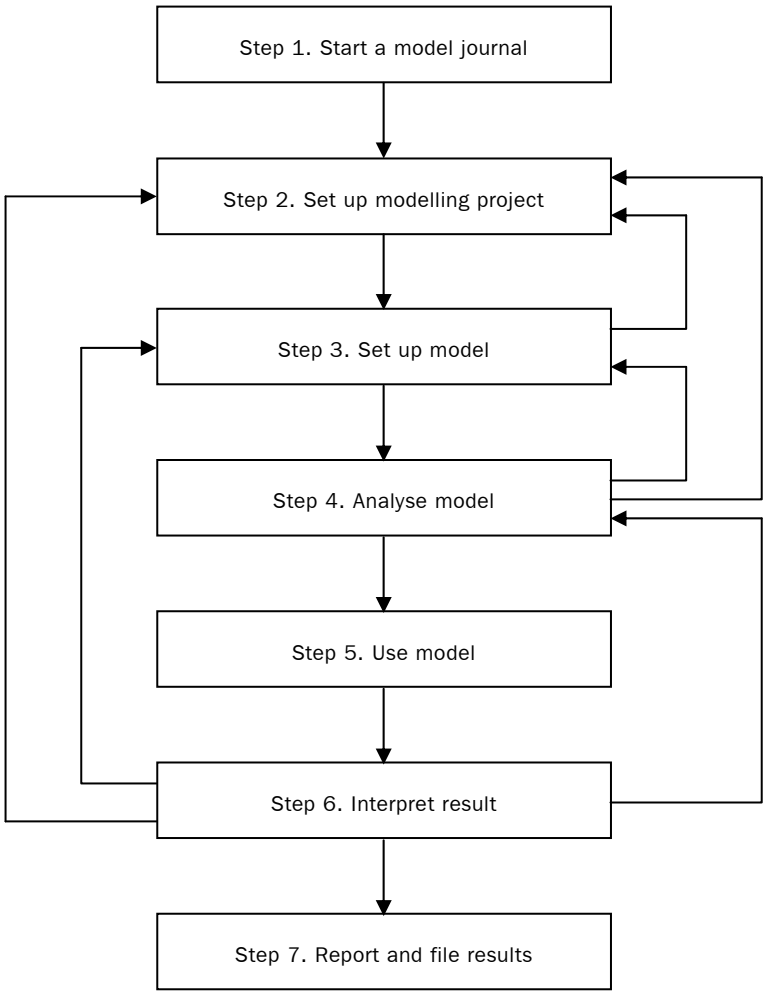


Figure 2: Summary of the Modelling Process (from STOWA 1999)

2.0 Set up of the Modelling Process

The initial steps of a modelling project are important, as they go on to affect all the subsequent modelling steps. Once a problem has been detected, for which a model would provide useful information, a number of preliminary modelling steps need to be taken. Such a problem may be an actual or potential effect. The problem may be a declining groundwater fed stream flow, salt water being pumped from wells, faecal contamination of a well, or drawdown interference between pumping wells, etc. A groundwater model can be used to understand better: whether the problem is likely, or, if it might already be occurring; the causes of the problem; and how to mitigate the problem.

For any problem, the specific questions that need to be answered to help with the problem need to be defined, and then the model objectives and requirements, and data requirements to allow these objectives to be met must be defined. Lastly a plan of how to go about the modelling process can be established. An important initial step is to record this in a modelling journal, as described below.

When these initial steps are carried out appropriately, the model outputs should be appropriate for its purpose and the modelling project will be carried out in the most efficient manner.

2.1 Set-up a Model Journal

A **model journal** records ALL modelling activity such as: what the original model objectives are and any changes to these as the modelling project progresses; what choices were made, such as model assumptions, data synthesis, etc; details of parameter combinations that are trialled during the calibration process; who did the work; what specific tasks were carried out, etc.

The benefits of the model journal extend both to those undertaking the modelling process (as modelling is an iterative process where previous steps frequently need to be revisited and remembered!), and anyone looking at using the model at a later date. Of all the modelling steps carried out this is the most frequently neglected, and this can waste a lot of time, particularly when previous tasks need to be repeated as there are no records of previous results or details of this work.

The STOWA (1999) guidelines include a template for a model journal, however, less formal modelling diaries, if complete, are just as useful.

The model auditor does not need to read the model journal, as sufficient detail for auditing should be provided in the model report. However, modelling projects that are undertaken using a journal have a greater likelihood of developing along a basis that will

more likely comply with these guidelines. The model journal (and report) needs to include information regarding all the model set up steps that follow in this document.

2.2 Defining the Problem and Determining the Model Objectives

2.2.1 Defining the Problem

There are often major differences between the perception of a problem from the viewpoints of a client and the modeller. Consequently, both the modeller and the client (such as a policy maker or a consent applicant) must consult until a common description of the problem is established, such that it can be modelled.

Firstly, the use of a model usually takes place within a larger context: a consent application, a regional plan, etc. It is important to establish the purpose of the application of the model, is it for analysis of policies, consent application, comparison of management options, scientific research, etc.

Secondly, sometimes there is both a client and one or more additional parties who must also be satisfied with the model outcomes. Discussing the model problem with additional interested parties should take place before modelling commences. This might include discussions with Regional Council consent investigating officers and Groundwater Section staff. This is an important step, as potentially fatal flaws in the modelling approach can be identified at the start of the project, rather than presenting the results of a study that may not be regarded as technically sound, or are based on flawed or unreliable data. It is recognised that Regional Councils are sometimes reluctant to discuss how a modelling project should be undertaken for liability reasons, however, input from Regional Councils at the start and during the modelling process is undoubtedly more efficient.

Once a common understanding between all parties with an interest in the model project has been reached, the problem to be modelled should be briefly defined, without details, in terms of the physical processes of concern, their time and spatial scale.

It is also important to consider at this stage whether a model is the only appropriate tool for exploring solutions to the problem, and to identify other alternatives to a model based approach.

2.2.2 Model Objectives

Model objectives should explain in detail the purpose or ‘desired end’ or ‘outcome’ of a groundwater model. For example, this may be to establish groundwater pumping restrictions to maintain spring fed stream flows. Alternatively, the desired end may be to establish separation distance rules between wells and septic tank discharges, so that faecal contamination of wells is mitigated. The definition of objectives follows from the definition of the problem, but specifies:

- *The reason (desired end) for solving the problem by means of a model;*
- *The questions to be answered by the model;*
- *The scenarios to be modelled;*
- *The model domain and the problem area.*

2.3 Model Requirements

To carry out any modelling project, the following factors must be determined on the basis of the model objectives defined:

- *Model complexity requirements;*
- *Model accuracy requirements;*
- *Communicating and reporting requirements;*
- *Availability of personnel with appropriate expertise;*
- *Time available to complete the modelling project and report;*
- *Sufficient budget for the personnel and time.*

i. The model objectives determine the type of modelling approach to be used. For example, a model that is used to explore policy options for preserving stream flows, will need to evaluate the relative effects of differing policy options and also indicate the level of certainty the model outputs are able to provide. For instance, a decision maker may be told that 'reducing stream depletion effects by 10% will preserve the in-stream environment, but at a significant social cost'. Does the inherent uncertainty surrounding the 10% figure make this a meaningless relationship, hence invalidating the decision? In this situation a relatively comprehensive modelling exercise is likely to be required. In contrast, a relatively simple model could be used to assess whether the stream depletion effects of a proposed groundwater abstraction are likely to be minor.

These examples illustrate that the model complexity appropriate for one set of the model objectives may be not be suitable for another more complex set of model objectives.

A model may be constrained due to the limitations placed on the modeller by budget, personnel requirements, the context of the project, the time constraints, and justification of the project. These limitations may constrain the extent and simulations allowed for by the modeller. During auditing, it is important to identify these constraints as being external to the model and note how they have affected the modelling process. Where a simple model is required, management constraints are generally not an issue. However, for more complex model projects, the "quick-cheap-good" paradox comes into play, where a client can readily obtain a model with one or two of these three attributes, but not all three.

An agreed **definition of the problem and model objectives** is a critical first step in any modelling exercise, as it helps define how the modelling should be undertaken. Consequently, it is important that both the model objectives and the framework within which the model is constructed are clearly stated in any groundwater study.

It is important to recognise that a model is always developed for a specific purpose and model simulations of scenarios that are not consistent with the original model objectives may be unreliable.

2.3.1 Model Complexity

An appropriate model complexity needs to be assessed to suit the study purpose, objectives and resources available for a model study. As the complexity of a modelling exercise increases, more accurate field data are required for both input and calibration. This involves consideration of:

- *The model objectives;*
- *The hydrogeological system;*
- *The available data;*
- *The management constraints.*

Table 1 lists typical types of model complexity for some types of model objectives.

Table 1: Appropriate Model Complexity for Differing Model Applications

Model complexity	Examples of types of models	Model purpose and typical characteristics	Examples of model objectives	Typical data requirements
Low	Often analytical equations or models	• Ranking model. • Simple worst case assessment. • Simple systems.	• Rank the relative stream depletion effects of bores adjacent to a surface waterway. • Determine the observation bore network to suit a pumping test. • Determine the preliminary dewatering requirements for an excavation or mine. • Assess the preliminary effects of discharge from wastewater plants or stormwater detection basins.	• Can be completed without detailed site specific data. • Parameters often obtained from literature review. • Requires application of experienced modelling judgement.
Medium	Analytical or numerical models	• Impact assessment model. • A specific question is posed. • Prediction of impacts of proposed development. • Conservative assumptions adopted where data or understanding is lacking, such that model predictions are conservative. • Prediction of contaminant transport.	• Determine dewatering rates for mines, construction, where dewatering cost becomes a significant factor in project viability, etc. • Define well head protection zones. • Determine dispersivities, flow paths, and capture zones for pollutants of groundwater. • 2D determination of heat transfer during injection of warm water.	• Some site specific data required, especially in more developed areas. • Dewatering problems require good data on aquifer geometry and parameters. • Water supply problems require good data on hydrogeological variability. • Contaminant problems requires tracer information and hydrogeological data.

Table 1 (continued)

Model complexity	Examples of types of models	Model purpose and typical characteristics	Examples of model objectives	Typical data requirements
High	Usually requires numerical modelling	• Suitable for predicting the response of a system to changes in hydrologic conditions, where the model has been calibrated to these specific objectives. • Required for reliable water resource allocation and optimisation, incorporating assessment of stream-aquifer interaction, groundwater dependent ecosystems, etc. • Required for complex contaminant tracking and transport modelling (3D).	• Determine sustainable yield of a groundwater system, and define optimal resource allocations and groundwater dependent ecosystem impacts, etc. • Determine the long term water balances and impacts within intensive irrigation areas. • Assess the performance of groundwater interception schemes. • Determines 3D flow paths and travel time for particles in contaminant transport. • 3D determination of heat transfer due to injection of warm or cold water.	Detailed and comprehensive data required, with ongoing monitoring and interpretation.

Adapted from MDBC Modelling guidelines (MDBC, 2000)

3.0 Model Conceptualisation

*"The differences between the geologic reality of heterogeneity and the simplifications that may be used in ground water models make it scientifically dangerous and potentially misleading to blindly apply generic ground water models to any specific hydrogeological situation." (*Water Science and Technology Board, 1990, p2.)

Model conceptualisation comprises four main stages. These are:

- *Site characterisation;*
- *Building a conceptual model;*
- *Choosing the model code;*
- *Discretisation of the data in time and space.*

These stages are all linked, and sometimes combined. For instance the choice of model code can sometimes include decisions on time and space discretisation. Furthermore, the stages are not always undertaken sequentially. Rather, an iterative process can occur, where earlier stages need to be revisited and refined.

There are a number of useful guidelines to assist a modeller develop a site conceptualisation, including STOWA (1999), ASTM (1994 and 1996), Anderson and Woessner (1992), MDBC (2000) and Hill (1998). The important components to be considered from the perspective of a model auditor are discussed below.

3.1 Site Characterisation

Site characterisation is the collection and collation of all available data relating to the aquifer system within which the groundwater problem occurs. At this stage it is important to know the exact nature of the data required in order to solve the problem. Data requirements for specific modelling problems are listed in Appendices A-D.

Site characterisation data involves any data that describe the geological framework in a spatial sense and the hydrogeological framework in a temporal and spatial sense, as listed in Table 2 below. The physical processes involved in the problem are identified at this stage. It is also necessary to collect system observation data, such as water levels, contaminant concentrations and flow rates, which are used as model calibration targets. Additional data, such as which parameters are well known and which are not, and the parameters that are interrelated, are also important to establish an understanding of the system, and for model calibration. It is also important to record details of how the measurements were made, who collected the data, how are measurements that are below detection limits treated, etc. Such details can be important when considering model validity.

Table 2: Site Characterisation Data

Site characterisation data	Additional data	Data collection information
• Boundaries – physical boundaries such as basement rock, or a lake; or flow boundaries such as rivers, drains or the coast. • Spatially varying hydrogeologic properties – transmissivity, storativity and how they vary through the aquifer. • Spatially and temporally varying hydrogeologic properties: flow regime, water balance, recharge/discharge sources and abstraction points, water quality data.	• Measurements (system observations) which will be used for comparison of model results – usually water levels, flows or concentrations and their variation with time. • Knowledge about the parameters – which are well known and which are not precisely known. • Statistical distributions (often only a range) of all parameters. • Relationships between parameters (co-variance) – i.e. rainfall recharge and water levels or recharge events and concentrations etc.	• Where the data is from • Whether the data is in digital form • How to deal with serious outliers • How to deal with missing values • The quality of the data • Who is responsible for the supply of the data

It is necessary to collate and analyse the available data to develop an understanding of the important aspects of the aquifer system, particularly the processes that most significantly control or impact on the groundwater flow system.

Site characterisation can be quite onerous for complex problems. As the associated risk of a model prediction increases, a more thorough site characterisation must be completed. Greater site characterisation requires more field work, including more monitoring wells, groundwater samples, and an increase in the number of laboratory chemical and microbiological determinands, and field parameters.

If there is a lack of data, it is likely that there will also be lack of understanding of aspects of the aquifer flow processes. In this case, the building of a complex model may not be justified. Alternatively, additional field work may be scheduled before a model can be built. Typical data requirements for groundwater models are listed in the following Tables 3a, 3b and 3c.

The key components of a **site characterisation** are:

(i) Data for all the relevant components of the aquifer system

(ii) Description of the mutual relationships between the aquifer system components - some analysis of the site characterisation data to determine the interaction of components of the aquifer system, i.e., a simple linear regression between groundwater levels and stream flows etc.

(iii) The boundaries of the aquifer system to be modelled or the relationships between the aquifer system being modelled and the wider aquifer environment. The system boundaries are the dividing line between the system and wider environment.

A model report should identify the sources of site characterisation data and its meta-data i.e., where the data came from, how and who measures it and the error or uncertainty associated with its measurement.

Table 3a: Site Characterisation Data Requirements – Hydrogeological Framework

Hydrogeological framework data (i.e. spatially varying only)	**Data sources**
• Physical system (geology, topography, surface drainage). • Aquifer extent, boundary types, elevations, thickness, confining beds, bedrock configuration • Aquifer hydraulic and storage parameters and spatial variability (transmissivity, hydraulic conductivity, anisotropy, specific yield, storage coefficient, porosity). • Bore hole locations	• Maps of hydrogeology (often in Regional, District of Unitary Council Resource reports, University research papers and theses,) • Topographical maps showing surface drainage features, and other survey data to specify drainage geometry (extent and elevation). • Bore construction and lithological logs, cross sections, bore completion reports. During installation of a bore, the drilling company completes bore detail records (initial water level, depth drilled, bore depth, screen top and bottom, pump type) that are normally submitted to the local authorities for their database. In commissioning the well, the drawdown and yield is determined, allowing for calculation of the specific capacity of the bore. • Aquifer tests and slug tests are ideally used to determine the hydraulic conductivities and storage characteristics specified in a model. Methods of evaluating aquifer tests are discussed in, for example, Kruseman and de Ridder (1994) and Brooks (1997). Aquifer parameters determined from aquifer tests can differ due to assumptions and limitations of each method. Aquifer tests use theoretically based assumptions that are not always met by the aquifer being tested. Limitations of the constant discharge test are that the aquifer thickness will vary over the test area but the analysis assumes constant thickness and infinite extent. Errors to be considered include barometric pressure, pumping variability, measurement error, precipitation rates and river effect. • Journal and conference papers, student theses. • Regional and City Council databases, Private company reports.

Table 3b: Site Characterisation Data Requirements – Hydrogeological Stresses

Hydrogeological stress data (i.e. varying in time and space)	Data sources
• Sources (e.g. a recharge site) and sinks (e.g. abstraction wells), and data to quantify their effect on drainage features and processes and on flows and aquifer water levels • Natural recharge and discharge areas, rates, patterns and durations • Stream-aquifer interaction • Land uses, irrigation, evapotranspiration, vegetation	• Rainfall and evapotranspiration records and any lysimeter data from natural recharge experiments. This information includes rainfall statistics, and any soil drainage information that relates rainfall on the ground to aquifer recharge. An accurate representation of the rates of groundwater recharge is important in modelling the water budget of an aquifer. Data regarding recharge rates can commonly be obtained from regional authorities or government organisations that have undertaken studies within their area. • Stream flow and level (stage data) records. Surface water flow gauging data, including the identification of areas of loss and gain to rivers from groundwater is required. • Groundwater level data from pumping and observation bores. • Abstractions from groundwater and surface water, including consented quantities and estimates of actual quantities. • Areas irrigated, method and duration of irrigation, crop types and areal distribution. • Projections of growth in demand for water and discharge of wastewater. • Groundwater and surface water quality measurements. • Regional and City Council databases, Private company reports.

Table 3c: Site Characterisation Data Requirements – Additional Contaminant Transport Data

Additional contaminant transport data	Data sources
• Identification of chemicals of concern in contaminant plume and Identification of target concentration. • Location, history and mass loading rate or removal rate for contaminant sources or sinks (such as a reactive barrier). These may vary in time. • Identification of down-gradient receptors. • Direction and rate of contaminant migration (varies in time). • Organic carbon content of strata. • Appropriate geochemical indicator parameters (e.g. dissolved oxygen, Eh, pH). • Distribution coefficients	• Sample analysis or literature values. • Drinking water guidelines, aquatic health guidelines etc. • Site history. • Topographic maps and well location maps. • Sediment and strata analyses. • Water quality analyses at a variety of sampling points, over a representative period of time. • Batch testing

3.2 Conceptual Model

The **conceptual model** describes in words and mathematical equations the key components of an aquifer system. These key components are the boundaries of the model domain area, and within the defined domain, the hydrogeological and physical framework, flow system components and their inter-relationships within this framework. This may be supported by maps, drawings, graphs and diagrams.

The process of building a conceptual model involves taking the site characterisation and applying some simplifying assumptions to it. It is important to consider the effect of these simplifying assumptions.

When determining a conceptual model, simplifying assumptions are necessary, as complete reconstruction of the field system is not feasible, and also there are rarely sufficient data for a comprehensive model. In addition, a complex model can in fact increase the predictive uncertainty of the model. The concept of parsimony is used in modelling, where parsimony means that the best approach is the simplest that fits the purpose of the application. So only the essential features that are important to the resulting decision, or design, should be included in a model, so that it has only as much complexity as is necessary.

The assumptions made at this stage of the modelling project are carried throughout the modelling project, so it is important that they are correct. Anderson and Woessner (1992) report that one of the main causes of discrepancies between the model predictions and the actual measured responses found after the event relate to an inaccurate conceptual model which is either invalid or incomplete. Other key inaccuracies are the assumed future stresses such as pumping and recharge rates.

Consideration of appropriate assumptions is based on answering a number of questions. For instance, the location of a stream and details of its flow, as noted in the site characterisation, must now be described in terms of the following questions (Note that the answers to these questions may require some further analysis.):

- *Is the stream in hydraulic connection with the aquifer?*
- *If the stream is in hydraulic connection with the aquifer, does the stream lose water or gain water from the aquifer, or both?*
- *Does the stage height of the stream vary significantly with time?*

The answers to these questions determine the form the stream will take as a model input. For example, where stream flows themselves are not being investigated by the model, the stream can be represented either as a recharge flow boundary, or as a constant head or general head boundary. Where the stream flows are being assessed in the model, the stream can be represented either as a drain (if the stream is only gaining water); or as a stream, if the stream is both losing or gaining water.

It is important to consider whether the conceptual model formed is the best one, given the problem, the model objectives, and the available data and techniques. This can best be determined by comparing the concepts with one another in an experimental manner, (i.e. make and compare the model with the various concepts and compare the results). Alternatively, a panel of experts could discuss the conceptual model at a meeting or workshop. Both options are time consuming. However, for complicated problems this step is useful. Where conflicts are found it may be important to revisit the site characterisation stage and gather more data.

3.2.1 Model Boundaries

Model boundaries describe the interface between the model domain and the surrounding environment, and are ideally based on actual physical or hydraulic boundaries. Whenever possible the natural hydrogeologic boundaries of the system should be used as model boundaries. Physical boundaries usually relate to the presence of an impermeable geological formation or a large body of surface water. (An impermeable boundary typically forms the lower and/or lateral boundaries of modelled systems. Anderson and Woessner, (1992) suggest a two order of magnitude contrast in hydraulic conductivity is sufficient for a physical boundary). Hydraulic boundaries occur as a result of hydrologic conditions, such as groundwater divides and streamlines, although these features are not permanent and may shift their location and magnitude (of flux or head). A careful assessment of the validity and stability of the hydraulic boundary during the model period must be made.

There are three major types of model boundary conditions, all of which may vary with time, as described in Table 4 below. Boundary conditions are located and oriented consistent with the physical and, or hydraulic features they represent. Table 4 below details boundary types.

Incorrect model boundary selection can compromise the validity of the entire modelling project. Ideally, model domain boundaries should be set far from the area of interest (e.g. a water supply bore field) so that the imposed stresses at the area of interest do not reach the boundaries. This is because many of the boundary conditions are approximate and can only be considered realistic when they are some distance from the area of interest. For example, when modelling drawdown effects, locating a constant head boundary within the extent of the drawdown cone will constrain the predicted drawdown. Sometimes it is not possible to locate boundaries far from the area of interest and in this case it is important that the simulated boundary effect is realistic.

A model report should document the type and location of boundaries, and explain the physical basis of the boundary.

3.2.2 Hydrogeological Framework

The use of geological maps, cross sections and bore logs combined with hydrogeologic properties, such as porosity and hydraulic conductivity, allows hydro-stratigraphic units to be defined, i.e. units with similar hydraulic properties. This information allows the strata data to be summarised as either an aquifer or a confining unit or layer (or something between the two). The extent and top and bottom elevations of these layers also need to be defined.

In addition, maps showing depth to water and the distribution of hydraulic conductivity and storativity characteristics for aquifers, aquitards and stream and lake bed sediments (defined on the basis of pumping tests and/or previous modelling studies) are used.

A model report should document the extent and depth ranges of these aquifer and confining layers, and explain the basis for these groupings. This will always include hydraulic conductivity similarity. The report should also include maps showing the distribution of aquifer parameters.

Table 4: Types of Boundary Conditions

Boundary Type	Description	Common Applications	Comments	Effects of boundary conditions
Specified Head	The head value is specified and the model calculates flow across the boundary to or from the model domain.	Rivers, lakes, coastlines, groundwater divides, known pumping water levels in bores, dewatering targets.	Commonly used because head data are easier to measure than flow data. A specified head allows an inexhaustible amount of water flow (calculated by the model) into or out of the model.	Models using this condition are the easiest to solve. However these boundaries constrain the solution to the greatest degree and can artificially constrain the solution to too great a degree.
Specified flow	The flow is specified and the model calculates the head at the boundary.	Impermeable boundary, groundwater divide or streamline, infiltration source, lateral inflow or outflow, evaporation sink, other known sink or source fluxes (e.g. leakage to or from an adjacent aquifer or pumping bore).	The 'no flow' boundary is a special version of the specified flow boundary, and is the most commonly used boundary, especially to define low permeability formations adjacent to or underlying aquifers or for stream lines (flow directions transverse to groundwater level contours).	Moderately difficult to solve, and involves moderate constraints on solution.
Head dependent flow	The model calculates the flow for the given head.	Leaky rivers, drains, flow to or from adjacent aquifers, basement leakage, springs (including general head boundaries).	Care is required in some cases, as the model – calculated flow is subject to a conductance parameter, which may need to vary with time, and this may violate some calibration assumptions.	Most difficult to solve, and involves the least constraints on the solution. Can form a very complex and sensitive boundary condition.

Adapted from MDBC (2000).

3.2.3 Hydrogeological Flow System

Piezometric maps are used to show groundwater flow direction, and the presence of recharge and discharge areas.

Hydrographs of water levels and stream levels and discharge rates are used to show the transient responses of these resource components to changes in recharge or discharge rates. Relationships between these components, such as between recharge and water levels or recharge and concentrations, are shown using plots, or statistical relationships such as linear regression analyses, etc.

Spatial and temporal distributions of rates of evapotranspiration, groundwater recharge and pumping, and surface-groundwater interaction may be required of the model.

These data are used to define a water balance for the aquifer systems. A water budget is prepared for the entire model area, (and can also be subdivided into smaller areas of greater complexity) where the differences between model inputs and outputs are equal to the changes in storage of the aquifer (as shown by the groundwater hydrographs).

A model report should describe the water balance in terms of the input and output flows of the aquifer system, and where applicable, changes in storage that occur when inputs and outputs to the system are not equal. The water balance can be broken down into sub-areas if the model area is large. The significant processes that drive the flow system should be identified, and any plots or statistical relationships that support this should also be included in the report.

3.2.4 Simplifying Assumptions

Simplifying assumptions introduce a bias into the model and its prediction, e.g. by fixing a parameter as a constant value, rather than a spatially or temporally variable one. These assumptions impose a bias on the parameters that calibrate the model. For example, a dispersivity value derived from tracer test data from a heterogeneous aquifer calibrated to a model which assumes aquifer homogeneity may give a lower dispersivity term than if a model representing the aquifer heterogeneity is used in the parameter determination. So, oversimplifying the essential features of an aquifer system by using too simple a model can introduce a bias into the model which in turn affects its parameterisation and predictions. It is important to consider whether the bias will significantly under- or overestimate the model predictions. Minimising simplifying assumptions in a model brings with it another problem in that the greater the model parameterisation, the greater the degree of predictive uncertainty associated with a model. Therefore, when considering simplifying assumptions for a model, there is a trade off to be made in terms of model bias and model predictive uncertainty.

How these assumptions impact on the question at hand needs to be considered e.g., a steady-state model used to represent a stormwater discharge could be extremely conservative. Alternatively, a simple steady-state model may be satisfactory, where the conservative case demonstrates that no adverse effects will occur. Another example where a model could be misleadingly conservative would be using a contaminant

transport model that assumes no adsorption or decay for a contaminant that is readily adsorbed or biodegraded.

Some other typical questions to ask when considering whether simplifying assumptions are appropriate in a conceptual model are:

- Can the groundwater flow or contaminant transport be characterised as one-, two- or three dimensional?
- Is the aquifer system composed of more than one aquifer, and is vertical flow between aquifers important?
- Is there recharge to the aquifer by precipitation or leakage from a river, drain, lake or infiltration pond?
- Is groundwater leaving the aquifer by seepage to a river or lake, flow to a drain, or extraction by a well?
- Does it appear that the aquifer hydrogeological characteristics remain relatively uniform, or do geologic data show considerable variation over the site?
- Do groundwater flow or contaminant source conditions remain constant, or do they change with time?
- Are the receptors located generally down-gradient of the contaminant plume?
- Are geochemical reactions taking place in the groundwater, and are the processes / reactions / geochemical conditions understood?

Other questions related to site specific conditions may also be asked. A list of relevant questions to ask specific to model types and how these relate to model assumptions are included in Appendices A – D.

The report should list the **simplifying model assumptions** used and discuss the impacts the assumptions are likely to have on the model predictions.

The following two sections “Discretisation in Space and Time”, and “Choice of Model Code” contain tasks that are closely related and interdependent. Although the Discretisation in Space and Time is described first, it will almost certainly have to be revisited after the Choice of Model Code has been made.

3.3 Discretisation in Space and Time

Discretisation choices determine where and when the model solutions will be calculated. Choosing an appropriate model time discretisation may affect which model is chosen and is based on consideration of the following questions:

- *Is the problem of concern a long term or short term effect?*
- *Is understanding of the development of the effect important?*
- *Does the proposed model stress, for example the pump rate or discharge rate, change with time?*

Time discretisation when only the magnitude of the effect is important

Where only long term effects are important, a steady state model can be used. A steady-state model assumes that the stresses have continued for so long that the aquifer system can be considered to be in equilibrium with the model stress.

Alternatively, if the model stress occurs for an insignificantly short time, a solution based on a singular stress being introduced instantaneously may be used (such as in a slug test or a tracer test).

Time discretisation when the magnitude and timing of the effect is important

For situations where the proposed model stresses are varying with time, the time discretisation needs to be consistent with these stress periods.

Where the time varying response of an aquifer to a stress is important, the time discretisation needs to be consistent with the detail required. For example, if it is important to establish the time of peak concentration in a down-gradient well, resulting from a short term discharge, time discretisation will be based on groundwater velocity.

Spatial discretisation

Numerical models are of two types, finite difference and finite element. In finite difference numerical models, the model domain is split up into a rectangular grid of rows, columns and layers. This produces model cells within which an average solution is calculated for each cell. Finite element models allow for more irregular shaped areas, where the model domain can be split up into irregular shaped elements and the solution is calculated for each element. In either model type the model grid must be sufficiently small in the area of interest or where steep hydraulic gradients will occur (e.g., around a seepage face, a drain, or pumping wells) to accurately represent local variations in soil properties, hydraulic head and groundwater concentrations.

Model conceptualisation summary

In terms of reporting, the Model conceptualisation section of the report depicts all parameters that were used to choose and develop the calibrated model. This report section should emphasise the rationale for modelled parameter values. Data gaps, anomalies, or uncertainties should be discussed. Input parameters include the following:

- Model grid size and spacing
- Layer elevations †
- Boundary conditions †
- Hydraulic Conductivity/Transmissivity †
- Recharge
- Any additional model input †
- Transient or steady state modelling
- Dispersion coefficients †
- Degradation rate coefficients †

† Requires values for each model layer

Finally, the modeller must clearly show how the spatial and temporal resolution and discretisation has been achieved.

3.4 Choice of Model Code

Once appropriate model assumptions and a first attempt at discretisation in space and time have been carried out, a model code consistent with these assumptions is selected. If necessary new software can be developed though this is generally not advisable unless you have sufficient expertise and there is really no other option.

If a number of modelling codes are all equally appropriate in terms of the model assumptions for the problem at hand, then the decision comes down to the following:

- *available hardware capabilities;*
- *available software;*
- *available expertise;*
- *available time;*
- *modeller's preference; and*
- *client's wishes.*

The guidelines do not specifically prescribe the type of modelling that should be carried out, as this needs to be evaluated on a case by case basis. Instead the assumptions inherent in different modelling algorithms are detailed in Appendices A – D. Models are grouped on the basis of the assumptions used, rather than discussing each individual model. Examples of situations where these assumptions would and would not apply are included. The implication of each individual assumption in the model not being consistent with the real hydrogeology is outlined where possible. Table 5 on the following page can be used as a general guide for assessing the appropriateness of a model.

Once the choice of model code has been made, a further iteration of discretisation in space and time will undoubtedly be necessary.

Table 5: Model Code Applicability

Model code groupings	Situations where generally appropriate
Analytical models	Field data show that groundwater flow or transport processes are relatively simple.
A one-dimensional groundwater flow or transport model	Initial assessments where the degree of aquifer heterogeneity or anisotropy is not known.
Two-dimensional models	• Those sites that have one or more groundwater sources/sinks (e.g. pumping or injection well, drain, river, etc.). • Those sites where the direction of groundwater flow is obviously in two dimensions (e.g. radial flow to a well or a single aquifer with relatively small vertical hydraulic head or contaminant concentration gradients). • Sites in which the aquifer has distinct variations in its hydraulic properties. • Sites where the impacts of transverse dispersion are important.
Three-dimensional flow and transport models	• Sites where the hydrogeologic conditions are well known. • Sites with multiple aquifers present, or the vertical movement of groundwater or contaminants is important.

3.5 What Can Go Wrong in Model Conceptualisation

Errors can be generated through inappropriate model design, selection of conditions, lack of information and oversimplification. Some examples of errors and pitfalls resulting from incorrect conceptualisation of a groundwater model are shown on the following pages in Table 6.

3.6 The Importance of Groundwater Monitoring

Groundwater monitoring is important to determine the performance of groundwater model predictions, such as future changes in hydraulic heads or the migration pathway and concentrations of contaminants or heat flux in groundwater. Field observation and monitoring should be included in all management and planning programs. The model may be revisited and refined on the basis of groundwater monitoring.

The degree of monitoring should be based on the level of confidence needed and model predictions. One must not solely rely on model predictions for management and planning decisions.

Table 6: Pitfalls in Conceptual Modelling and the Consequences

Conceptual stage	Pitfalls – comments, consequences and errors
Discretisation	
Grid/mesh design	Does design meet guidelines regarding maximum rate of change in cell dimension?
x, y, z restrictions	Limits results, may have a bearing on boundary conditions
Binding of layers together	Limit simulation of flow fields for individual layers
Excessive discretisation - i.e. excessive number of hydraulic conductivity zones with no physical basis.	A firm physical basis (aquifer tests and geological characterisations) is needed when assigning hydraulic conductivity zones. Assigning hydraulic conductivity zones solely to improve calibration is not justified and a large number of hydraulic conductivity zones generally indicates over-calibration, a lack of site-specific data, or a lack of understanding of groundwater modelling data requirements. (DEQ, 2001)
Hydraulic blockages/fractures	Results are representative of the large-scale, bulk material only. Misinterpretation of system detail, presence of faults.
Time steps	Are time steps sufficiently small? For transient models, are initial conditions appropriate?
Inputs	
Wellhead protection area delineations: pumping rate does not represent average day, peak month pumping rate.	The pumping rate for an average day of the month with the highest demand is usually used for the modelled pumping rate specified for wellhead protection delineations (DEQ, 2001).
Well not specified correctly - i.e. well screen assigned incorrectly, pumping schedule not accurate, pumping rate not appropriate for problem.	The well parameters must be specific, especially screen length, for accurate modelling. In a case where no screen has been defined the model may be very distorted in order to get the model to "work properly' (DEQ, 2001). Pumping rates need to be specified to represent the actual conditions.
Incorrect sign for pumping or recharge.	It is common practice to express pumping rates as a negative value, and injection and recharge as positive values in groundwater modelling programs (DEQ, 2001).

Table 6 (continued)

Conceptual stage	Pitfalls – comments, consequences and errors
Using interpolated input data.	Interpolated data must be viewed with caution and scientific judgement used when applying the results. For example, the up-gradient narrowing of a wellhead protection area delineation is generally an artefact of an interpolated potentiometric surface. Therefore, it is completely acceptable to allow for the uncertainty relating to this interpolation by either defining the maximum width of the delineation as a constant width (DEQ, 2001) or a constant angle of safety either side of the groundwater flow direction.
Aquifer stresses (pumping, recharge, evapotranspiration, etc.) not specified over entire transient simulation period.	Increased opportunities for mistakes may arise with the added complexity of transient models and can also mask data input errors, such as failing to define pumping rates, recharge rates, river stages, etc. for the full time period (DEQ, 2001). Therefore, it is important for the model auditor to understand what the results mean and if they make sense. For example, the results indicate water mining beginning after six years of a 10-year simulation period. Therefore, it is advisable to check that the recharge rates were defined for years 6 through 10. (DEQ, 2001)
Inconsistent parameter units - i.e. days and seconds, gallon per minute and cubic feet per day.	It is important to use consistent units when modelling. Inaccuracies can occur easily if the same units are not used. For example, days are selected for the time unit and feet for the length unit, then recharge and hydraulic conductivity must be in feet per day, pumping rates must be in cubic feet per day, constant head boundaries and grid dimensions must be in feet, etc. (DEQ, 2001).
Model parameterisation assumptions	
Density assumptions	Incorrect flow direction and calibration constants. This is especially significant in contaminant and pollution modelling. Typically a constant density is assumed.
Heterogeneity assumptions	This affects travelling time and breakthrough curves in both saturated and unsaturated strata.
Geo-hydrochemical process assumptions	This relates to assumptions regarding sorption, decomposition, geochemical reactions, organics in the system.
Unsaturated flow assumptions	In reality hysterisis (or residual water rententivity) is not taken into account. However this would be important if considering a hydrocarbon mass flux of a contaminant entering groundwater etc.

Table 6 (continued)

Conceptual stage	Pitfalls – comments, consequences and errors
Mass input assumptions	In some cases the model input requires additional assumptions which may not be compatible with the conceptual model, thus requiring an additional calculation. For example some models require the contaminant source flux to be defined in terms of a groundwater concentration. If the contaminant source is from above ground, and no groundwater concentration measurements are available (such as for a predictive model) – the modeller must (I) assume an aquifer depth that the source has fully mixed with, AND (ii) if the flow of the contaminant source is significant compared to the groundwater flow, the modeller must account for the increased flow of groundwater in the aquifer.
Lack of understanding of site hydrogeological processes - i.e. excessive recharge, aquifer thickness/permeability not known, fully penetrating streams, isotropic/homogenous conditions.	Field observations are required to define the hydrogeological characteristics of a site, before the site can be accurately modelled (DEQ, 2001). There must be some physical justification for use of model parameters, and spatial variations of them for calibration purposes. In cases such as recharge and effective porosity, textbook values can be used conservatively (DEQ, 2001). Each discrete unit is attributed values for all parameters, therefore there is a need to decrease the degrees of freedom by zoning parameters. The pitfall of this method is that the scale in which the model parameters are given are not in keeping with discretisation (STOWA, 1999). Point data are scaled to "block effective" and this can affect the sensitivity to heterogeneities (STOWA, 1999).
Boundaries	
Lack of far-field data	There needs to be a valid basis for specifying boundary conditions and parameters in modelled areas outlying the area of interest (DEQ, 2001). Have the boundary conditions been adequately described, and are they justified? The area (and therefore the boundary conditions) need to be large enough not to distort the aquifer's response to stresses in the area of interest and if there is insufficient far-field data then the effect of assumed conditions on model response must be evaluated (DEQ, 2001).
Closure criteria	Have closure criteria used for stopping the model been appropriately defined and achieved?
Placing model boundaries too close to area of interest, which may include pumping centre.	DEQ (2001) recommended checking the reasonableness of the flow through any suspicious boundary zone as it is not possible to quantify if a model boundary is "too close" to the area of interest, thereby inhibiting the response to stresses by the aquifer.

Table 6 (continued)

Conceptual stage	Pitfalls – comments, consequences and errors
Model code	
Oversimplification of problem - i.e. 2D model when obviously 3D flow.	The appropriate dimension should be used during modelling. Problems where groundwater flow is in 2D, such as radial flow, should be modelled in 2D. In situations of multiple aquifers or where vertical flow occurs, a 3D model is more appropriate (DEQ, 2001).
Inappropriate model code selection.	Model selection depends upon the modelling objectives and the hydrogeological conditions of the site. It is inappropriate to attempt to define the optimum placement and pumping rate for an extraction well and monitoring system with a simple model incapable of representing known hydrogeological features of a complex site, such as rivers, lakes, variable aquifer thickness or hydraulic conductivity, 3-D groundwater flow, or multiple aquifers. Conversely, wellhead protection areas are frequently delineated by reverse particle tracking on a confirmed potentiometric surface. A buffer area to account for dispersion processes and other uncertainties is often added to the final delineation. In these cases, use of a MODFLOW-based model may significantly increase data requirements, modelling effort, and cost without a proportional improvement in delineation accuracy.
Water balances	Errors propagated later through the model.

4.0 Calibration

'It is the mark of an instructed mind to rest satisfied with the degree of precision which the nature of the subject permits and not to seek an exactness where only an approximation of the truth is possible.'
Aristotle

Model calibration solves a problem inversely by adjusting the unknowns (e.g. aquifer parameters and rainfall recharge) until the solution matches the knowns (e.g. water levels). When a model has been calibrated it shows that the model can reproduce the behaviour of the aquifer system under a certain set of conditions. The smaller the deviation between calibrated model results and the field observations the better the model. The calibration process lessens the range of uncertainty associated with model predictions.

Model calibration consists of changing model input parameter values, within realistic limits, in an attempt to match field conditions. Data describing field conditions may consist of measured hydraulic heads, groundwater or stream flow rates, or contaminant plume migration rates. Model calibration requires that field conditions at a site are properly characterised, such that the model can be calibrated to a set of conditions that are representative of actual field conditions. Therefore, it should be appreciated that calibration should only be undertaken by those who understand the entire modelling process. In an ideal situation, when a model is calibrated there should be some prior assessment of the degree of fit required. In reality, calibration can be subjective, and will in part be dependent on the quality of data used in the model.

If calibration of a model is not carried out the range of possible model predictions is much greater than when a model is calibrated. This may reduce the usefulness of the model . However, an uncalibrated model is a useful tool in cases where a rapid modelling assessment is required to confirm that, despite worst case assumptions, an effect would be minor. In such a case it is important to provide information that demonstrates, the 'reasonableness' of the model output. Typically models that are not calibrated may be used for initial assessments, as a screening tool or for guiding data collection activities.

For calibration to be meaningful or valid requires a degree of rigour. As with site characterisation, a number of authors provide guidelines for model calibration, most notably, ASTM (1994 and 1996), Anderson and Woessner (1992), and Hill (1998). The process is discussed here from the model audit perspective.

Before starting the calibration stage it is important to determine the acceptable goodness of fit otherwise the calibration process could be deemed to be subjective.. Typically the following data types are used as calibration targets, as shown in Table 7.

Table 7: Calibration Targets

Data type	Source
Hydraulic head data	Water level time series and drawdown curves
Hydraulic head gradients (groundwater flow directions)	As shown by piezometric contours and calculations of vertical gradients from a multi-level piezometer system, or a compact well field containing wells of differing depths.
Water balance information	Stream or river flow loss data, or drain flow data
Contaminant concentrations	Contaminant migration rates, contaminant migration directions, plume dimensions, contaminant breakthrough curves
Established relationships between these data types	River flow and groundwater levels or groundwater levels and concentration values.

The use of multiple types of data for model calibration is advocated. A model calibrated with hydraulic head, changes in surface flow and travel time data is more reliable than one calibrated by hydraulic head alone. The more data involved in the model calibration, the more the model is constrained by what is known of the hydrogeology of the system.

The calibration process typically involves a steady-state and transient simulation. Steady-state conditions are where the aquifer system is considered to be in equilibrium and the model is calibrated to a set of spatial hydraulic head or contaminant concentration data that represents this equilibrium condition. Steady-state conditions are either represented by a long term average hydrological balance or conditions where aquifer storage changes are not significant (e.g. insignificant ground water level fluctuations). In contrast, transient simulations involve the changes in systems such as hydraulic head or contaminant concentrations with time.

Even when developing a transient model, initially it is common practice to calibrate the model to steady-state conditions to develop a broad hydraulic conductivity distribution. This is because aquifer storage effects are not involved in the steady-state calibration process. Transient models may be calibrated without first simulating steady-state flow conditions, but not without some difficulty.

4.1 Parameterisation

Model calibration requires the trial and error of many different combinations of model inputs. Usually there is a large number of parameters in a model which may or may not be spatially distributed and/or

correlated. In most cases, the amount of field data does not permit all parameter values to be optimised and so the modeller must reduce them. This is done in a number of ways including:

- Sensitivity analysis;
- Zonation on the basis of geological and hydrogeological maps;
- Zonation based on geostatistical relationships between parameters.

Sensitivity analysis

Sensitivity analyses are carried out for both analytical and numerical models. Model sensitivity analysis identifies the parameters that are most important for model reliability by varying model input parameters over a reasonable range (usually this is the range of uncertainty in value of the model parameter) and observing the relative change in model response. Its purpose is to identify those parameters which are most important in determining aquifer behaviour. Priorities can then be set by ranking the key parameters in order of importance to reduce model uncertainty.

A sensitivity analysis can also be used to provide a focus for later field investigations and monitoring.

Where model calibration is maintained throughout the sensitivity analysis, it can indicate the likely error range in the model output. The process in this case is called predictive uncertainty analysis (see Section 5). It is important to note that this is only true when calibrated conditions are maintained.

Zheng and Bennett (1995), discuss sensitivity analyses in some depth and should be referred to for more information.

Zonation on the basis of geological maps

Zonation is carried out for numerical models, essentially defining areas where one or more parameters are assumed to be constant. This is usually based on areas of similar geology and hydrogeology. Typically, zonation is carried out for hydraulic conductivity, storativity and porosity parameters. The calibration process adjusts the parameter value for each of these zones until the fit between model outcomes and field observations is as good as possible. If the match between modelled and measured values obtained on the basis of geology/hydrogeology based zones is not good enough, then extra zones are introduced into the model domain at locations where the modeller feels they will do the most good, although this process of inserting extra zones is somewhat subjective.

Zonation on the basis of geostatistical relationships

Zonation can also be based on geostatistical methods to interpolate between the points where aquifer parameters have been measured with confidence. The most popular method used is kriging, which is a statistical method used for spatial interpolation that chooses the best linear unbiased estimate for the variable in question. The variable is assumed to be a random function whose spatial correlation structure is defined by a variogram. A variogram is a measure of the change in the variable with changes in location. Clearly, a higher correlation between measured and calculated values is expected for smaller distances between those points.

Kriging provides an estimate of the interpolation error in the form of the standard deviation of the kriged values, which is useful when considering the reasonableness of parameters. Unlike some other spatial interpolation methods, kriging preserves the field value at measuring points.

4.2 Calibration Techniques

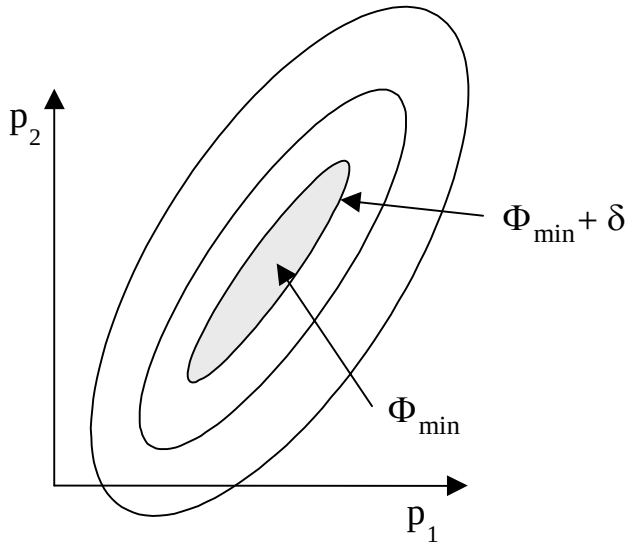
The success of model calibration is measured in both quantitative (statistical) terms and qualitative (pattern matching) terms. Qualitative assessment of calibration is commonly undertaken by comparing patterns such as piezometric contours showing groundwater flow. Quantitative measures usually involve mathematical and graphical comparisons between measured and simulated heads, flows or concentrations and the calculation of statistics regarding residuals (i.e., the difference between the measured and simulated heads, flows or concentrations). The relationship that describes these residuals is called the objective function. The objective function can be mathematically formulated and expressed in a number of ways. Its most simple and commonly used forms are one of the following single figure values:

- The relative error;
- The average value of the residual error;
- The maximum residual error;
- The sum of the squared residuals.

Where a number of differing types of parameters and/or variables are used to determine the objective function, weighting of the various terms can be undertaken to emphasise certain aspects of the system to a greater or lesser extent. Figure 3 shows an example of how the objective function may vary with varying combinations of two parameter values.

Calibration can be undertaken either manually or it can be automated, or the two techniques can also be combined.

Figure 3: Objective Function Contours in Parameter Space; Linear Model, where p_1 and p_2 define



terms associated with two parameters. (reproduced from PEST Manual, Doherty, 2000)

Trial and error calibration

In trial and error calibration, initial parameter values are adjusted in sequential model runs to match the calibration targets. This process is influenced by the expertise and bias of the modeller, and is labour intensive. Those in favour of manual optimisation point out that the modeller gains greater feeling for the characteristics of the model, and is able to use unquantifiable information. However, although an experienced modeller can achieve good results, the approach is not particularly reproducible. In addition, it seldom results in the true optimum of the objective function being obtained.

Because of the shortcomings of manual optimisation, there is currently a trend away from manual 'trial and error' towards automated calibration.

Automatic optimisation

Automatic optimisation is similar to the trial and error method in that model simulations are repeated each time a parameter is altered. However, the automatic optimisation code automatically checks the match between model outputs and field data and adjusts the parameters in a systematic way to minimise an objective function.

A significant advantage of automatic optimisation is that many methods also generate information on the reliability (uncertainty) of the model. This information is then used in the uncertainty analysis. However, one disadvantage of automatic optimisation is the blind trust that is inherent in the method without incurring the benefits of the 'hands-on' approach.

A useful recent development for models with spatially varying parameters is the new PEST-Advanced spatial parameterisation software which allows a model to be calibrated on the basis of pilot points (Doherty, in prep.). Parameter 'pilot points' are assigned on the basis of kriging and are located in the predefined zone areas. This allows the automatic optimisation to employ both the prior geological knowledge that defined the zones and the geostatistical relationships between data to determine the optimum parameter distribution that minimises the objective function.

A model report should include maps, tables and graphs showing the comparisons between field and model simulations achieved through the calibration process. These should emphasise the limitations of the calibrated model. Professional judgement is required by each modeller and model reviewer when evaluating the calibration results. There are no universally-accepted calibration criteria that apply in all cases, therefore it is important that the modeller makes every attempt to minimise the difference between model simulated and field conditions.

It is important to appreciate that automatic optimisation or calibration cannot take into consideration the conceptual basis of flow systems or contamination. Experience has shown that automatic calibration will sometimes produce solutions that are erroneous or misleading.

4.3 Model Verification

The terms 'verification' and 'validation' are not used in this report to imply that a model is completely robust (cf. Konikow and Bredehoeft 1992). The common test of model verification or model validation requires splitting the calibration data set into two, or better, to use completely independent data. In the former method, the model is calibrated to the first part of the data set. The calibrated model is then run in predictive mode to check whether the prediction reasonably matches the observations of the reserved data set, that was excluded from the initial calibration. The process of model verification may result in further calibration refinement of the model. After the model has successfully reproduced measured changes in field conditions, it is ready for predictive simulations and predictive uncertainty analysis.

4.4 Analysing the Calibration

Both the quantitative and qualitative measures must be met if a reasonable calibration has been achieved. These measures are summarised in Table 8 below. The deviations between the model results and the field observations can be due to conceptual errors, parameter values and their uncertainties, measuring errors of field data and errors in assumptions and stresses in the model.

A model may still be used even where it has not been calibrated acceptably as long as the uncertainty surrounding any of the model predictions is rigorously analysed. This will ensure that the model is not afforded too much confidence.

Table 8: Criteria for Calibration

Quantitative performance measures	**Criterion**
Water balance and mass balance (for numerical models.	A numerical model output always includes a water balance for flow models, and also a mass balance for contaminant transport models. The discrepancy between inputs and outputs should be less than 1% (and must be no greater than 2%) to ensure that the model calibration is not numerically unstable (for each stress period and cumulatively for the entire model), (MDBC 2000).
Iteration criterion. The calculated error term is the maximum change in heads (for each node or cell) between successive iterations of the model.	The iteration convergence criterion should be one to two orders of magnitude smaller than the level of accuracy required in the model outputs, i.e. heads, concentrations, flows etc.
The objective function (statistical measures of differences between modelled and measured head data).	This should be a minimum and, ideally, defined prior to calibration, otherwise calibration is subjective. Refer to Table 9 for list of residual head statistics criteria.
Residual errors should be random.	Mathematical and graphical comparisons of measured and simulated water levels, flows, concentrations etc. should be checked to see that the errors are random. If it appears that there may be non-random systematic error - the model conceptualisation should be revisited.
Qualitative performance measures	**Criterion**
Match to piezometric pattern.	Subjective assessment of goodness of fit
Match to contaminant breakthrough curves – peak concentration and time to peak.	Subjective assessment of goodness of fit
Match to hydrographs.	Subjective assessment of goodness of fit
Distribution of aquifer properties.	Subjective assessment of reasonableness, given hydrogeological knowledge, measured ranges of values and associated non–uniqueness of values.

Table 9: Quantitative calibration criteria

Description of measure	Equation	Comment
Residual	$R_i = H_i - h_i$ where: R_i = residual H_i = measured head at location i h_i = modelled head at location i	The smaller the residual the better the calibration.
Mean error (ME)	$\frac{1}{n}\sum_{i=1}^{n}(H_i - h_i)$	A mean error incorporates both negative and positive residuals. Therefore a small mean error may not indicate a good calibration.
Mean absolute error (MAE)	$\frac{1}{n}\sum_{i=1}^{n}\lvert H_i - h_i\rvert$	A small MAE may indicate a good calibration.
Root mean squared error (RMS)	$\frac{1}{n}\sum_{i=1}^{n}\sqrt{(H_i - h_i)^2}$	A small RMS may indicate a good calibration.
Sum of residuals	$\sum_{i=1}^{n} W_i\lvert H_i - h_i\rvert$ where: W_i = weighting from 0 to 1	Useful for comparing successive model runs. The measure is dependent on sample size. Weights are used to emphasise more or less reliable data, change the emphasis of a specific parameter or area.
Correlation function – R	$\frac{\sum(h_i - \bar{h})(H_i - \bar{H})}{\sqrt{\sum(h_i - \bar{h})^2}\sqrt{(H_i - \bar{H})^2}}$ where: $\bar{h}$ and $\bar{H}$ are the average of the modelled and measured heads respectively	May tend to one for perfect calibrations.

Table 9 (Continued)

R^2	$\frac{\sum_{i=1}^{n} W_i\left(H_i - \overline{H}\right)^2}{\sum_{i=1}^{n} W_i\left(h_i - \overline{H}\right)^2}$ where : $\overline{h}$ and $\overline{H}$ are the average of the modelled and measured heads respectively	May tend to one for perfect calibrations
Weighted least squares – S(b) – used to describe parameter estimation	$(H - h(b))^T \underline{w} (H - h(b))$ where : b = vector containing parameter estimates h(b) = matrix of modelled heads which is a function H = matrix of measured heads	This is a matrix function, is used in parameter estimation software.
Maximum likelihood – S'(b)	$(ND + NPR)\ln 2\pi - \ln\lvert\underline{w}\rvert + (H - h(b))^T \underline{w} (H - h(b))$ where : ND = number of observations NPR = number of prior information values $\lvert\underline{w}\rvert$ = determinant of the weight matrix	This is a matrix function, is used in parameter estimation software.

Note 1: In Table 9, heads have been used to represent the observations for comparison with model output. However, other measurements such as flows could be used in the above equations.

Note 2: In Table 9 (and companion tables in Appendices A-D) it is noteworthy that 'good' correlation coefficients and similar measures of quantitative calibration criteria are not necessarily incontrovertible indicators of a 'good' model (see, for example Konikow and Bredehoeft 1992).

4.5 The Non-Uniqueness Problem and what can be done about it

As discussed at the start of these guidelines, groundwater flow and transport models are typically non-unique and therefore contain an inherent uncertainty, i.e. when a model is calibrated to measured data, there is always a range of combinations of possible inputs that allow adequate reproduction of these data. This is shown in Figure 3 which depicts a situation where there is a high degree of parameter correlation – that is, one parameter can be varied in harmony with another with virtually no effect on the objective function. Thus the solution to the inverse problem (i.e. the model calibration problem) is non-unique.

It is important to understand that a well calibrated model, with a good fit between field data and model simulations is not a guarantee of a 'good' model. Calibration only constrains the range of what could possibly occur given appropriate model parameter ranges, it does not give 'the right answer'. Furthermore, the uncertainty of model predictions increases when the model is used to consider situations that are not represented in the calibration data. The section on predictions and predictive uncertainty discusses this issue further, and outlines methods to address predictive uncertainty.

4.6 Calibration Errors

Common calibration errors are outlined in Table 10 as follows.

Table 10: Calibration Errors

Calibration targets	
Target wells clustered in a small portion of the model (i.e. lack of far field calibration data).	Calibration statistics are meaningful to the entire model only when target wells are distributed over the majority of the model domain (DEQ, 2001).
Target wells too close to, or within, specified head boundaries .	If a target well is too close to, or within, specified head boundaries, the aquifer's response at the well to stresses will be artificially limited by the boundary (DEQ, 2001). Target wells should be distributed over the model domain and generally away from the constraints of specified head boundaries such as flowing rivers(DEQ, 2001).
Solver/numerical instability	
Misinterpreting mass balance information.	The mass balance report includes statistics on the percent discrepancy between water added to the model and water removed from the model (DEQ, 2001). The solver used within the model will always attempt to minimise this discrepancy. Thus this is an indicator of solver accuracy for the specified model inputs, but cannot indicate how well the model replicates the hydrogeological characteristics of the site (DEQ, 2001).

Table 10 (Continued)

Forcing fit to unsuitable calibration targets	
Forcing questionable data to fit.	Scientific judgement is needed when using data that have been forced to fit, such as when a hydraulic head contour is forced to make a sharp turn to fit an observation at a single well, that observation may not be accurate (DEQ, 2001). Similarly, if early-time aquifer test data do not fit a curve, chances are the pump had not settled down, there was some well bore storage, or something similar that caused the discrepancy (DEQ, 2001).
Forcing a fit: using unrealistic data values or over-discretizing an aquifer or aquitard layer.	If the model can only achieve reasonable calibration statistics using unreasonable data values or by artificially assigning numerous zones of hydraulic conductivity, recharge, etc., the hydrogeology of the site has not been fully understood (DEQ, 2001). Proper characterisation of the site in and near the area of interest is necessary. The use of un-weighted criteria in the model can cause an imbalance and result in superfluous information and unrealistic calibration (STOWA, 1999). During calibration if steady state is assumed, i.e. storage is neglected and average flow is used, the model could be less sensitive in terms of groundwater levels. If the data used to calibrate the model are from a dynamic system, errors can result in the hydraulic head and “long term” memory (STOWA, 1999). Thus, there is a need to recalculate calibration dynamic data into steady state before it is used (STOWA, 1999).
Using interpolated data distribution rather than point data.	Interpolated data carries an uncertainty with it from the interpolation process. It is unacceptable to calibrate a model to interpolated data for hydraulic head, solute concentration, etc. or to a model output from another model of the same site (DEQ, 2001). The only meaningful comparison is to actual, measured data points. During parameterisation and discretisation the point data is scaled to “block effective” data that may not be sensitive to heterogeneity (STOWA, 1999).
Hydraulic blockages/fractures.	Results may be representative of aquifer properties on a large scale only. Misinterpretation of system due to ignorance of faults and fractures.

5.0 Predictions and Predictive Uncertainty Analysis

'Using scientifically based models, you will often predict an incorrect future with great accuracy, and when using complex, non-identifiable models, you may be capable of predicting the correct future with great uncertainty'. Beck (1987)

The aim of most groundwater flow and contaminant transport models is to predict some future groundwater flow or contaminant transport condition. Predictions are undertaken by running the model with the adopted parameters (calibrated or most reasonable uncalibrated), and imposing a predicted stress which represents the expected future conditions.

However, model uncertainties make any model prediction no better than an approximation. For this reason, it is often desirable that model predictions should be expressed as one of a range of possible outcomes that reflect the uncertainty in model parameterisation. In addition, every effort should be made to define the extent of this range. This process is called predictive uncertainty analysis, and is concerned with the cumulative uncertainty produced from uncertainties in the data and calibration process that are then translated into the uncertainty of the model results.

Predictions are made with both calibrated and uncalibrated models. Usually, less complex models are used when the model is not calibrated to any data. Calibrated models have the huge advantage of constraining the range of predictions, where it can be demonstrated that the model can reasonably accurately simulate measured data. Because of this, calibrated models can be much more useful when considering management decisions. Model predictive uncertainty is related to the following three issues:

(i) *Model calibration, parameter uncertainty and predictive uncertainty*

Parameters are measured imperfectly, so there is an error (or uncertainty) associated with a parameter even at the exact point at which a parameter is measured. Furthermore, parameter measurement is dependent on the volume of the aquifer involved in the measurement. The variability of parameters measured increases as the volume of aquifer involved in the measurement decreases e.g. hydraulic conductivity values determined from slug tests compared to larger scale pumping tests.

This means that parameters measured at points in space should not be considered unique, but rather as a value plus or minus some error term.

Further, the impacts of aquifer heterogeneity and model bias (from model assumptions) complicate this parameter uncertainty. By definition, measurements of aquifer parameters vary considerably with aquifer heterogeneity. In a model, values derived from a measurement at a point are extrapolated to points where there are no data. This introduces further random error into the model.

In calibrating a model to the available measured data, an average broad parameter distribution is achieved. Calibration of the model is therefore constrained by a set of calibration constraint data as measured at boreholes, but there are many more points in the model domain which are inaccessible via the traditional calibration process. In the 'real world', which includes all points in a model domain, there may be more parameter heterogeneity occurring between the measurement points that do not affect calibration which can affect predictions made with the model.

(ii) Model calibration and model assumptions, bias and uncertainty

Models represent the 'essential' features of the real world. What an 'essential' feature constitutes depends on the features germane to the problem at hand.

As discussed in Section 4, model assumptions impose a bias on the parameters that calibrate the model. For example, a dispersivity value derived from tracer test data (from a heterogeneous aquifer) calibrated to a model which assumes aquifer homogeneity may give a lower dispersivity term than if a model representing the aquifer heterogeneity is used in the parameter determination. So, over-simplifying a model to its essential features can introduce a bias into the model which in turn affects its parameterisation and predictions.

Alternatively, when a more complex model can be employed, the heterogeneous spatial patterns of aquifer parameters, model boundaries and stresses can be described in as much detail as possible. For this to be meaningful, a reasonable amount of field data must be gathered. However, some assumptions will remain, AND the uncertainty of the increased model input parameter data becomes more significant. In fact, it can be demonstrated that the higher the level of 'system detail' that a model attempts to simulate (e.g. contaminant movement in areas of high geological heterogeneity, the response of a catchment to extreme climatic events, nuances of groundwater-surface water interaction, etc), the greater the uncertainty with which such predictions are made – the groundwater equivalent of the Heisenberg Uncertainty Principle.

(iii) Uncertainty in system stresses

Post-auditing involves revisiting the model, once the predicted time period has occurred, and allows the modeller to check the model predictions for future scenarios and assumptions made for the system stresses such as rainfall, stream-flows and groundwater usage against what really occurred. Many published model post-audits show that models have not been very successful at prediction primarily because the predicted stresses imposed on the model differed from those that occurred in reality (Zheng and Bennett (1995) in MDBC 2000).

MDBC (2000) discusses methods for estimating system stress uncertainty, particularly recharge uncertainty which is important for sustainable yield estimates. Where a Monte Carlo approach is used on system stresses, there is an assumption of a degree of randomness associated with each stress. The use of the Monte Carlo approach in addressing parameter uncertainty is discussed in Section 5.1 below in more detail.

All **model predictions** have a degree of uncertainty associated with them due to uncertainties associated with parameters, model assumption and future stresses. Because of this it is important to present model predictions as part of a possible range of outcomes.

5.1 What Methods are Currently Available to Address Predictive Uncertainty?

5.1.1 Stochastic Methods

Stochastic methods are used to address both the model uncertainty and the stress definition uncertainty.

Stochastic modelling employs numerous model runs, where each of the model inputs is defined as a distribution rather than a single variable. Each of the many possible combinations of model inputs are then used in a separate model simulation. Random sampling of these distributions using methods such as MONTE CARLO or LATIN HYPERCUBE sampling techniques are often used. Multiple realisations of aquifer properties are used in model simulations in order to build up a distribution of possible model outcomes. The benefits of stochastic models are that the modelling uncertainty is emphasised, and in some cases the likelihood of any of the model outcomes is estimated.

However, for analysing model predictive uncertainty, stochastic modelling can be time consuming when there is more than a handful of adjustable parameters, where millions of model runs can be required. In addition most stochastic simulations fail to ensure that every possible realisation produces a realistic simulation in terms of the criteria used for model calibration. This is a significant shortcoming, as calibration constraints significantly reduce the level of uncertainty associated with model predictions.

A variety of software packages can be used to determine uncertainties. Software packages, such as @Risk (for analytical equations) and numerical models PMWIN and Stochastic MODFLOW/MODPATH, provide a facility for generating stochastic fields and running simulations for multiple realisations.

Another possibility for uncertainty analysis is in using inverse modelling software. Merrick and Doherty, 1998 advocate the use of “rapid-fire re-calibration” (RFRC) that leads to multiple calibrated models for the one area, where the equivalent models differ in assumed fixed aquifer properties, or stresses, or boundary conditions. The uncertainty in the model predictions can be estimated by running conventional scenario analyses with all of the models.

Most stochastic methods neglect the random heterogeneities that can exist between the calibration points and consequently do not make a stochastic model, but are rather a

stochastic approach wrapped around a deterministic model. A small handful of authors are exploring calibration constrained Monte Carlo methods (US Department of Energy, 1999 , La Venue et al., 1995 and RamaRao et al., 1995). To the extent that this has been done, these methods rely on complex purpose built software (i.e. they can only be used with one specific model), are inflexible and are numerically intensive and therefore are not widely used. An efficient, flexible and readily usable method has yet to be found, so rigorous predictive uncertainty analysis is still within the realms of theoretical research, not environmental management practice.

5.1.2 The Worst Case Approach

The worst case approach represents one end of the stochastic continuum. The worst-case approach adopts one set of the most conservative 'worst case' model inputs, and runs the model one time with these inputs. For uncalibrated models, it has the benefits of being simple, and it addresses the uncertainty of these analyses by calculating the most conservative of a range of possible model outputs. It is an appropriate method when very conservative decisions have to be made in water management problems.

When more 'reasonable' worst case assessments are required, a calibrated model is used. However, determining the combination of worst case parameters that still honour calibration constraints requires the calibration of numerous models to determine which is the worst case and so is very time consuming.

One method to minimise the time requirements for worst case assessments for calibrated models is to use the automated calibration software PEST. This software allows the worst case for a calibrated model to be determined quite simply, by running the software in predictive analysis mode (Doherty, 2000). Figure 4 shows contours of increasing conservative predictions as a function of combinations of two parameters. In Figure 5, the calibration objective function is superimposed on these contours, such that the shaded area in the objective function represents an 'acceptable' match with field conditions. The point where the most conservative contour intersects with the calibrated shaded area, represents the critical point, or worst case combination of parameters. The predictive analysis option identifies the parameter combinations that occur at this point and then runs the predictive simulation using this parameter combination, thereby ensuring that the worst case prediction is compatible with calibration constraints.

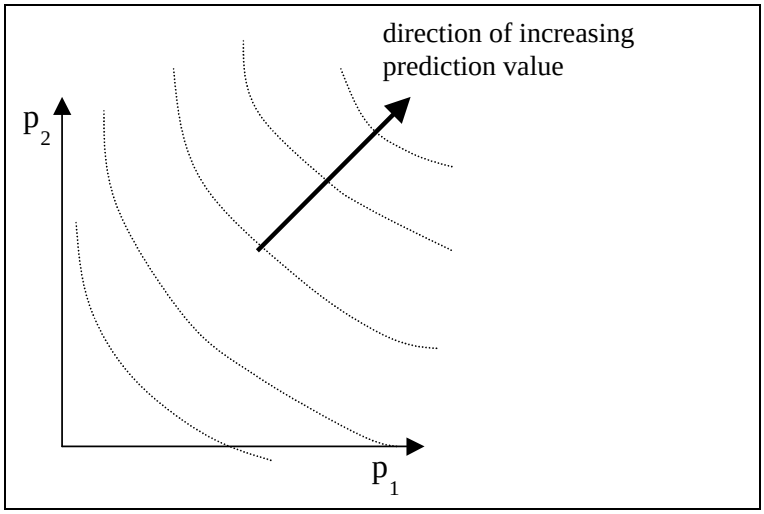


Figure 4: Contours of a Model Prediction in Parameter Space

(reproduced from PEST manual, Doherty 2000)

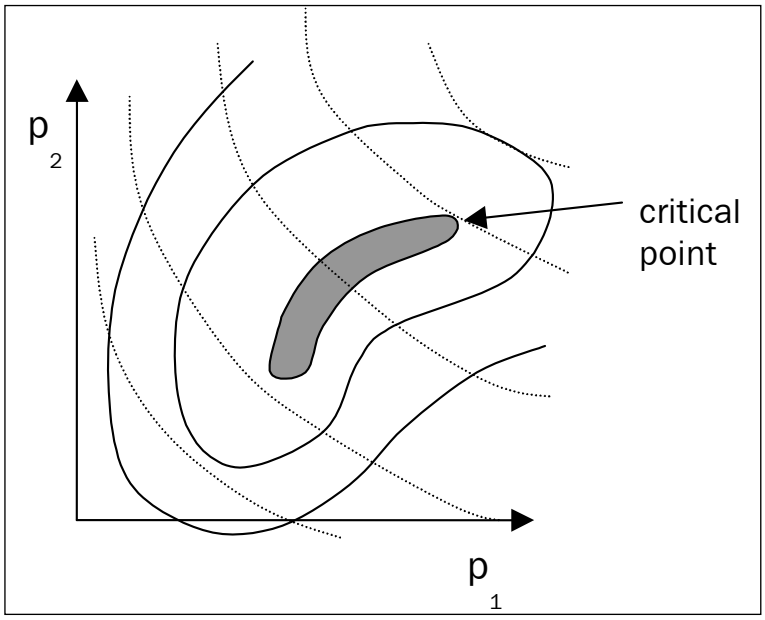


Figure 5: The "Critical Point" in Parameter Space (reproduced from PEST manual, Doherty 2000)

5.1.3 Response Functions

Response functions are used to compare the relative response of a system to the range of possible spatial distributions of a specific stress or prediction. For instance a model may be being used to investigate the relative impacts on stream flow, from groundwater abstractions occurring at differing locations. For this case, the model would be run many times, with one groundwater abstraction per model run. The relative impact of each groundwater abstraction on stream flows would then be able to be assessed.

Response functions essentially sidestep the issue of model predictive uncertainty and instead only assess the relative impacts of a prediction. It does not address the magnitude of a prediction or the uncertainty surrounding the prediction.

Response functions can be useful when investigating where to target monitoring and management efforts.

5.1.4 Performance Monitoring Plan

Models may be used as predictive tools, however field monitoring must be incorporated to verify model predictions. Performance monitoring is required to compare future field conditions with model predictions. The degree of monitoring required to compare future field conditions with model predictions depends on the level of confidence in the model results and the associated level of risks. The length of the performance monitoring period should be based, in part, on model predictions, but more importantly on actual data trends from the monitoring events, and on professional judgement. The performance monitoring plan should include proposed well locations, screen locations, pumping rates, etc.

5.2 Predictive Errors

Common prediction errors are outlined in Table 11 on the following page.

Table 11: Prediction Errors

Prediction errors	
Omitting results inconsistent with your preconceptions.	Uncertainties can arise in predictive results due to errors in the calibrated model and assumptions used to determine the future hydrogeological stresses. An example of this inaccuracy may be if 100% capture of a plume is achieved in the model, but model simulations show that some particles from the source area are not captured. Others could include ignoring the distribution of contaminants and trying to demonstrate a different flow direction inconsistent with measured hydraulic heads or groundwater chemistry (DEQ, 2001).
Not incorporating data variability or uncertainty into the analysis.	Model parameters can never be precisely known. Measured data can show variability that may be an indication of measurement uncertainty or the result of real physical differences. To bracket the model results, the modeller can use a range of data values that reflect data variability. A conservative approach that recognises the uncertainty inherent in modelling displays a firm understanding of the goals of groundwater modelling (DEQ, 2001). For example, during delineation of a wellhead protection area, an appropriately conservative approach would be to use the lowest estimate of transmissivity or hydraulic conductivity to determine the width of the protection area and the highest value to determine the length (DEQ, 2001).
Unquestioned acceptance of model output.	One should always question the model predictions before submitting a model for review. The accuracy of computer modelling is no better than the accuracy of the data used in the analysis (DEQ, 2001). Model results should agree with the modeller's understanding of the site hydrogeology and sound hydrogeological principles.

5.3 Interpretation and Reporting Model Predictions and Results

Model predictions are commonly the main or only section read by interested parties. Consequently, these results need to be clearly and prudently presented. The steps that should be followed by the modeller are shown in Figure 6. Text, figures and tables should be presented in condensed and full form (normally in the appendices) by the modeller. In the step to "discuss the results" the modeller should compare the results with that from other studies and explain any unanticipated results (STOWA, 1999). A direct link between the conclusion drawn from the results and the research question should be clearly evident (STOWA, 1999).

An important step is to check if the goals have been met, and if they have not, the modelling process should begin again by adjusting the conceptual model. A summary of results including statistical analysis should be presented and a comparison with common practices provided. Finally, analyses of the consequences of the research question should be presented. This may expose gaps in domain knowledge, the need for further field observations or a follow-up project is initiated (STOWA, 1999).

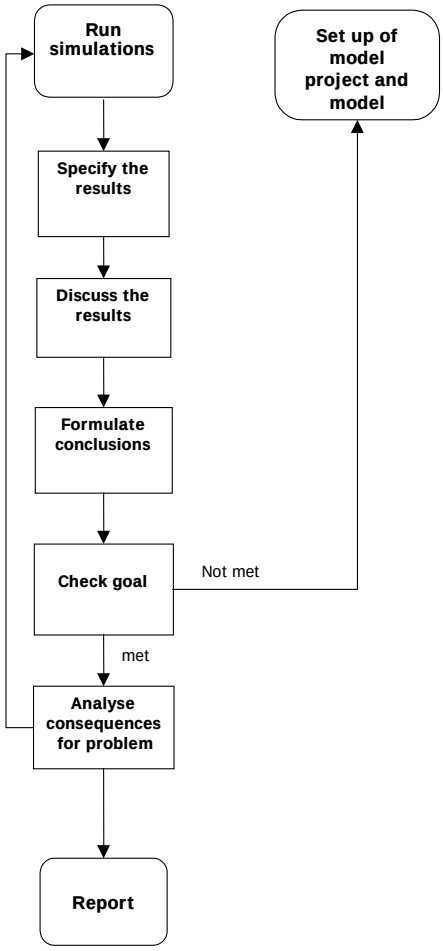


Figure 6: Interpreting model results

6.0 Documentation and Model Report

'The road from science through the model to advice is veiled...' STOWA 2000.

The model report should be of sufficient quality to allow an auditor (or any other third party) to reproduce the model study (including its results) and/or proceed from where the study left off. The report should therefore give a clear indication of the validity, utility and restrictions of the model results. There should also be a model archive comprising the model journal, files, pre- and post-processing documents (text, figures, spreadsheets, etc), such that the model could be regenerated for review (or further refinement).

The model report focuses on the entire modelling process, and all of the components that make up the modelling process must also be discussed therein. The report must detail the process by which the model was selected, developed, calibrated, verified and utilised. There must be sufficient information to allow the auditor to check for errors and to assess whether the uncertainty surrounding model predictions is well enough understood and described. The auditor must ascertain whether decisions should be made on the basis of the model predictions and results. Special care must be taken in representing model results to indicate inherent inaccuracies in the theoretical equations, boundary conditions and other conditions of the codes (Water Science and Technology Board, 1990).

The report must include the following information:

- A description of the purpose and scope of the model application.
- Presentation of the hydrogeological data used to characterise the site.
- Documentation of the source of all data used in the model, whether derived from published sources or measured or calculated from field or laboratory tests.
- Description of the model conceptualisation.
- Identify the model selected to perform the task, its applicability and limitations.
- A discussion of the modelling approach.
- Documentation of all calculations.
- Summary of all model calibration, history matching and sensitivity analysis results.
- Presentation of all model predictive simulation results as a range of probable results given the range of uncertainty in values of model parameters.

The following sections, as outlined in Table 12, could be included, as appropriate, in a modelling report. In some cases, additional information may be necessary to convey a complete understanding of the groundwater model.

Table 12: Example of sections that could be included in a Report

Report section	Detail
Executive Summary	The executive summary is a concise statement of the site problem, model development, management scenarios assessed, modelling conclusions and the uncertainties associated with these conclusions, and recommendations.
Introduction	The introduction communicates the purpose, goals, desired outcomes and the objectives of the project.
Hydrogeological Characterisation	This includes hydrogeological parameters, catchment description, site description, current concepts used.
Conceptual Model and Plan	Detailed information and an outline of the conceptual model and plan including: • The basic features used to represent the physical system; • Aquifer geometry, types and parameters; • The model grid including nodal spacing, the extent and orientation, layers, flow between layers; • Initial and boundary conditions; • Natural recharge and discharge; • Abstractions; • Surface water-groundwater interactions; • Simulation and discretisation time; • How non-uniqueness has been addressed; • Methods of uncertainty and error analysis; • Plan for review of the model in the future.
Calibration and Sensitivity Analysis	Measures of calibration of model performance and sensitivity: • Water balances; • Iteration residual errors; • Statistics, plots and uncertainty results; • Comparisons between predicted and measured groundwater heads, groundwater-surface water interactions; • Approach and outcome of sensitivity analysis.
Prediction and Sensitivity Analysis	Conclusions from assessment of simulated sustainability and management scenarios; Uncertainties and sensitivity analysis results from simulations.

Table 12 (continued)

Model Limitation	Limitations in the conceptual model, calibration and predictions. Methods for resolving these issues.
Performance Monitoring Plan	Timeframe for monitoring of model prediction against actual data. Possible amendments to model if required.
Conclusions and Recommendations	Conclusions and recommendations with regard to the model and the site. Include a discussion of any model limitations and uncertainties. Conclusions can also illustrate how the objectives of the modelling effort were obtained.
References	Full references of all cited work.
Tables	Well logs • well name; • x y co-ordinate data; • top of casing; • ground elevation; • well screen interval; • piezometric elevation data; † • bottom of layer elevations; † • hydraulic conductivity/transmissivity; †‡ Groundwater quality information; Aquifer or slug tests; Model calibration and prediction error results. Sensitivity analysis results.
Figures	All figures should have: • North Arrow • Date • Title Bar • Scale Bar • Legend Regional Location Site plan Cross sections Maps showing aquifer elevation and confining layers Measured hydraulic head distribution Areal hydraulic conductivity/transmissivity If appropriate: areal recharge area Model grid Simulation and prediction maps.

† Requires values for each model layer
‡ Clarify from which type of test (aquifer, slug, etc.)

Other data may be required, depending on the conditions at the site. These additional subjects should be reflected within the body of the report. Examples of additional data or information might include monitoring or management plans, additional figures and tables, or report sections.

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8.0 Glossary

ADVECTION The transport of a contaminant that occurs by the movement of flowing groundwater.

ANALYTICAL MODEL An analytical model is based on simplified versions of the partial differential equations which describe groundwater flow and contaminant transport in groundwater. The simplifications, based on a number of assumptions, allow an exact solution of these equations to be determined. This is in contrast to the complex numerical expressions required to solve the partial differential equation. They can be solved by hand, or by simple computer programs (e.g. WinFlow, TwoDan), but allow only limited complex spatial or temporal variability. They are useful to provide rough approximations for many applications with little effort.

ANISOTROPY If the hydraulic properties of an aquifer measured at a point vary according to the direction of flow, the aquifer is anisotropic at that point.

AQUIFER A geological material such as sand, gravel, limestone or fractured rock in which water may be stored and from which it may be efficiently retrieved. An aquifer is sufficiently permeable to transmit significant quantities of water.

AQUIFER, CONFINED An aquifer that is overlain by a confining bed. The hydraulic conductivity of the confining bed is significantly lower than that of the aquifer. In a confined aquifer the water level in a well usually rises above the aquifer, due to the water pressure within the aquifer being greater than atmospheric pressure.

AQUIFER, PERCHED A region in the unsaturated zone where the soil may be locally saturated because it overlies a low-permeability unit.

AQUIFER, SEMICONFINED An aquifer confined by a low-permeability layer that permits water to flow through it slowly. During pumping of the aquifer, recharge to the aquifer can occur across the confining layer and along the aquifer unit. Semi-confined aquifers may exhibit leaky artesian or leaky confined characters.

AQUIFER, UNCONFINED Also known as water-table and phreatic aquifer. An aquifer in which there are no laterally continuous confining beds between the zone of saturation and ground surface. The water table is in equilibrium with atmospheric pressure.

BORE (WELL) A structure drilled or dug below the surface to obtain water from an aquifer system.

BOUNDARY CONDITIONS

Specified Head (or Fixed or Constant Head) This condition is where the groundwater level (or head, water pressure) is known at the boundary of the model domain. It may, or may not be constant. This boundary is usually only applicable some distance from the area of interest in the model. (also referred to as a Dirichlet condition or first type boundary).

Specified Flow This condition is where the flow into the aquifer at the boundary of the model domain is known and may, or may not be constant. This may be used where a steady amount of leakage into the aquifer occurs from, for example, river leakage or a lake. (also referred to as a Neumann condition or a second type boundary).

Head-dependent Flow This condition is where flow into the aquifer is dependent on the water levels within the aquifer. (also referred to as a Cauchy condition or a third type boundary).

CALIBRATION The process by which the model parameter inputs (usually the aquifer hydraulic properties and boundary conditions), are adjusted within realistic limits, to produce the best match between model outputs and the measured data that form calibration targets. The calibration targets are usually water-level, flow or concentration values.

CALIBRATION, INITIAL CONDITIONS Initial conditions provide a starting point for both steady state and transient simulations. The initial hydrologic conditions for a flow system that are represented by its aquifer head distribution at some particular time corresponding to the antecedent hydrologic conditions in that system.

CALIBRATION, STEADY STATE The calibration of a model to a set of hydrologic conditions that represent (approximately) an equilibrium condition, with no accounting for aquifer storage changes.

CALIBRATION, TRANSIENT or DYNAMIC The calibration of a model to hydrologic conditions that vary dynamically with time, including consideration of aquifer storage changes in the mathematical model.

COMPLEXITY The degree to which a model application resembles, or is designed to resemble, the physical hydrogeological system (Ritchey and Rumbaugh, 1996). There is a hierarchical classification of three main fidelities in order of increasing fidelity: Screening, Engineering Calculation and Aquifer Simulator. Higher fidelity models have a capability to provide for more complex simulations of hydrogeological process and/or address resource management issues more comprehensively.

CONCEPTUAL MODEL A simplified and idealised representation (usually graphical) of the physical hydrogeologic setting and our hydrogeological understanding of the essential flow processes of the system. This includes the identification and description of the geologic and hydrologic framework, media type, hydraulic properties, sources and sinks, and important aquifer flow and surface-groundwater interaction processes.

CONFINING LAYER A body of relatively impermeable material that is stratigraphically adjacent to one or more aquifers. It may lie above or below the aquifer.

DENSITY The mass or quantity of a substance per unit volume. Système Internationale (SI) units are kilograms per cubic metre or grams per cubic centimetre.

DETERMINISTIC A description of a parameter or a process with uniquely defined qualities. A deterministic parameter has, or is assumed to have, a unique value or a unique spatial distribution. The outcome of a deterministic process is known with certainty. There is, or is assumed to be, a clear cause-and-effect relation between independent and dependent variables.

DIRICHLET CONDITION Also known as a Specified, Fixed or Constant Head Boundary, or Third Type Boundary Condition. A boundary condition for a groundwater model where the head is known and specified at the boundary of the flow field, and the model computes the associated groundwater flow.

DIFFUSIVITY The ratio of transmissivity to storage coefficient in an aquifer.

DISCHARGE The volume of water flowing in a stream or through an aquifer past a specific point in a given period of time.

DISCHARGE AREA An area in which there are upward components of hydraulic head in the aquifer.

DRAWDOWN A lowering of the water table of an unconfined aquifer, or of the potentiometric surface of a confined aquifer. Drawdown is the result of pumping of groundwater from wells.

GROUNDWATER The water contained in interconnected pores located below the water table.

GROUNDWATER DIVIDE The boundary between two adjacent groundwater basins. The divide is represented by a high in the water table surface.

GROUNDWATER FLOW MODEL An application of a mathematical model to represent a site-specific groundwater flow system.

HETEROGENEOUS An aquifer or aquitard medium which consists of different (non-uniform) characteristics in different locations.

HOMOGENEOUS An aquifer or aquitard medium with identical (uniform) characteristics regardless of location.

HYDRAULIC CONDUCTANCE A term which incorporates model geometry and hydraulic conductivity into a single value for simplicity. Controls rate of flow to or from a given model cell, river reach, etc.

HYDRAULIC CONDUCTIVITY Is a measure of the capacity of a medium to transmit water.

HYDRAULIC GRADIENT The change in total head with distance in a given direction which yields a maximum rate of decrease in head.

HYDROLOGIC CONDITIONS A set of groundwater inflows, outflows, boundary conditions and hydraulic properties that causes potentiometric heads to adopt a distinct pattern.

ISOTROPY The condition in which hydraulic properties of an aquifer or aquitard are equal in all directions.

KARST Karst topography is developed over limestone or other calcareous rocks. It is commonly characterized by sinkholes, caves, and underground river systems.

LOCAL GROUNDWATER SYSTEM Aquifers which respond rapidly to recharge due to a shallow water table and/or close proximity of the recharge and discharge sites. These types of flow systems occur almost exclusively in unconfined aquifers.

METADATA (-INFORMATION) Data on data location, how it was measured, by whom it was measured, the accuracy of data etc.

MODEL - *mathematical model* A mathematical model is a set of equations, which, subject to certain assumptions, quantifies the physical processes active in the aquifer. While the model itself obviously lacks the detailed reality of the groundwater system, the behaviour of a valid model approximates that of the aquifer.

MODEL - *analytical model* Refer to Analytical Model

MODEL - *numerical model* Refer to Numerical Model.

MODELLER Person using the model.

MONTE CARLO ANALYSIS A set of model simulations for alternative model realisations, on the assumption that aspects of the model are stochastic. A *realisation* is one of many possible model representations in terms of its aquifer parameters, boundary conditions or stresses.

NON-UNIQUENESS The condition that many different possible sets of model inputs can produce nearly identical computed aquifer head distributions for any given model (see heuristic representation given in Appendix A and Section 3 - Ritchey and Rumbaugh, 1996).

NUMERICAL MODEL A model of groundwater flow in which the aquifer is described by numerical equations, with specified values for boundary conditions, that are usually solved on a digital computer. In this approach, the continuous differential terms in the governing hydraulic flow equation are replaced by finite quantities. The computational power of the computer is used to solve the resulting algebraic equations by matrix arithmetic. In this way, problems with complex geometry, dynamic response effects and spatial and temporal variability may be solved accurately. This approach must be used in cases where the essential aquifer features form a complex system, and where surface-groundwater interaction is an important component (i.e. high fidelity models).

OBSERVATION WELL A non-pumping well used to observe the elevation of the water table or the potentiometric surface. An observation well is generally of larger diameter than a piezometer.

PARAMETER A quantity that is supposed to be constant but is not exactly known.

PIEZOMETER A non-pumping well, generally of small diameter, that may be used to measure the elevation of the water table or potentiometric surface. A piezometer generally has a short screen through which water can enter, it therefore measures hydraulic head at that point.

POROSITY The ratio of the volume of void spaces in a rock or sediment to the total volume of the rock or sediment.

POROSITY, EFFECTIVE The volume of the inter-connected void spaces through which water or other fluids can travel in a rock or sediment divided by the total volume of the rock or sediment.

POROSITY, PRIMARY The porosity that represents the original pore openings when a rock or sediment formed.

POROSITY, SECONDARY The porosity that has been caused by fractures or weathering in a rock or sediment after it has been formed.

POST-AUDIT Comparison of model predictions with what actually happened.

POTENTIOMETRIC (PIEZOMETRIC) SURFACE A surface that represents the level to which water will rise in tightly cased wells. The water table is a particular potentiometric surface of an unconfined aquifer (see SATURATED ZONE).

PUMPING TEST Also known as an aquifer test. A test made by pumping a well for a period of time at a measured rate and observing the change in hydraulic head in the aquifer. A pumping test may be used to determine the capacity of the well and the hydraulic characteristics of the aquifer.

RECHARGE The process which replenishes groundwater, usually by rainfall infiltrating from the ground surface to the water table and by river water entering the water table or exposed aquifers. The addition of water to an aquifer.

REGIONAL GROUNDWATER SYSTEMS Extensive aquifers which take longer than local systems to respond to increased groundwater recharge because their recharge and discharge sites are separated by large distances (>10 km), and/or they have a deep water table. Unconfined aquifers with deep water tables that are part of regional flow systems may become, in effect, local flow systems if there is sufficient recharge to cause the water table to rise close to the surface (<5 m) (Tóth 1963, in Freeze and Cherry 1979).

RESIDUAL The difference between the computed and observed value of a variable at a specific time and location.

SATURATED ZONE The zone in which the voids in the rock or soil are filled with water at a pressure greater than atmospheric. The water table is the top of the saturated zone in an unconfined aquifer.

SCOPE The set of conditions under which a model may be applied.

SENSITIVITY ANALYSIS The measurement of the uncertainty in a calibrated model as a function of uncertainty in estimates of aquifer parameters and boundary conditions.

SIMULATION One complete execution of a groundwater modelling program, including input and output.

SPECIFIC CAPACITY The time-dependent ratio of the rate of discharge of water from the well to the drawdown of the water level in the well. Specific capacity should be described on the basis of the number of hours of pumping prior to the time the drawdown measurement is made. It will generally decrease with time as the drawdown increases.

SPECIFIC DISCHARGE Also known as Darcian flow velocity. An apparent velocity calculated from Darcy's law; represents the flow rate at which water would flow in an aquifer if the aquifer were an open conduit.

SPECIFIC STORAGE The amount of water per unit volume of a saturated formation that is expelled from storage due to compression of the mineral skeleton and the pore water.

SPECIFIC YIELD The ratio of the volume of water that a given mass of saturated soil or rock will yield by gravity to the volume of that mass.

STOCHASTIC A description of a parameter or a process with random qualities. A stochastic parameter has a range of possible values, each with a defined probability. The outcome of a stochastic process is not known with certainty.

STORAGE COEFFICIENT (STORATIVITY) The volume of water that a conductive unit will expel from storage per unit surface area per unit change in head. In a confined aquifer, it is computed as the product of specific storage and aquifer thickness. In an unconfined aquifer, it is equal to specific yield.

SYSTEM A whole (often a part of reality) consisting of inter-related entities.

THEIS EQUATION An equation for the unsteady flow of groundwater in a fully confined aquifer to a pumping well.

TOPOGRAPHIC DIVIDE The boundary between adjacent surface water boundaries. It is represented by a topographically high area.

TORTUOSITY The actual length of a groundwater flow path, which is sinuous in form, divided by the straight-line distance between the ends of the flow path.

TOTAL DISSOLVED SOLIDS (TDS) A measure of the salinity of water, usually expressed in milligrams per litre (mg/L). Sometimes TDS is referred to as total dissolved salts, or as TSS, total soluble salts.

TRANSMISSIVITY The rate at which water is transmitted through a unit width of aquifer of confining bed under a unit hydraulic gradient. The product of saturated thickness and hydraulic conductivity.

UNCERTAINTY ANALYSIS The quantification of uncertainty in model results due to incomplete knowledge of model aquifer parameters, boundary conditions or stresses.

UNCONFINED AQUIFER An aquifer that contains the water table and is normally exposed to the surface. Occasionally there may be a layer overlying this type of aquifer protecting it from the surface.

UNSATURATED ZONE Also known as the zone of aeration and the vadose zone. The zone between the land surface and the water table. It includes the root zone, intermediate zone, and capillary fringe. The pore spaces contain water at less than atmospheric pressure, as well as air and other gases. Saturated bodies, such as perched groundwater, may exist in the unsaturated zone.

VALIDATION See VERIFICATION.

VERIFICATION A test of the integrity of a model by checking if its predictions reasonably match the observations of a reserved data set deliberately excluded from consideration during calibration.

WATER BUDGET An evaluation of all the sources of supply and the corresponding discharges with respect to an aquifer or a drainage basin.

WATER TABLE The upper level of the unconfined groundwater, where the water pressure is equal to that of the atmosphere and below which the soils or rocks are saturated. It is the location where the sub-surface becomes fully saturated with groundwater, the level at which water stands in wells that penetrate the water body. Above the water table, the sub-surface is only partially saturated (often called the unsaturated zone). The water table can be measured by installing shallow wells across the water table and then measuring the water level in those wells.

WELL EFFICIENCY The ratio of idealized drawdown in the well, where there are no losses resulting from well design and construction factors, to actual measured drawdown in the well.

WELL, FULLY PENETRATING A well drilled to the bottom of an aquifer, constructed in such a way that it withdraws water from the entire thickness of the aquifer.

WELL, PARTIALLY PENETRATING A well constructed in such a way that it draws water directly from a fractional part of the total thickness of the aquifer. The fractional part may be located anywhere in the aquifer.

WELL SCREEN A tubular device with either slots, holes, gauze, or continuous-wire wrap as an integral part of the well casing. The water enters the well through the well screen.

Appendix A

Appendix A – Analytical flow models

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Tables

1.0 Description

An analytical flow model provides an exact solution to a groundwater flow equation by creating a range of simplifying assumptions regarding the natural flow system. These assumptions generally include aquifer homogeneity and commonly involve no spatial variability of model inputs. The groundwater flow equation is typically used to determine drawdown interference effects, stream depletion effects, or most simply, the water balance of an aquifer. Analytical flow equations are solved by hand or by using simple computer programs.

Analytical flow models provide solutions for estimating effects such as drawdown interference, stream depletion rates, and groundwater mounding. Analytical flow models are typically used for:

- Simple worst case assessments of drawdown interference, stream depletion or aquifer sustainability.
- Ranking of development options in terms of their risk to other wells, stream flows or the sustainability of an aquifer (exact magnitude is not important).
- Where there are insufficient data, hours or budget to allow for a more sophisticated approach and/or the level of uncertainty associated with more simple models is acceptable.

These models are commonly used for Assessment of Environmental Effects reports (AEE's) submitted with consent applications to assess the impact of a proposed development. Partly, this is because there is commonly insufficient information prior to development to allow a more complex model to be used.

Table A1 lists several analytical flow models available – they are all for exploring the impact of drawdown effects or aquifer test analysis.

Table A1: Commonly available analytical codes for groundwater flow.

Code	Description
SUPRPUMP	Used to analyse pump tests and assess aquifer drawdown effects. Provides solutions for confined and leaky aquifers, with anisotropy and no flow or recharge boundaries.
AQTESOLV	Used to analyse pump tests assess aquifer drawdown effects. Provides solutions for confined and leaky aquifers, with anisotropy and no flow or recharge boundaries.
JSTEP	Used to analyse step discharge pump tests.
MOUNDT	Used to assess mounding of water table in response to an areal recharge

2.0 Analytical flow models – how do they work?

The mathematical model for three dimensional movement of groundwater of constant density through porous strata can be described by the following partial differential equation.

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

where:

K_{xx}, K_{yy} and K_{zz} = values of hydraulic conductivity along the x, y and z coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity.

h = the potentiometric head

W = a volumetric flux per unit volume and represents sources and/or sinks of water

S_s = specific storage of the porous material

t = time

In most realistic situations these factors may be difficult to quantify, and may vary in time and/or space. Mathematical models for such problems may require complex numerical expressions and a considerable amount of data to characterise the problem. However, when carrying out preliminary assessments, it is often justifiable to make the following types of simplifying assumptions:

- The aquifer is of infinite extent
- Initial conditions of a flat (horizontal) water table.
- The aquifer is homogeneous
- The well fully penetrates the aquifer
- The river fully penetrates the aquifer

When these assumptions can be made it is possible to use relatively simple analytical equations (or models) to estimate groundwater flow problems. For example, the equations on the following pages are examples of those available for drawdown, mounding and stream depletion assessments.

The Theis (1935) equation is probably the best known analytical equation and is commonly used to determine drawdown around a pumping well.

Hantush (1967) created a number of equations, such as the mounding equation quoted on the following page. Hantush also presented solutions to approximate water table rise, water table decay and for an infinitely long recharging strip.

Jenkins (1977) formulated an equation to estimate stream depletion resulting from groundwater extraction from a well.

Drawdown assessments (Theis 1935)

$$h_o - h = \frac{Q}{4\pi T}\int_u^\infty \frac{e^{-u}}{u}du$$

$$u = \frac{r^2 S}{4Tt}$$

Where

Q is the constant pumping rate (L^3/T)

h is hydraulic head (L)

h_o is hydraulic head before pumping started (L)

$h_o - h$ is the drawdown (L)

T is aquifer transmissivity (L^2/T)

t is time since pumping (T)

r is radial distance from the pumping well (L)

S is aquifer storativity (dimensionless)

Mounding assessments (Hantush, 1967):

$$h_m^2 - h_i^2 = \frac{V}{2\pi K}\left\{W(u_o) + \left(\frac{1-e^{u_o}}{u_o}\right)\right\}$$

which, if $u_o \le 0.05$ can be written as

$$h_m^2 - h_i^2 = \frac{V}{2\pi K}\left[W(u_o)+1\right]$$

$$= \frac{V}{2\pi K}\ln\left(6.11vt/R^2\right)$$

where $u_o = R^2/4vt$ and $W(u)$ is the well function for nonleaky aquifers.

where h_m = maximum height of the water table

h_i = initial height of water table

$V = w\pi R^2$

w = constant rate of percolation

K = hydraulic conductivity

$v = K\bar{b}/\varepsilon$

ε = storativity

$\bar{b} = 0.5\left[h_i(0) + h(t_1)\right]$ constant of linearization

t_1 = the period at the end of which h is to be estimated

t = time since the incident of percolation

R = radius of the circular recharging area

Stream depletion assessments

Jenkins Method for stream depletion:

$$\frac{q}{Q} = erfc\left(\sqrt{\frac{sdf}{4t}}\right) = 1 - erf\left(\sqrt{\frac{sdf}{4t}}\right)$$

where

$$erf\ \ x = \text{the error function of x} = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,dt = 1 - erfc\ \text{x}$$

$$erfc\ \ x = \text{the complementary error function of x} = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}\,dt$$

$$\text{sdf} = \frac{\text{a}^2 S}{T}$$

where

T = transmissivity (L^2/T)

S = specific yield of the aquifer (dimensionless)

t = time during pumping period, since pumping began (T)

Q = the net steady pumping rate (L^3/T)

q = the rate of depletion of the stream (L^3/T)

a = the perpendicular distance from the pumped well to the stream (L)

sdf = stream depletion factor (T)

3.0 Calibration targets for analytical flow models

3.1 Calibration parameters

The following is a list of parameters that are altered in the calibration of an analytical flow model. A full description of these parameters is outlined in Section 5 of this appendix.

Calibration parameters

- Storativity
- Transmissivity
- Leakage rates from under or overlying aquifers
- Stream bed conductance

3.2 Calibration Targets

Both qualitative and quantitative calibration criteria are used to measure the success of an analytical flow model calibration. As summarised below.

Qualitative calibration criteria

- Comparison of drawdown curves (water level – time data)
- Assessment of the 'reasonableness' of the input parameters

These are subjective assessment measures.

Quantitative calibration criteria

- Calculation of water level residuals

  Mean, root mean square, standard deviations etc (for statistics as outlined in Table A2 below)

Table A2: Quantitative calibration criteria. Criteria in this table are to be used only as a guide to model calibration success; they should not be used without analysis and reference to the hydrogeological basis of the model (cf. Table 9 of main report).

Description of measure	Equation	Comment
Residual	$R_i = H_i - h_i$ where: R_i = residual H_i = measured head at location i h_i = modelled head at location i	The smaller the residual the more likely the calibration is correct.

Mean error (ME)	$\frac{1}{n}\sum_{i=1}^{n}\left(H_i - h_i\right)$	A mean error incorporates both negative and positive residuals. Therefore a small mean error may not indicate a good calibration.
Mean absolute error (MAE)	$\frac{1}{n}\sum_{i=1}^{n}\left\|H_i - h_i\right\|$	A small MAE may indicate a good calibration.
Root mean squared error (RMS)	$\frac{1}{n}\sum_{i=1}^{n}\sqrt{\left(H_i - h_i\right)^2}$	A small RMS may indicate a good calibration.
Sum of residuals	$\sum_{i=1}^{n} W_i\left\|H_i - h_i\right\|$ where: W_i = weighting from 0 to 1	Useful for comparing successive model runs. The measure is dependent on sample size. Weights are used to emphasize more or less reliable data, or change the emphasis of a specific parameter or area.
Correlation function – R	$\frac{\sum(h_i - \bar{h})(H_i - \bar{H})}{\sqrt{\sum(h_i - \bar{h})^2}\sqrt{(H_i - \bar{H})^2}}$ where: $\bar{h}$ and $\bar{H}$ are the average of the modelled and measured heads respectively	May tend towards one for perfect calibrations.
R^2	$\frac{\sum_{i=1}^{n} W_i\left(H_i - \bar{H}\right)^2}{\sum_{i=1}^{n} W_i\left(h_i - \bar{H}\right)^2}$ where: $\bar{h}$ and $\bar{H}$ are the average of the modelled and measured heads respectively	May tend towards one for perfect calibrations

Note 1: Heads have been used to represent the observations for comparison with model output. However, other measurements such as flows could be used in these equations of statistical measure.

Note 2: Statistical calibration criteria such as correlation coefficient should be used as a measure of the validity of a model only with caution, as described in Section 4.3 of the main report.

4.0 Predictive uncertainty and numerical models

As discussed in Section 5 of the main report, model predictive uncertainty is related to model assumptions and parameter uncertainty. In addition, model errors clearly compromise model predictions. Because of this the model auditor needs to:

- Consider the degree to which the model assumptions are different from the real world and assess what the likely bias on predictions may be as a result of model assumptions.
- Consider the possible range of parameters and their natural variability or heterogeneity, measurement errors, interpretation of measurement errors, or lack of measurements. The auditor also needs to check that the model solutions are within a realistic realm, as some combinations of parameters, within realistic ranges, can produce unrealistic solutions.
- Undertake checks for model errors.

When addressing model uncertainty, the chief aim is to identify the limiting case for the model prediction (often called worst case). For example, if the model is being used to determine drawdown interference effects, what is the biggest drawdown interference that could occur, given the information available? The model auditor needs to be satisfied that this limiting worst case has been realistically identified in such a way that it takes into account the model uncertainty.

4.1 Model assumptions and model predictive uncertainty

Assumptions that are of significance in terms of analytical flow models are discussed below.

4.1.1 Assumption as to whether the aquifer is confined, unconfined, or leaky

Many analytical flow solutions make an assumption as to whether the aquifer is confined, leaky or unconfined. A confined aquifer is defined as being bounded above and below by an impermeable layer. An unconfined aquifer is bounded below by an impermeable layer but there is no impermeable layer above the aquifer, instead the water table forms the top of an unconfined aquifer. A leaky aquifer (also called a semiconfined aquifer) is an aquifer which has either or both an upper or lower boundary as a low permeability layer (low relative to the aquifer permeability), which allows water to move through it from a lower or higher aquifer. For a leaky aquifer a distinction is made between low permeability layers that simply transmit water, and those that also store water. An unconfined aquifer has a characteristic S shape drawdown-time curve when plotted on a log-log scale. The early time part of the curve gives an initial storage coefficient that relates to the instantaneous release of the water from the aquifer, with associated expansion of the water and compaction of the aquifer. Whereas the later part of the curve relates to the draining of stored water (specific yield) The early time storage coefficient can not be used to accurately determine long term drawdown.

When making a prediction for a drawdown interference, the most conservative drawdown interference occurs when assuming a confined aquifer (with the associated low storage coefficient). Assumption of a leaky aquifer model is less conservative than a non-leaky one, for an aquifer with an overlying confining layer. That is, it underestimates the drawdown.

If the analytical equations are being used to determine aquifer parameters, such as transmissivity or storage coefficient, the choice of an assumed aquifer type will bias the calculation of the parameter.

4.1.2 Assumption of boundaries

A common assumption of analytical flow solutions is that the aquifer is of infinite extent (flow boundaries only at infinity) and has a flat (horizontal) water table. However, where appropriate, this very simplistic environment can be modified to one where no-flow boundaries are present. A typical no-flow boundary might be a non-conformable alluvial gravel aquifer

system overlying basement metamorphic or igneous rocks. In many cases a flow boundary may involve recharge, such as one involving groundwater relationships with a lake or river.

When making predictions of drawdown interference, assuming a recharge boundary lowers the predictive drawdowns, while assuming a barrier (no-flow boundary), increases the predictive drawdowns. If using the models to calculate aquifer parameters, again these assumptions will bias the calculation.

4.1.3 Assumption of steady or transient (unsteady) flow

Analytical models can be set up for both steady flow or transient (unsteady) flow conditions. Steady-state flow is independent of time. For example steady state flow assumes that the water level in a pumped well and in surrounding wells does not change with time. Steady-state flow could occur when a pumped aquifer is recharged by an outside source by the same rate as the pumping well. In practise, steady state flow is assumed if the changes in water level in wells with increasing time can be assumed to be negligible.

In contrast transient or unsteady-state flow is assumed where water levels are changing significantly with time. Usually in the initial stages of pumping from a well, an unsteady-state is assumed, while the steady-state is used for later time data.

When making drawdown predictions, use of solutions that assume steady-state has been reached will calculate the maximum likely effect.

Similarly in stream depletion calculations, as the stream is depleted, the flow cannot be considered to be steady. Making this assumption of steady flow will overestimate the stream depletion.

4.1.4 Assumption of a homogeneous/isotropic aquifer

Analytical flow models assume a homogeneous and isotropic aquifer. However most aquifers composed of sedimentary deposits are more likely to be heterogeneous and anisotropic. Where an aquifer is significantly anisotropic or heterogeneous this will impose a bias on model predictions.

For drawdown assessments, solutions are available that account for vertical and horizontal anisotropy. Aquifer heterogeneity is only accounted for where a lower permeability strata can be represented as an aquifer boundary. Not accounting for heterogeneity is likely to overestimate drawdown in some areas and underestimate it in others.

For stream depletion predictions, ignoring the presence of lower permeability strata overestimates the stream depletion rate. The most important heterogeneity for stream depletion assessments relates to the stream bed clogging layer. Sophocleous et al. (1995) reported that a ratio of 0.01 between aquifer and stream bed hydraulic conductivities will cause the stream depletion to be overestimated by up to 71% when compared to a numerical model which did represent this heterogeneity.

4.1.5 Penetration of the stream and well

Some aquifers are so thick that it is not justified to assume a fully penetrating well. Partial penetration of a pumping well, causes the flow velocity in the immediate vicinity of the well to be higher than usual, causing extra head losses around a well. Most analytical solutions assume that wells or streams fully penetrate the aquifer, however where observation bores are near to the pumping bore (i.e., a distance of around 1.5 – 2 times the aquifer thickness), this assumption will result in underestimation of aquifer transmissivity.

There are analytical solutions available for both drawdown assessments and stream depletion assessments that allow for partial penetration.

4.2 Parameter uncertainty and predictive model uncertainty

The uncertainty of parameters is related to their natural variability and heterogeneity, measurement errors, interpretation of measurement errors, or lack of measurements. The factors that govern flow and aquifer response in groundwater are:

- Aquifer parameters, such as transmissivity and storativity, aquifer thickness and aquitard thickness.
- Aquifer recharge/boundaries.
- Well location and pumping rate.
- For stream depletion, stream parameters such as streambed conductance and stream width may also be required (Hunt method).

Parameters are always measured imperfectly, so there is an error (or uncertainty) associated with a parameter even at the exact point at which a parameter is measured. Furthermore, parameter measurement is dependent on the volume of the aquifer involved in the measurement. The variability of parameters increases as the measurement volume decreases.

This means that parameters measured at points in space should not be considered unique, but rather as a value plus or minus some error term. The model auditor needs to assess whether the uncertainty of these parameters has been taken into account. Table A3 provides a brief summary of how the input parameters affect a model solution.

Table A3. Input Parameters – How They Affect Assessments

	Most Conservative (worst case)	Least Conservative	Auditor check
Transmissivity (T)	Stream depletion: High T Drawdown: Low T for wells close to the pumping well and high T for wells far from the pumping well	Stream depletion: Low T Drawdown: High T for wells close to the pumping well and low T for wells far from the pumping well	
Storativity (S)	Stream depletion: Low S: (not reasonable given theory) Drawdown: Low S	Stream depletion: High S Drawdown: High S	
Well location	Small distances to well or stream	Large distances to well or stream	
Pump rate (Q)	Maximum	Average, or actual use from a ‘wet’ year	

5.0 Data requirements

Analytical flow assessments can be completed without detailed site specific data or with some site specific information, parameters often obtained from literature review, requires experienced judgement.

Parameter	Aquifer Thickness (b)
Units	m
Description	Where a model defines the solution in 2 dimensions, an aquifer thickness must be specified.

Parameter	Aquitard Thickness (b')
Units	m
Description	Where a model defines the system in 2 dimensions, an aquitard thickness may need to be specified

Parameter	Cartesian Coordinates (x, y, z)
Units	m
Description	The position of components of the aquifer system need to be specified in space. The model is defined in two dimensions, using a 2D coordinate system (e.g. where the x axis is the groundwater flow direction and along the y axis is perpendicular to the groundwater flow direction). The model is defined in three dimensions, using a coordinate system, where the x axis is the groundwater flow direction and along the y axis is perpendicular to the groundwater flow direction, and the z axis represents depth.

Parameter	Hydraulic conductivity (K)
Units	m/day
Description	The volume of water that will move through a porous medium in unit time under a unit hydraulic gradient through a unit area measured at right angles to the direction of flow. Hydraulic conductivity parameter contains properties of the fluid (water) and of the saturated porous medium. It is defined as: $K = \frac{k\rho_{water} g}{\mu}$ Where: k = intrinsic permeability of the strata g = acceleration due to gravity ρ_{water} = density of water μ = viscosity of water

Parameter	Transmissivity (T)
Typical Units	m^2/day
Description	Transmissivity is the product of the average hydraulic conductivity K and the saturated thickness of the aquifer.

Parameter	Storage Coefficient (S)
Units	dimensionless
Description	The storage coefficient of the aquifer from which groundwater abstraction occurs (i.e. the volume of water released per unit volume of aquifer for each unit decline in the piezometric surface).

Parameter	Pumping Rate (Q)
Typical Units	m^3/day or L/s
Description	The average abstraction rate from a well over a fixed period of time. Note: The principle of superposition applies to drawdown and to stream depletion rates. Therefore, for example, the effect of intermittent pumping can be simulated by the addition of effects resulting from a sequence of pumping and recovery. Jenkins (1977) concludes that "*within quite large ranges of intermittency, the effects of intermittent pumping are approximately the same as those of steady, continuous pumping of the same volume.*" Therefore averaging of abstraction rates over a longer time period (e.g. an irrigation season) provides a useful estimate of drawdown and stream depletion in many cases.

Parameter	Separation Distance (l)
Typical Units	metres (m)
Description	The lateral separation distance from the abstraction well to another well or to the nearest edge of the stream water, measured perpendicular to the stream flow.

Parameter	Pumping Period (t)
Typical Units	days
Description	The duration of the pumping period of interest.

Parameter	Streambed conductance (λ)
Typical Units	m/day
Description	A measure of the vertical hydraulic conductance through the streambed to the underlying aquifer. Streambed conductance can be defined as:

	$$\lambda = \frac{K'W}{M}$$ where K‘ is the hydraulic conductivity of the strata in the streambed (m/day) W is the width of the streambed (m) M is the thickness of the streambed across which K‘ is measured (m)

6.0 Errors

Errors can be generated through inappropriate model design, selection of conditions, lack of information, carelessness and oversimplification. Some errors are therefore the application of inappropriate model assumptions, as discussed in Section 4 of this appendix.

Table A4 provides a check list which model auditors can use as they consider the validity of a model prediction. Meeting all the requirements outlined in the checklist does not guarantee good model predictions, but will assist an auditor to make their assessment.

Table A4: Checklist for analytical flow model errors

Data gathering errors	Potential implication for solution	Auditor check	OK - tick	Comments
Field measurements of parameters incorporate inherent inaccuracies	These are errors are associated with human error or an instrument error. For example simple water level measurements have an error of around 0.5 cm.	Have measuring errors been assessed?		
Extrapolation of data.	During aquifer tests it is important that measurements of water level or flow and time are recorded accurately rather than extrapolating the measurement to a theoretical time measurement schedule.	Have water level time measurements been made accurately?		
Lack of background trend information	During aquifer tests it is important to correct for any antecedent water level trend, i.e. a seasonal rise in water level resulting from winter recharge, etc.	Has background water level data been monitored prior to test?		
Data input errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Inconsistent parameter units - i.e. days and seconds, gallons per minute and cubic feet per day.	It is important to use consistent units when modelling. Inaccuracies can occur easily if the same units are not used. For example, days are selected for time unit and feet for length unit, then recharge and hydraulic conductivity must be in feet per day, pumping rates must be in cubic feet per day, constant head boundaries and grid dimensions must be in feet, etc.	Are the model units consistent for all parameters – i.e. days and seconds, cubic metres per day etc?		
Incorrect sign for pumping or recharge.	It is common practice to express pumping rates as a negative value, injection and recharge as positive values in groundwater modelling programs	Are the correct signs for pumping and recharge used?		
Well not specified correctly	The well parameters must be specified, especially screen length, for accurate modelling. In a case where no screen has been defined the model may be very distorted in order to get the model to 'work properly'. Pumping rates need to be specified to represent the actual conditions.	Have the well location, screen depths and pumping rates been specified correctly?		

Model assumption errors	Potential implication for solution	Auditor check	OK - tick	Comments
Variable or constant density assumptions	Neglecting density variations can give incorrect indications of flow field.	Are there density variations within the flow field and if so have they been accounted for?		
Inappropriate model selection given model assumptions re boundaries and initial conditions and parameterisation/ oversimplification of the problem.	It is inappropriate to attempt to define the optimum placement and pumping rate for an extraction well and monitoring system with a simple analytical model incapable of representing known hydrogeological features of a complex site, such as rivers, lakes, variable aquifer thickness or hydraulic conductivity, 3-D groundwater flow, or multiple aquifers. Similarly it is important that the model assumptions best reflect the aquifer characteristics, i.e. confined, unconfined, etc.	Is it appropriate to use an analytical model for the problem being assessed? If it is – has the correct solution been chosen, i.e. for an unconfined aquifer, etc?		
Calibration errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Forcing questionable data to fit	If early-time aquifer test data do not fit a curve, perhaps the pump had not settled down, there was some well bore storage, or something similar that caused the discrepancy.	Have questionable data been forced to fit?		
Sensitivity analysis	A sensitivity analysis should be used a part of the calibration process – so that calibration efforts are targeted to the parameters to which model predictions are most sensitive.	Has a sensitivity analysis been undertaken? Which were the most sensitive parameters?		
Prediction errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Omitting results inconsistent with your preconceptions	The wrong answer – you will be found out, eventually.	Have all data been used?		
Blind acceptance of model output	A model's accuracy is no better than the accuracy of the data. Make sure that the model results agree with your understanding of the site hydrogeology and sound hydrogeological principles.	Has the data accuracy been considered?		

Predictive uncertainty must be addressed.	Given the non-uniqueness of models, it is important the uncertainty of predictions is explored and the limiting scenario (worst case) is reported.	Has predictive uncertainty analysis been undertaken?		
The correct predictive simulations must be undertaken to fulfil model purpose		Does the model fulfil its purpose?		

7.0 Case study

7.1.1 Model purpose and background

An estimate of the potential drawdown effect at a neighbouring well was determined assuming 100 days of continuous pumping. The well is 60 m deep and draws water from a leaky semiconfined aquifer. The neighbouring domestic water supply bore is located 200 m distant, is 30 m deep and is screened in an unconfined aquifer above the semiconfined aquifer. Water levels in the unconfined aquifer vary from 11 – 22 m below ground level. Water levels in the semiconfined aquifer vary from 15 – 30 m below ground level.

7.1.2 Model details

Pumping time: 100 days

Pumping rate: 7.5 L/s for 15 hours per day, 7 days per week

Aquifer transmissivity was estimated on the basis of drillers specific capacity tests, from 3 wells less than 1 000 m distant, within the same aquifer as the pumping bore. This estimate is based on a regression relationship between specific capacity and transmissivity measurements in the area, and has a r^2 of 0.66 (Bal 1996). Transmissivity was estimated to be 300 m^2/day.

Aquifer storativity was estimated based on the geometric average of pumping tests in the area as 0.004.

The Theis aquifer drawdown model was used, and assumes a confined aquifer setting, which was considered an appropriately conservative assumption to make in this instance.

7.1.3 Model calibration

The model was not calibrated to any field measurements.

7.1.4 Model predictions and predictive uncertainty

A single model prediction was made. The prediction was assumed to be conservative, given that the Theis model was used, which would tend to overestimate drawdown effects in this setting, as drawdown in a confined aquifer would be greater than in a leaky semiconfined aquifer with the same aquifer parameters. A sensitivity analysis of the model predictions, to explore the impacts of the parameter uncertainty, was not undertaken.

Table A5: Case study - checklist for analytical flow model errors

Data gathering errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Field measurements of parameters incorporate inherent inaccuracies	These are errors are associated with human error or an instrument error. For example simple water level measurements have an error of around 0.5 cm.	Have measuring errors been assessed?		No checks made on field data
Lack of precise data	Extrapolation of data, such as transmissivity, over large distances gives rise to uncertainties, especially in aquifers known to be inhomogeneous.	Density distribution of original data		No checks made on field data
Extrapolation of data.	During aquifer tests it is important that measurements of water level or flow and time are recorded accurately rather than extrapolating the measurement to a theoretical time measurement schedule.	Have water level time measurements been made accurately?		No checks made on field data
Lack of background trend information	During aquifer tests it is important to correct for any antecedent water level trend, i.e. a seasonal rise in water level resulting from winter recharge etc.	Has background water level data been monitored prior to test?		No checks made on field data
Data input errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Inconsistent parameter units - i.e. days and seconds, gallons per minute and cubic feet per day.	It is important to use consistent units when modelling. Inaccuracies occur if the same units are not used. For example, days are selected for time unit and metres for length unit, then recharge and hydraulic conductivity must be in metres per day, pumping rates must be in cubic	Are the model units consistent for all parameters – i.e. days and seconds, cubic metres per day, etc?	√	

	metres per day, constant head boundaries and grid dimensions must be in metres, etc.			
Incorrect sign for pumping or recharge.	It is common practice to express pumping rates as a negative value, injection and recharge as positive values in groundwater modelling programs	Are the correct signs for pumping and recharge used?	√	
Well not specified correctly	The well parameters must be specified, especially screen length, for accurate modelling. In a case where no screen has been defined the model may be very distorted in order to get the model to "work properly'. Pumping rates need to be specified to represent the actual conditions.	Have the well location, screen depths and pumping rates been specified correctly?	√	
Model assumption errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Variable or constant density assumptions	Neglecting density variations can give incorrect indications of flow field.	Are there density variations within the flow field and if so have they been accounted for?	√	Constant density assumption is appropriate

Inappropriate model selection given model assumptions re boundaries and initial conditions and parameterisation / over-simplification of the problem.	It is inappropriate to attempt to define the optimum placement and pumping rate for an extraction well and monitoring system with a simple analytical model incapable of representing known hydrogeological features of a complex site, such as rivers, lakes, variable aquifer thickness or hydraulic conductivity, 3-D groundwater flow, or multiple aquifers. Similarly it is important that the model assumptions best reflect the aquifer characteristics, i.e. confined, unconfined, etc.	Is it appropriate to use an analytical model for the problem being assessed? If it is – has the correct solution been chosen, i.e. for an unconfined aquifer, etc?		The simple analytical model is appropriate for the modelling problem. Using the Theis model in this setting is unrealistic and will tend to overestimate drawdown effects. While this was done intentionally to make a conservative assessment, it would be prudent to use correct model assumptions and instead assess the sensitivity of that solution to the range of parameters likely at the site.
Calibration errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Forcing questionable data to fit	If early-time aquifer test data don't fit a curve, perhaps the pump hadn't settled down, there was some well bore storage, or something similar that caused the discrepancy.	Have questionable data been forced to fit?		No calibration
Sensitivity analysis	A sensitivity analysis should be used a part of the calibration process – so that calibration efforts are targeted to the parameters to which model predictions are most sensitive.	Has a sensitivity analysis been undertaken? Which were the most sensitive parameters?		No calibration

Prediction errors	Potential implication for solution	Auditor check	OK - tick	Comments
Omitting results inconsistent with your preconceptions				Only one result reported.
Blind acceptance of model output	A model's accuracy is no better than the accuracy of the data. Make sure that the model results agree with your understanding of the site hydrogeology and sound hydrogeological principles.	Has the data accuracy been considered?		The parameter inputs have a considerable range of uncertainty associated with them. The specific capacity – transmissivity relationship is very approximate as is the average storativity value.
Predictive uncertainty must be addressed.	Given the non-uniqueness of models, it is important the uncertainty of predictions is explored and the limiting scenario (worst case) is reported.	Has predictive uncertainty analysis been undertaken?		Not undertaken.
The correct predictive simulations must be undertaken to fulfil model purpose		Does the model fulfil its purpose?	√	A drawdown assessment was made.

Appendix B

Appendix B – Analytical Contaminant Transport Models

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1.0 Description

An analytical contaminant transport model is based on an exact solution to equations that simulate contaminant transport by creating a range of simplifying assumptions regarding the contaminant migration. Applications of analytical contaminant transport models include: calculation of maximum plume lengths; comparison of plume impacts of alternative discharge scenarios; aquifer vulnerability studies; capture zone assessments. Contaminant transport analytical equations are solved by hand calculator or using simple computer programs.

Because of the simplifications inherent in analytical contaminant transport models, it is not possible to account for field conditions that vary in space. However, the use of analytical solutions is justifiable in cases such as:

- Initial assessments where a high degree of accuracy is not needed.
- Simple worst case assessments of contaminant concentrations and/or arrival times, where conservative assumptions are used to address the issues of model uncertainty.
- Prior to beginning field investigations to aid in the design of data collection programs.
- To check the results of a numerical solution.
- Ranking of development or rule options where there is a contamination risk (for cases where exact magnitude is not important).
- Where the level of uncertainty associated with the more simple analytical models is acceptable as the field conditions support the simplifying assumptions.

The data requirements for analytical models are simple:

- Mass of contaminant introduced into the aquifer and its extent in time and space.
- Model domain is an infinite aquifer, or a laterally bounded aquifer, and/or an aquifer of finite thickness.
- Average hydrogeological parameters, such as the groundwater flow velocity, dispersion characteristics, and aquifer porosity.
- Average geological, thermal and chemical processes such as adsorption, biological decay, radioactive decay, thermal decay, and sometimes, chemical transformations.

These models are frequently used for Assessment of Environmental Effects reports (AEE's) submitted with consent applications to assess the impact of a proposed development. Partly, this is because there is commonly insufficient information prior to development to allow a more complex model to be used.

Table B1 lists several analytical models available for 2-D and 3-D analysis of contaminant transport under homogeneous, isotropic conditions.

Table B1: Commonly available analytical codes for contaminant transport in groundwater.

Code	Description
AT123D	Used to analyse 3D saturated flow contaminant transport for point, line and areal sources, of instantaneous, fixed or continuous duration. The code assumes a constant dispersivity. Allows for adsorption and decay of contaminants.
DISPSOLV	Used to analyse 2D and 3D saturated flow contaminant transport for instantaneous and continuous contaminant point sources. Identifies the maximum plume length for the entire range of possible velocities, in a single model run, allowing identification of a worst case plume length. The code assumes a scale dependent velocity.
VIRALT	Used to analyse 3D saturated flow contaminant transport for point, line and areal sources, of instantaneous, fixed or continuous duration. The code assumes a constant dispersivity. Allows for adsorption and decay of contaminants. Provides for attenuating processes that occur in the unsaturated zone.
PLUME	Used to analyse 3D saturated flow contaminant transport for point, line and areal sources, of instantaneous, fixed or continuous duration. The code assumes a constant dispersivity. Allows for adsorption and decay of contaminants. Allows a constant groundwater concentration to be defined instead of a mass flux.

2.0 Analytical contaminant transport models – how do they work?

As groundwater moves through an aquifer it does so at a range of differing velocities, as shown in Figure B1.

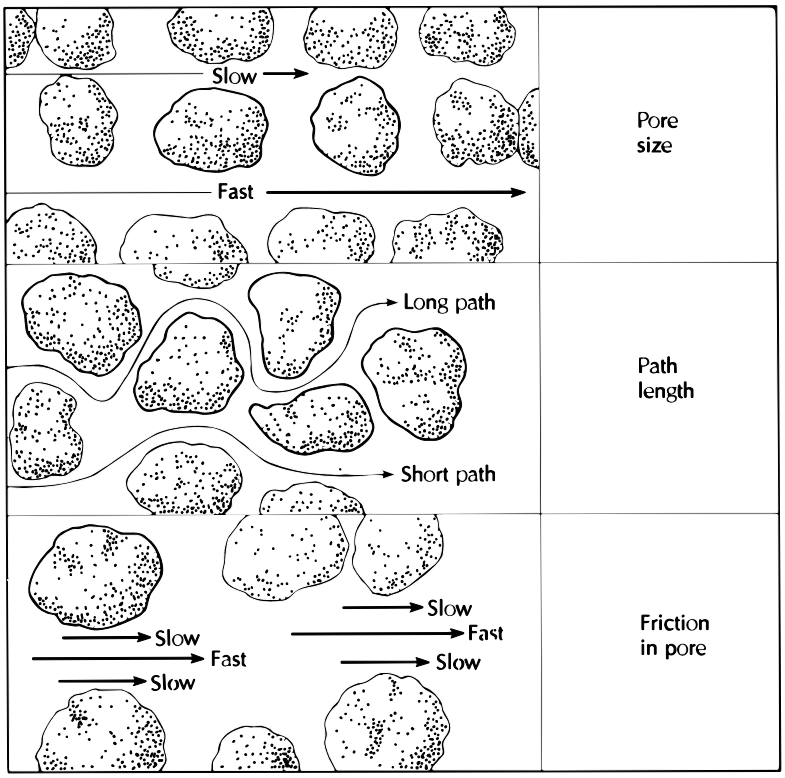

Figure B1. Factors causing pore velocity variations (Fetter 1994).

In contaminant transport problems this variation in pore velocity is addressed by using a mean groundwater pore velocity plus a mechanical dispersion term. Where mechanical dispersion describes the mixing that occurs as a consequence of the local variations in pore velocity around some mean pore velocity.

A composite 'dispersion' term is made up of both mechanical dispersion and chemical diffusion. However, diffusion is usually negligible compared to mechanical dispersion except in very slow moving groundwater systems.

Three dimensional movement of contaminant in groundwater of constant density through porous strata can be described by the following partial differential equation.

$$\frac{\partial}{\partial x}\left(D_1\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial y}\left(D_2\frac{\partial}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_2\frac{\partial}{\partial z}\right)=\frac{u}{\sigma}\frac{\partial c}{\partial x}+\frac{\partial c}{\partial t}$$

where:

D_1, D_2 and D_3 = Dispersion coefficients along the x, y and z coordinate axes, where the x axis is parallel to the major axes of groundwater flow velocity.

u = the pore velocity

c = concentration

σ = porosity

t = time

By making some specific simplifying assumptions, such as: the groundwater flow is steady with a uniform velocity; the aquifer media is homogeneous and of infinite extent; the contaminant source occurs at a point and is uniformly continuous; and the contaminant decays at an exponential rate; this equation can be written much more simply as:

$$c(x,y,z,\infty) = \frac{\dot{M}_3}{4\sigma\pi}\sqrt{\frac{1}{AD_xD_yD_z}}\exp\left(\frac{xu}{2D_x} - \sqrt{AB}\right)$$

$$where\ A = \frac{x^2}{D_x} + \frac{y^2}{D_y} + \frac{z^2}{D_z}$$

and

$$B = \lambda + 0.25\frac{u^2}{D_x}$$

where

$x, y, z =$ cartesian coordinates

$D_1 =$ longitundinal dispersion coefficient

$D_2 =$ lateral dispersion coefficient

$D_3 =$ vertical dispersion coefficient

$t =$ time

$\lambda =$ radioactive decay constant

$\sigma =$ porosity

$M_2 =$ contaminant mass per unit area

$u =$ pore velocity

$c =$ contaminant concentration

Analytical contaminant transport models can be grouped as follows.

(1) The most simple analytical contaminant transport equation is the mass mixing model. In this model dispersion is neglected. The mass mixing model assumes the contaminant source is fully mixed within a specific width and depth of the aquifer and ignores biological and chemical processes. The mass mixing model is frequently used to determine the impacts of nitrate leaching from farming activities, refer to Figure B2.

(2) The advection dispersion equation, where a contaminant source is described as a mass flux prior to entering groundwater, as used in AT123D and DISPSOLV.

(3) The advection dispersion equation, where a contaminant source is described as a concentration in groundwater, as in the PLUME suite of models by Domenico (see Domenico and Schwartz 1990).

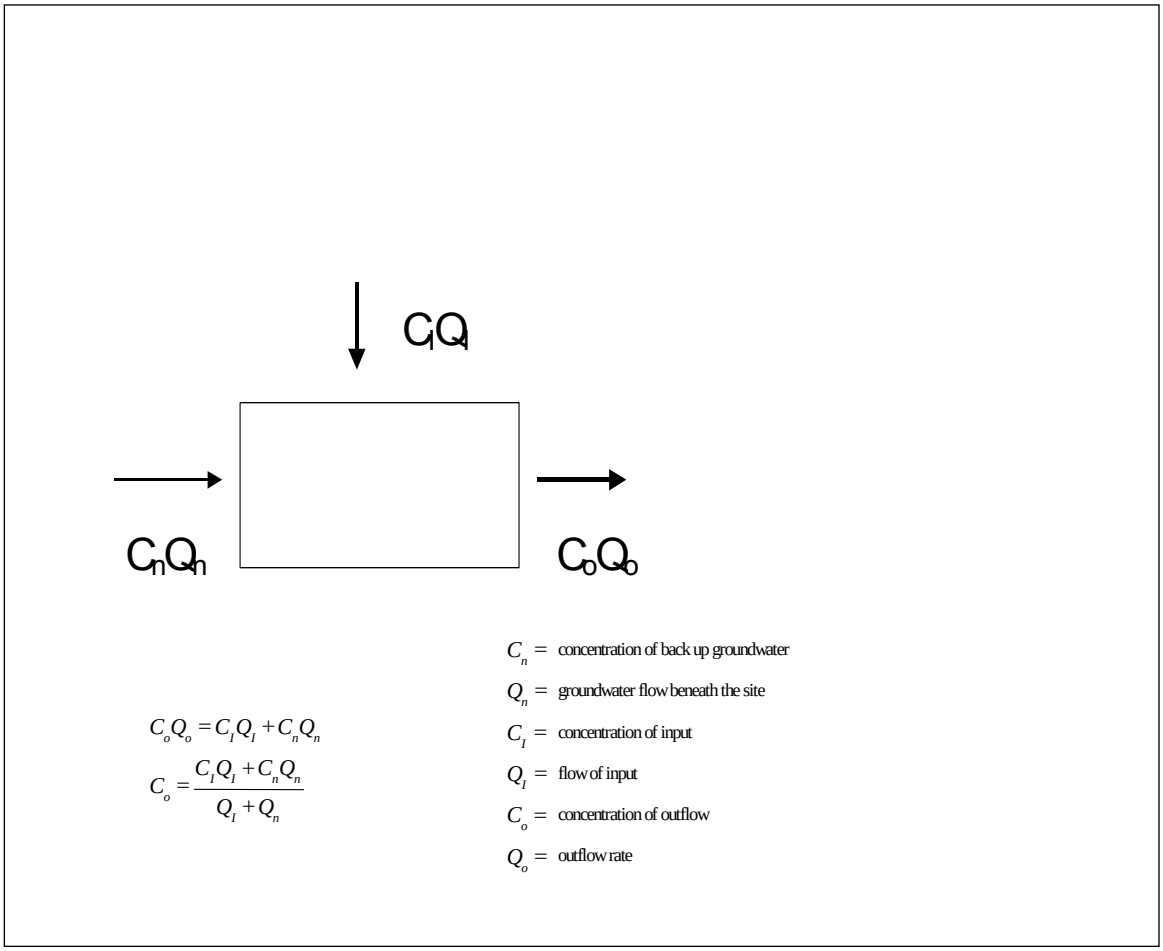

Figure B2. Mass mixing model

3.0 Calibration targets for analytical contaminant models

3.1 Calibration parameters

The following is a list of parameters that are altered in the calibration of an analytical contaminant model. A full description of these parameters is outlined in Section 5 of this appendix.

Calibration parameters

- Mean pore velocity (if coupled with a flow model – this will already be determined)
- Heterogeneity (if coupled with a flow model – this will already be determined)
- Dispersivity
- Diffusion coefficient
- Adsorption coefficient
- Degradation rate
- Source locations
- Source history
- Retardation

3.2 Calibration Targets

Both qualitative and quantitative calibration criteria are used to measure the success of an analytical flow model calibration. As summarised below.

Qualitative calibration criteria

- Plume patterns
- Concentration time plots for a well (breakthrough curves)

These are subjective assessment measures.

Quantitative calibration criteria

- Peak concentrations and time to peak concentrations
- Concentration - time measurements
- Model error: maximum, minimum, root mean square and standard deviations.

Table B2: Quantitative calibration criteria. Criteria in this table are to be used only as a guide to model calibration success; they should not be used without analysis and reference to the hydrogeological basis of the model.

Description	Equation	Comment
Residual	$R_i = C_i - c_i$ where: R_i = residual C_i = measured head at location i c_i = modelled head at location i	The smaller the residual the more likely the calibration is correct.
Mean error (ME)	$\frac{1}{n}\sum_{i=1}^{n}(C_i - c_i)$	A mean error incorporates both negative and positive residuals. Therefore a small mean error may not indicate a good calibration.
Mean absolute error (MAE)	$\frac{1}{n}\sum_{i=1}^{n}\lvert C_i - c_i\rvert$	A small MAE may indicate a good calibration.
Root mean squared error (RMS)	$\frac{1}{n}\sum_{i=1}^{n}\sqrt{(C_i - c_i)^2}$	A small RMS may indicate a good calibration.
Sum of residuals	$\sum_{i=1}^{n} W_i\lvert C_i - c_i\rvert$ where: W_i = weighting from 0 to 1	Useful for comparing successive model runs. The measure is dependent on sample size. Weights are used to emphasize more or less reliable data, or change the emphasis of a specific parameter or area.
Correlation function – R	$\frac{\sum(c_i - \bar{c})(C_i - \bar{C})}{\sqrt{\sum(c_i - \bar{c})^2}\sqrt{(C_i - \bar{C})^2}}$ where: $\bar{c}$ and $\bar{C}$ are the average of the modelled and measured concentrations respectively	May tend towards one for perfect calibrations.

R^2	$\frac{\sum_{i=1}^{n} W_i \left(C_i - \bar{C}\right)^2}{\sum_{i=1}^{n} W_i \left(c_i - \bar{C}\right)^2}$ where : $\bar{c}$ and $\bar{C}$ are the average of the modelled and measured concentrations respectively	May tend towards one for perfect calibrations
Weighted least squares – S(b) – used to describe parameter estimation	$(C - c(b))^T \underline{w} (C - c(b))$ where : b = vector containing parameter estimates c(b) = matrix of modelled concentrations which is a function of b C = matrix of measured concentrations	This is a matrix function used in parameter estimation software.
Maximum likelihood –S'(b)	$(ND + NPR)\ln 2\pi - \ln\lvert\underline{w}\rvert + (C - c(b))^T \underline{w}(C\ c(b))$ where : ND = number of observations NPR = number of prior information values $\lvert\underline{w}\rvert$ = determinant of the weight matrix	This is a matrix function used in parameter estimation software.

Note: Concentrations have been used to represent the observations for comparison with model output. However other measurements, such as flows could be used in the above equations.

4.0 Model predictive uncertainty

As discussed in Section 4 of the main report, model predictive uncertainty is related to model assumptions and parameter uncertainty. In addition, model errors clearly also compromise model predictions. Because of this the model auditor needs to:

- Consider the degree to which the model assumptions are different from the real world and assess what the likely bias on predictions may be as a result of model assumptions.
- Consider the possible range of parameters and their natural variability or heterogeneity, measurement errors, interpretation of measurement errors, or lack of measurements. The auditor also needs to simply check that the model solutions are within a realistic realm, as some combinations of parameters, within realistic ranges, can produce unrealistic solutions
- Undertake checks for model errors.

When addressing model uncertainty, the chief aim is to identify the limiting case for the model prediction (often called 'worst case'). The model auditor needs to be satisfied that this limiting worst case has been realistically identified in such a way that it takes into account the model uncertainty.

4.1 Uncertainty relating to model assumptions

As discussed earlier, analytical contaminant transport models incorporate a number of simplifying assumptions. These simplifying assumptions impose a bias on the model results. The most significant of model assumptions for analytical contaminant transport models which affect model predictions are summarised as follows:

- Aquifer homogeneity and the associated constant pore velocity.
- Aquifer homogeneity and dispersivity.
- Constant versus scale dispersivity.
- Assumptions regarding biological and chemical processes.
- Assumptions regarding the mass flux entering groundwater.
- Assumptions regarding the configuration of the source in time and space.
- Assumptions regarding the discretisation for model solutions, especially where a worst case is to be identified.

It is important for the auditor and the modeller to consider whether these assumptions are acceptable given the issue of concern.

4.1.1 Assumption of aquifer homogeneity and pore velocity and dispersion

Assuming a homogeneous aquifer is to also assume a constant mean groundwater pore velocity term. Yet we know that when migrating through a heterogeneous aquifer, groundwater moves through zones of varying permeabilities with associated differing flow velocities as seen in Figure B1. Because of this a contaminant mass in groundwater is distributed over a range of different permeability zones and migrates away from its source at differing mean pore velocities and with differing dispersion. Theoretically, where the complete range of local pore velocity variations is represented in the model, the mechanical dispersivity term is not required.

When using analytical contaminant transport models which assume homogeneity, an indication of this contaminant migration is obtained by assuming the mass migrates at a median pore velocity, representative of the range of velocities which will be encountered along any particular flow path, plus a dispersion term.

However, a representative median pore velocity and associated dispersion value are difficult to determine. Moreover the worst case for a pore velocity does not automatically fall at either end of a reasonable range, where biological and chemical removal processes occur. In one study, the average velocity did not predict the peak or maximum measured concentrations well (Moore and Scott, 2000). In worst-case assessments it is important to predict the peak concentrations. Consequently the impact on model predictions from the entire range of reasonable median velocities needs to be explored. This is a time consuming task, however some software, for example DISPSOLV (Scott and Smith, 1995, ECan, 2002) automates this exploration of velocities. Similarly, the model independent parameter estimation software PEST includes a sensitivity analysis option 'SENSAN' which allows the impact on model predictions from the range of any model inputs to be explored automatically.

When a homogeneous aquifer model is calibrated to tracer test data from a heterogeneous aquifer, the mechanical dispersivity term is higher than if a model representing some strata heterogeneity is used.

4.1.2 Scale and constant dispersivity

The dispersion process is a scale-dependent phenomenon i.e., more dispersion occurs with increasing distance from the source. A number of authors (see bibliography in Xu and Eckstein 1995) have described the relationship of increasing dispersivity with increasing scale of experiment. Some of these relationships assume a linearly increasing dispersivity with travel distance, as shown in Figure B3. below. Others, such as Neuman (1990) assume that the increase is non linear. These are shown in Figure B4 and Table B7.

Calibration to tracer test data in Canterbury indicates that dispersivity values in Canterbury alluvial gravels are lower than indicated by these relationships (ECan 2002). This report concludes, that on the basis of these calibrations, a very low longitudinal scale dependent dispersivity term of 0.03 may be appropriate for alluvial gravel aquifers.

Table B3: Reported dispersivity relationships

Reported by	Scale dispersivity relationship
Xu and Eckstein (1995)	Longitudinal dispersivity = $3.28 \times 1.2(\log_{10}(0.3048x)^{2.958}$ or Longitudinal dispersivity = $3.28 \times 0.83(\log_{10}(0.3048x)^{2.414}$
Neuman (1990)	If $x<100$ m Longitudinal dispersivity = $0.017(\log x)^{1.5}$ If $x>100$ m Longitudinal dispersivity = $0.32(\log x)^{0.83}$
Gelhar (1986)	Longitudinal dispersivity = $0.1x$
Ayra (1986)	Longitudinal dispersivity = $3.28 \times 0.177(0.3048\ x)^{0.728}$

The relationship between distance scale and dispersivity is a significant limitation for standard analytical solutions which assume that dispersivity is a constant. An approach used to overcome that limitation is using a different value of dispersivity for each distance under consideration. Hunt (1998) has produced new analytical solutions that treat dispersivity as a scale-dependent parameter, allowing all distances from the source to be considered in one solution.

Interestingly the solutions using the two different equations are sometimes quite different, giving a good example of model bias.

The differences between the constant dispersivity and scale-dependent dispersivity solutions can be seen by comparing

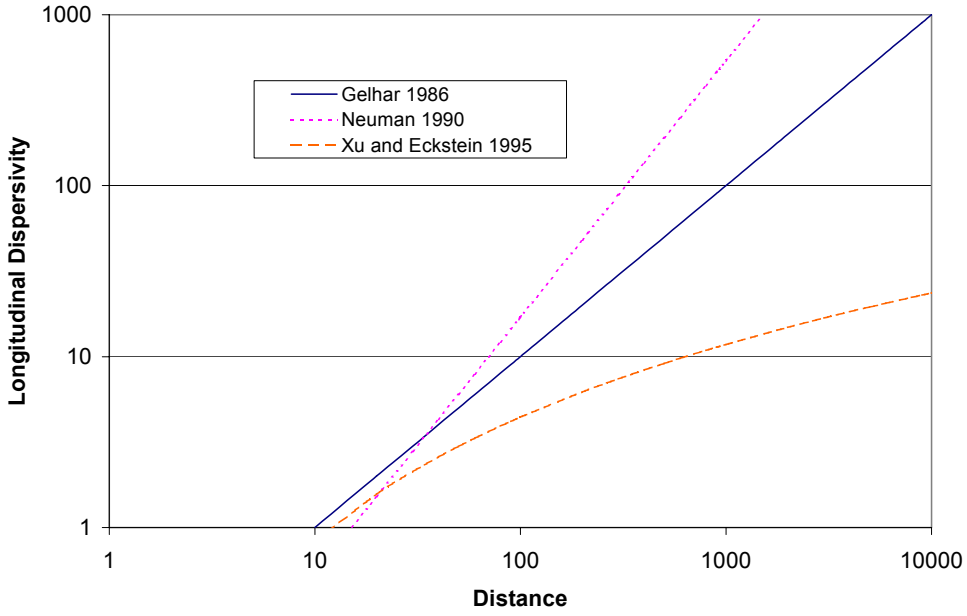

Figure B3: Scale dependent dispersivity relationships

the simulated breakthrough curves for the 2D instantaneous case with the following parameters: Mass flux = 10^6 units/day/m; Effective porosity = 0.1; Pore velocity = 10 m/day; Distance = 100 m.

For a conservative source (Figure B4) the constant dispersivity solution produces a maximum concentration approximately 50% of the scale-dependent dispersivity solution. The constant dispersivity solution uses a single dispersivity value based on the distance between the contaminant source and the observation point. Compared to the scale-dependent case this effectively over-estimates the amount of dispersion occurring before the peak concentration is reached at the observation point and so results in an under-estimate of peak concentration.

When a decaying source is considered, the comparison between the constant dispersivity and scale-dependent dispersivity solutions becomes more complicated. Figure B5 compares the solutions where the decay rate is 1 day^{-1} (equivalent to a half-life of about 0.7 days) and shows that in this case the constant dispersivity solution over-estimates the peak concentration. This counter-intuitive result is presumably a consequence of the fact that the constant dispersivity solution exaggerates the initial rate of dispersion and so allows a higher proportion of the contaminant to reach the observation point quicker, thereby reducing the time dependent decay effect.

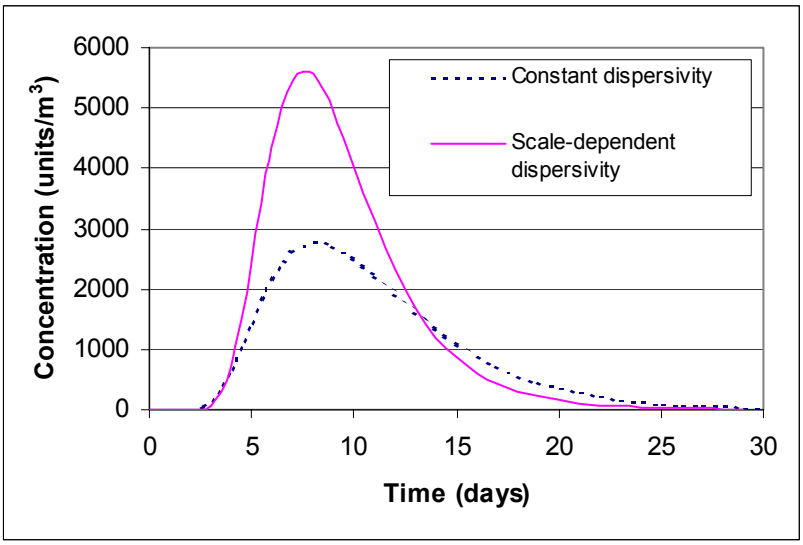

Figure B4: Comparison of simulated breakthrough curves for constant dispersivity and scale-dependent dispersivity for an instantaneous source without decay, at an observation point located 100 m from the source.

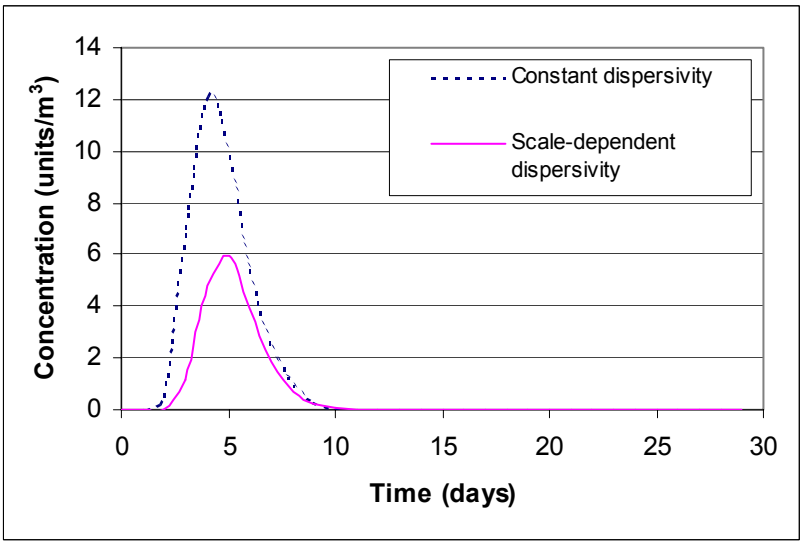

Figure B5: Comparison of simulated breakthrough curves for constant dispersivity and scale-dependent dispersivity for an instantaneous source with decay (λ= 1 day^{-1}), at an observation point located 100 m from the source.

For purely predictive models, where the dispersivity term has not been determined in model calibration, a low dispersivity value should be used for worst case assessments.

4.1.3 Line and area sources and fixed time duration sources

Some analytical models provide solutions for contaminants entering groundwater at a point on the groundwater surface; while others provide solutions for a line source on the groundwater surface or area sources. For example AT123D (Yeh, 1993), allows solutions for a point, an areal or a line source; however it does not provide for a scale dependent

dispersivity term. DISPSOLV (Smith and Scott, 1995 and ECan 2002) allows solutions for a point source only. Using a point source to represent a line or areal source will overestimate the down gradient concentrations near the source.

Similarly, some analytical models calculate solutions for instantaneous or continuous sources only, whereas other solutions allow for fixed time duration discharges of contaminant sources. If a fixed duration discharge is estimated by assuming a continuous source, this will tend to over-estimate concentrations.

4.1.4 Accuracy / step size with respect to space and pore velocity dependence / processing time and hardware requirements

All models, including analytical models, require that the user specify the spatial and temporal conditions at which the solution is calculated. Where a solution for the range of possible input values is also explored, one of the possible solutions will become the worst case. The extent to which the range is sampled affects the accuracy with which the worst case is determined. The greater the number of solutions, the more accurate the estimate of the 'worst case'. However, increasing the number of solutions required creates a proportional increase in the time required for the model run.

4.1.5 Biological and chemical processes

Most analytical contaminant transport models provide solutions for contaminants that decay biologically or chemically. Some also allow for retardation of contaminants, where they adsorb onto sedimentary particles within the aquifer. Using solutions that do not account for these processes where they occur will tend to over-estimate the solutions.

4.1.6 Assumptions regarding mass input or mass flux

In some cases it is difficult to determine a reasonable mass flux. Either the flow rate of the contaminant entering the aquifer or the concentration of the contaminant entering the aquifer may be unknown or difficult to determine. A large number of assumptions are then made, regarding, for instance, what may occur in the unsaturated zone before the contaminant flux reaches groundwater, or the volume of contaminated soil that rainfall recharge is percolating through. Depending on the assumption, this may under or over-estimate the likely mass flux.

4.2 Parameter uncertainty and predictive model uncertainty

The uncertainty of parameters related to their natural variability and heterogeneity, measurement errors, interpretation of measurement errors, or lack of measurements. The factors that govern contaminant transport in groundwater are:

- Mass of contaminant
- Porosity
- Groundwater pore velocity and mechanical dispersion and diffusion
- Biodegradation of the contaminant
- Reactions of the contaminant with the aquifer strata
- Reactions of the contaminant with other solutes

Of these parameters the solution is most sensitive to the mass of the contaminant and then to groundwater pore velocity, dispersivity and porosity. Consequently the focus of parameter uncertainty rests on these factors, which are discussed further in this section.

Parameters are always measured imperfectly, so there is an error (or uncertainty) associated with a parameter even at the exact point at which a parameter is measured. Furthermore, parameter measurement is dependent on the volume of the aquifer involved in the measurement. The variability of parameters increases as the measurement volume decreases.

This means that parameters measured at points in space should not be considered unique, but rather as a value plus or minus some error term. The model auditor needs to assess whether the uncertainty of these parameters has been taken into account. Table B4 provides a brief summary of how the input parameters affect a model solution.

Table B4. Input Parameters – How They Affect Assessments

	Most Conservative (worst case)	**Least Conservative**	**Auditor check**
Mass or Mass Flux	High mass flux	Low mass flux	
Velocity	Variable	Variable	
Decay rate	No decay	High decay rate	
Porosity (neglecting the impact on the velocity term)	Low porosity	High porosity	
Adsorption	High adsorption	No adsorption	
Dispersivity	Low dispersivity	High dispersivity	

NOTE: Porosity is related to the aquifer pore velocity where v = (Ki)/n, and the worst-case pore velocity is variable depending on the contaminant and decay rate. However, when the whole range of velocities is examined, it is not important to consider the impact of porosity on the pore velocity term. However porosity also occurs in the contaminant transport equation, independent of pore velocity, with the mass flux being divided by the porosity term. In this instance the worst-case porosity term is the lower end of the realistic range.

5.0 Data requirements

Typical analytical transport model inputs are described in this section. These inputs can be based on site specific information if a site specific prediction is required, or general regional flow data if the model is being used for exploration of a general case or literature values for a theoretical assessment. Generally, because of the simplifications of these models they are less suitable for accurate site specific predictions. The following text boxes in this section illustrate the data required for analytical transport models.

5.1 Mass of contaminant

Parameter	Input Mass/Mass Flux
Units	kg or Number or kg /day or Number/day
Description	The mass flux enters the groundwater at a point, or along a line or over an area (the most conservative assumption is that the mass enters groundwater at a point). If the source is instantaneous an input mass is entered. Where the source is continuous the mass entering groundwater each day is entered, and this is called the mass flux.
Discussion	Although this is an apparently simple definition when the concentration and flow rate are defined, the ways of calculating mass flux where one of these parameters is not defined are many and varied. The following discussion identifies some factors, which may need to be considered. **Contaminant mass is discharged to unsaturated strata before percolating to groundwater** A conservative and sometimes unrealistic mass flux assumes that there is no attenuation in unsaturated strata. This assumption is realistically conservative if the groundwater table occurs in very shallow gravel strata. A worst-case assumption is often made that the mass flux is directly entering groundwater, rather than first travelling through the unsaturated zone. Because this approach ignores processes in the unsaturated zone, such as adsorption, volatilisation and biodegradation, it will tend to overestimate mass flux. If groundwater is deep, this assumption becomes unrealistic, particularly for decaying contaminants. It is important that the greater degree of groundwater protection associated with a greater depth to the groundwater is reflected in the mass flux value. **Neither the contaminant concentration nor the flow rate are defined** In some situations, neither the contaminant mass nor the flow rate is well defined. This can be the case where a contaminant is being leached from contaminated soil, either by infiltrating rainwater or groundwater throughflow. ***Flow rate is not defined*** In these situations the flow rate is estimated by considering either the rainfall infiltration rate (if leaching is occurring via rainfall infiltration) or by groundwater throughflow (if groundwater is in contact with contaminated soil). For rainfall infiltration through contaminated soil consideration of the area of contaminated soil and rainfall infiltration is necessary, e.g. for a fuel spillage adsorbed onto soil in the unsaturated strata above a water table. Where contaminated soil is in contact with groundwater, the mass flux can then be calculated by assessing the groundwater flow through the contaminated strata. This may be necessary where free phase hydrocarbon product is sitting on top of the water table, contaminated soil is inundated by high groundwater levels, or in a landfill where high groundwater levels inundate the base of the landfill.

To consider the relevant groundwater flow rate, we need to determine the following; the thickness of the flow zone; the depth over which the waste is in contact with groundwater flow or the smear zone of hydrocarbons caused by a fluctuating water table; and finally the width of the contaminated zone. We can calculate the mass flux by multiplying the concentration by the groundwater throughflow beneath the site, using the following equation:

Groundwater throughflow rate = K i A

where:

K = Hydraulic conductivity,

i = Hydraulic gradient, and

A = Area of groundwater contamination.

Determining concentration in water when the soil concentration is known

The concentration of contaminants in leachate or groundwater throughflow can be related to the soil contaminant concentration by considering the distribution coefficient for the contaminant.

$C_{soil} = K_d C_{water}$

where:

K_d = distribution coefficient,

C_{soil} = concentration of contaminant in soil, and

C_{water} = concentration of contaminant in water.

This calculation assumes equilibrium conditions between the soil and water partitioning. The mass flux is then calculated knowing the rainfall recharge rate and the leachate concentration.

Note: Some contaminants are present in soil in a number of phases. For example hydrocarbons can be present in the sorbed phase, a soluble phase, a vapour phase and an immiscible (free) phase.

Determining concentrations in water where there are no soil concentrations

We commonly know neither the concentration of a contaminant in the contaminated soil nor in the groundwater source. Sometimes the concentration of leachate or the contaminated groundwater must be measured, or literature values can be referred to. A few approaches used to estimate the source concentration in contaminated soil or groundwater are discussed below.

Using groundwater monitoring data. Where there are actual groundwater monitoring data, these can be used to calibrate a model to determine the mass flux (i.e. back calculate the mass flux using a groundwater contaminant model).

Leachate tests (laboratory). A sample of the contaminated soil or landfill is collected and tested. There are many methods available including:

Column test. The sample is packed into a column and an appropriate solvent (e.g. local rainwater) is poured onto the column and the concentration of the leachate collected at the bottom of the column is analysed.

	Tumble test. The sample is mixed with a solution in a container and then tumbled for several hours. The solution is then poured off and analysed. *Lysimeter measurements*. A lysimeter allows the collection of in situ soil water in the unsaturated zone (much like a piezometer allows the collection of groundwater). *Literature values.* There are many papers available that cite concentrations of elements in landfill leachate and stormwater. In the absence of any field data, these literature concentrations can be used to estimate mass flux. Alternatively physical relationships cited in the literature, such as the solubility of an element and the partitioning of an element between soil and water (K_d), and the limits to the partitioning (Raoult's Law) can be used to estimate a mass flux. 'Raoult's Law' determines the maximum solubility of a hydrocarbon as: $C_{wmax} = x_i S_i$ where: C_{wmax} = maximum concentration in water x_i = mole fraction of compound, (e.g. mole fraction of benzene/gasolene = 0.03) S_i = solubility of compound, (e.g. water solubility of benzene = 1800 mg/L)

Boundary Condition	**Instantaneous or Continuous or Fixed Duration Mass Input**
Description	Instantaneous source - a slug of contamination is instantaneously injected into the aquifer. In reality nothing can be introduced instantaneously, it always takes some time. However sources which are introduced quickly into an aquifer, compared to the time frame of interest, can be considered to be introduced instantaneously. For example, this would be the case for a spill which may enter groundwater over the period of one hour, and the nearest point of concern is approximately 3 days travel distance away. Continuous source – a contaminant is continuously injected into an aquifer at a constant rate. Check – most models use a daily time frame. Any mass input that is constant on a daily basis can be considered a continuous source. A domestic waste water discharging every day to ground can be considered to be a continuous source. Fixed duration sources – a contaminant is injected into an aquifer at a specified rate for a specified amount of time. Irrigation of wastewater to land over a summer irrigation period could be considered a fixed duration source.

5.2 Model Domain and discretisation

Parameter	Maximum Distance
Units	m
Description	Some models require the maximum distance of concern to be defined, so that solutions for distances within the specified range are calculated. Distances are specified along the x –axis, the direction of groundwater flow. Solutions are determined at distances within the defined range, on the basis of the number of steps defined.

Parameter	Discretisation of the model in space and time - Number of Steps
Units	Integer
Description	Most models require that the solution domain is discretised in time and space. The greater the degree of discretisation the better the definition of the maximum plume length curve. However a larger number of steps requires a longer solution time.

Assumption	2 or 3 dimensions/infinite and semi-infinite
Description	The solution is defined in two dimensions. Concentrations are calculated over a groundwater surface, using a 2D coordinate system (e.g. where the x axis is the groundwater flow direction and along the y axis is perpendicular to the groundwater flow direction). This option assumes that the contaminant is fully mixed over the depth of the aquifer. The solution is defined in three dimensions. Concentrations are calculated in three dimensions, using a coordinate system, where the x axis is the groundwater flow direction and along the y axis is perpendicular to the groundwater flow direction, and the z axis represents depth. As this option allows contaminants to move in 3 dimensions it is usually more realistic. Semi-infinite – the contaminant is released into the top of the aquifer. Infinite – the contaminant is released into the middle of an aquifer that is so thick that its top and bottom boundaries have no effect on the migration of the contaminant. Note: Where a 2 dimensional solution domain is selected, an aquifer thickness must also be defined. The 2 dimensional solution assumes a well mixed source, with no further mixing, for instance where there are bounding surfaces to the aquifer.

Parameter	Aquifer Thickness
Units	m
Description	Where a model defines the solution in 2 dimensions, an aquifer thickness must be specified and the mass flux is divided by the aquifer thickness. The aquifer thickness determined should really be considered an effective aquifer thickness, over which the contaminant is likely to spread. More conservatively, the aquifer thickness can be based on the depth to the likely receptors.

5.3 Hydrogeological parameters

Parameter	**Effective porosity (σ or n)**			
Units	e.g.: m^3 / m^3			
Description	The dimensionless ratio of the volume of interconnected voids to the bulk volume of the aquifer matrix. Note that "total porosity" is the ratio of all voids (including non-connected voids) to the bulk volume of the aquifer matrix. The difference between total and effective porosity reflects lithological controls on pore structure.			
Typical values for alluvial aquifers	**Porosity**	**Method of Measurement**	**Location**	**Reference**
	0.25	Field density tests	Heretaunga Plains	Thorpe et al. (1982)
	0.2	Repacked aquifer material in laboratory column	Templeton	Sinton et al. (1997)
	0.19	Repacked aquifer material in laboratory column	Burnham	Close and Pang (1999)
	0.2 – 0.3	Resistivity results	McLeans Island	Broadbent and Callander (1991)
	0.25 – 0.35	Seismic results	Canterbury Plains Quaternary sediments	Broadbent (1978)
Typical values for other types of strata	The following values in this section are taken from Domenico and Schwartz (1990):			
Rock type	Range of porosities			
SEDIMENTARY				
Gravel, coarse	0.24 – 0.36			
Gravel, fine	0.25 – 0.38			
Sand, coarse	0.31 – 0.46			
Sand, fine	0.26 – 0.53			
Silt	0.34 – 0.61			
Clay	0.34 – 0.60			
SEDIMENTARY ROCKS				
Sandstone	0.05 – 0.30			
Siltstone	0.21 – 0.41			

Limestone, dolostone	0 – 0.20
Karst limestone	0.05 – 0.50
Shale	0 – 0.10
CRYSTALLINE (IGNEOUS & METAMORPHIC) ROCKS	
Fractured crystalline rock	0 – 0.10
Dense crystalline rock	0 – 0.05
Basalt	0.03 – 0.35
Weathered granite	0.34 – 0.57
Weathered gabbro	0.42 –0.45

Parameter	**Pore Velocity (v)**
Units	m/day
Description	The pore velocity, v, (also known as the contaminant transport velocity) is calculated as follows: v = (-Ki)/n where: n = porosity i = hydraulic gradient K = hydraulic conductivity Note 1: Beware, in heterogeneous aquifers pore velocities determined from tracer tests are quite different to those calculated from pumping test results, refer to the following page and Sections 4.1.1. and 4.1.2 in this appendix. Note 2: Beware the term 'velocity' is also used to describe the flux velocity, (be sure you know which one you are dealing with!). The flux velocity is the volumetric flow rate (or flux) divided by the cross-sectional area normal to flow. U = -Ki
Guidance on selection	Because of aquifer heterogeneity, there is often a discrepancy between the mean groundwater pore velocities often apparent from tracer test studies and those calculated from pumping test data (for estimates of K and n) and piezometric maps. For example, using typical hydraulic conductivity values derived from pumping test results in alluvial gravel aquifers (ranging from 10 m/d to 200 m/d), hydraulic gradients from piezometric contour maps (ranging from 0.01 to 0.001) and a typical porosity for gravel strata (ranging between 0.2 and 0.4), gives velocities from less than 1 m/day up to 10 m/day. However, tracer tests in Canterbury alluvial

	aquifers indicate much faster pore velocities ranging from 5 to 200 m/day. The likely explanation for this difference is that in a pumping test the calculated hydraulic conductivity is based on the drawdown response as water is drawn from both low and high permeability strata. In contrast, for a tracer test, hydraulic conductivity is calculated based on the time of maximum concentration at any observation point, which is related to the fastest moving groundwater (flowing through the most permeable pathway within the aquifer strata). The following approach for choosing reasonable ranges of pore velocity estimates is advocated: • For heterogeneous strata, such as alluvial gravels, pore velocity estimates should be based on tracer test data. Where there are no data available in a specific area, reference should be made to the data available in the literature for similar strata. In alluvial gravel aquifers, tracer tests at Burnham, Templeton and Heretaunga Plains studies, as described by Sinton et al. (1997) and Pang and Close (1999) and Thorpe et al. (1982) respectively indicate peak concentration velocities of between 60 – 140 m/day. On the basis of these velocities it may be necessary to recognise that the maximum pore velocity could be as high as 200 m/day. • For homogeneous strata such as sand or beach gravels calculated pore velocity (v) estimates from pumping test data are likely to be appropriate, using the equation $v = (Ki)/n$.

Parameter	**Dispersivity** **Longitudinal dispersivity a_L** **Transverse dispersivity, a_T** **Vertical dispersivity, a_V** **Longitudinal scale dispersivity, E1** **Transverse scale dispersivity, E_2** **Vertical scale dispersivity, E_3**
Units	m
Description	Dispersion refers to the process whereby a plume will spread out in a longitudinal direction (along the direction of groundwater flow), transversely (perpendicular to groundwater flow), and vertically downwards due to mechanical mixing in the aquifer and chemical diffusion. Dispersion occurs as a result of two processes - chemical diffusion and mechanical dispersion. Diffusion originates from mixing caused by random molecular motions due to the kinetic energy of the contaminant. Mechanical dispersion is mixing that occurs as a consequence of local variations in velocity around some mean velocity. Dispersivity is defined in three dimensions, in the direction of groundwater flow – longitudinal dispersivity (α_L), perpendicular to the direction of groundwater flow – transverse dispersivity (α_T), and with depth (α_V), – vertical dispersivity. Dispersivity values increase with scale; i.e. the further away from a source, the greater the contaminant is dispersed. More recently, scale dispersivity terms have been defined (Hunt, 1998) as follows: $(\alpha_L) = E_1 x$, where (α_L) is the longitudinal dispersivity, x is the distance from source, and E_1, is the longitudinal dispersivity dimensionless coefficient. Similarly, $(\alpha_T) = E_2 x$, where (α_T) is the transverse dispersivity, x is the distance from source, and E_2, is the transverse dispersivity dimensionless coefficient, and $(\alpha_V) = E_3 x$, where (α_V) is the vertical dispersivity, x is the distance from source, and E3, is the vertical dispersivity dimensionless coefficient.

Parameter	**Hydraulic conductivity (K)**
Units	m/day
Description	The hydraulic conductivity is defined as the volume of water that will move through a porous medium, in unit time, under a unit hydraulic gradient, through a unit area measured at right angles to the direction of flow. The hydraulic conductivity parameter contains properties of the fluid (water) and of the saturated porous medium (the aquifer). It is defined as: $K = \frac{k\rho_{water} g}{\mu}$ Where: k = intrinsic permeability of the strata g = acceleration due to gravity ρ_{water} = density of water μ = viscosity of water Hydraulic conductivity can vary in differing directions and this feature is called anisotropy. Anisotropy especially occurs in water laid sediments which are often stratified and have a greater conductivity in the direction of flow. The major axes of hydraulic conductivity are defined as K_{xx}, K_{yy} and K_{zz}. Anisotropy is usually represented on a layer by layer basis in numerical models, where the magnitude of the anisotropy and its principal direction are defined. Hydraulic conductivity also varies spatially from one point in the aquifer to another, this property is called heterogeneity. Heterogeneity can be represented in a numerical model by having different zones of hydraulic conductivity. Both heterogeneity and anisotropy affect groundwater flow.
Typical values <u>*Sedimentary*</u> Gravel Coarse sand	Values taken from Domenico and Schwartz (1990) $3 \times 10^{-4} - 3 \times 10^{-2}$ $9 \times 10^{-7} - 6 \times 10^{-3}$
Medium sand Fine sand Silt, Loess Till Clay Un-weathered marine clay	$9 \times 10^{-7} - 5 \times 10^{-4}$ $2 \times 10^{-7} - 2 \times 10^{-4}$ $1 \times 10^{-9} - 2 \times 10^{-5}$ $1 \times 10^{-12} - 2 \times 10^{-6}$ $1 \times 10^{-11} - 4.7 \times 10^{-9}$ $8 \times 10^{-13} - 2 \times 10^{-9}$

Sedimentary rocks	
Karstified and reef (bioherm) limestone	$1 \times 10^{-6} - 2 \times 10^{-2}$
Limestone, dolostone	$1 \times 10^{-9} - 6 \times 10^{-6}$
Sandstone	$3 \times 10^{-10} - 6 \times 10^{-6}$
Siltstone	$1 \times 10^{-11} - 1.4 \times 10^{-8}$
Salt	$1 \times 10^{-12} - 1 \times 10^{-10}$
Anhydrite	$4 \times 10^{-13} - 2 \times 10^{-8}$
Shale	$1 \times 10^{-13} - 2 \times 10^{-9}$
Crystalline rocks	
Permeable basalt	$4 \times 10^{-7} - 2 \times 10^{-2}$
Fractured igneous and metamorphic rock	$8 \times 10^{-9} - 3 \times 10^{-4}$
Weathered granite	$3.3 \times 10^{-6} - 5.2 \times 10^{-5}$
Weathered gabbro	$5.5 \times 10^{-7} - 3.8 \times 10^{-6}$
Basalt	$2 \times 10^{-11} - 4.2 \times 10^{-7}$
Massive (un-fractured) igneous and metamorphic rocks	$3 \times 10^{-14} - 2 \times 10^{-10}$

Parameter	**Hydraulic Gradient (i)**
Units	unitless (m/m)
Description	The slope of the potentiometric surface. In unconfined aquifers, this is equivalent to the slope of the water table. The hydraulic gradient is typically calculated by constructing potentiometric surface maps using static water level data from monitoring wells and estimating the slope of the potentiometric surface. Typically it can range from 0.01 - 0.0001.

5.4 Chemical or biological processes

Parameter	**Decay Coefficient (λ)**			
Units	1/day			
Description	The decay coefficient is used to represent both radioactive decay and biological die-off of the source. In both cases the initial concentration of a contaminant is continually decreasing as follows; $N(t) = N_0 e^{-\lambda t}$ Where, N is the number of elements in the contaminant source (i.e. faecal coliforms, atoms, etc.), t is time and λ is the rate constant for decay. $T_{1/2} = 0.693/\lambda$, where $T_{1/2}$ is the half life and $T_{90} = 2.303/\lambda$, where T_{90} is the time where 90% die off has occurred.			
Discussion	*Chemicals.* Decay rates are usually derived from laboratory experiments. There are many references which list decay rates for many substances, i.e. Howard et al., (1991) list environmental decay rates for soil, water and air environments for a comprehensive range of chemicals *Microbes.* For microbes, the decay rates appear to vary significantly depending on the environment they are in. This is at least partly because the measured decay rates for microbes assessed through tracer tests also account for other removal processes dependent on aquifer strata such as filtration, sedimentation and adsorption (Sinton, 1997). As with any data derived from model calibration to test data, the decay rates that are obtained are very unlikely to be a unique solution. Some decay rates for microbial tracer tests in Canterbury are shown in the table below. NOTE: If a decay rate derived from model calibration to tracer test data is used, then it is important that a model with similar assumptions is used, i.e. with the same model bias.			
Some examples of decay rates	Contaminant	λ (day $^{-1}$)	T_{50} (half –life)	T_{90}
	Benzene	$0.07 - 9.5 \times 10^{-4}$	10 days to 24 months	33 days – 2424 days
	Toluene	0.1 – 0.025	7 days to 4 weeks	23 days – 92 days
	Ethylbenzene	$0.12 - 3.0 \times 10^{-3}$	6 days to 228 days	19 days – 768 days
	Xylene	$0.05 - 1.9 \times 10^{-3}$	2 - weeks to 12 months	46 days – 1212 days
	Faecal coliforms Oxidation pond effluent	0.37 day $^{-1}$	1.8 days	6.2 days
	Faecal coliforms Septic tank effluent	$\lambda = 0.8$ day $^{-1}$	0.87 days	T_{90} = 2.9 days,

Parameter	Kd = distribution coefficient (used for adsorption assessments)
Units	mL/g
Description	The coefficient that describes how much sorption of contaminants to the solid aquifer matrix there will be. The degree of sorption depends on both aquifer and constituent properties. Increasing Kd values are indicative of a greater tendency for sorption. Usually estimated from soil and chemical data using variables described below; Koc = organic carbon-water partition coefficient, foc = fraction organic content on uncontaminated soil where Kd = Koc x foc Also derived from batch experiments.

Parameter	Organic Carbon Partition Coefficient (Koc)
Units	(mg/kg) (L/kg) (mg /L) or (mL/g)
Description	Chemical-specific partition coefficient between soil organic carbon and the aqueous phase. Larger values indicate greater affinity of contaminants for the organic carbon fraction of soil. This value is chemical specific and can be found in chemical reference books. Note there is a wide range of reported values for Koc in chemical reference literature, listing relationships between Koc and solubility of Koc and the octanol-water partition coefficient (Kow). Some typical examples are: Benzene 38 L/kg Toluene 135 L/kg Ethylbenzene 95 L/kg Xylene 240 L/kg

Parameter	Fraction Organic Carbon (foc)
Units	Unitless
Description	Fraction of the aquifer soil matrix comprised of natural organic carbon in uncontaminated areas. More natural organic carbon means higher adsorption of organic constituents on the aquifer matrix. Typical Values range from 0.0002 - 0.03. The fraction organic carbon value should be measured if possible by collecting a sample of aquifer material from an uncontaminated zone and performing a laboratory analysis (e.g. ASTM method 2974-87 or equivalent).

6.0 Typical errors

Analytical models are simple to use; errors resulting from their careless use are less likely to occur. However the following types of errors are significant in these types of models:

- Inappropriate model simplifying assumptions for a given modelling problem
- Failure to use appropriate assumptions – or using a mismatch of assumptions when determining mass flux
- Failure to explore the impact on model predictions caused by the uncertainty of parameters

Model simplifying assumptions

Perhaps the most significant of model errors for analytical contaminant transport models is that of inappropriate model simplicity or model assumptions for a given model problem. Given that plume migration is dominated by aquifer heterogeneity the assumption of aquifer homogeneity is possibly the most important simplification of an analytical model . Consequently, a model auditor needs to consider whether neglect of heterogeneity impacts is important for the modelled problem being considered. For ranking of the feasibility of development options, or generic worst case type assessments heterogeneity is unlikely to be a problem. However, for consideration of the location of appropriate monitoring wells, heterogeneity will impact on the solution and needs to be represented using a numerical model with site measurements to gain a more accurate description of the aquifer system.

The most extreme model in terms of simplification is the mass mixing model. This model is really only appropriate for estimating the long term average concentration increases that may occur over an aquifer as a result of widespread land use changes which introduce a contaminant into water. It is not possible to estimate the development and migration of a contaminant plume with these types of models.

Less well understood biases from model assumptions are those from scale dispersivity assumptions – as discussed in Section 4 of this Appendix. where it is noted that the same scale dispersivity relationships will give different solutions where equations are based on the constant dispersivity assumption compared to those based on the scale dependant dispersivity assumption. This is because the constant dispersivity relationship assumes that all the mass is dispersed at a rate appropriate for one specific scale. Whereas the scale dependant equations assume the mass is dispersed at an increasing rate as scale increases. If the contaminant is conservative, the constant dispersivity solution underestimates concentrations, whereas for the decaying contaminant investigated, the constant dispersivity solution overestimated the concentration.

Inappropriate assessment of mass flux

Sometimes there is inconsistency between assumptions used in the analysis of field data to determine a model input parameter and the contaminant transport model assumptions which creates a model error. One example encountered was where a mass mixing model was used to determine the groundwater source concentration for input into an advection dispersion model. The mixed concentration was determined C_o (from Figure B2), and then input into the advection dispersion model which had a natural background flow of Q_n (from Figure B2) and not the total flow of Q_o which represents the additional drainage flow. The consequences of this error is to reduce the mass flux and therefore the calculated output concentrations.

Similarly another example, discussed in the case study in Section 7 of this Appendix, describes the contaminant source as a groundwater concentration occurring over a specified volume of the aquifer. However, when the model was used to explore the impact of various velocities on plume length, the mass flux in the model varied with groundwater velocity, which does not make sense for a stormwater discharge into a soak hole. However, varying the mass flux with groundwater velocities would be an appropriate assumption in some settings, for example, where the contaminant source was hydrocarbon spill floating on the water table.

Failure to explore the impact of parameter uncertainty on model predictions

Because of the uncertainty surrounding any parameter used in a model, it is potentially misleading to simply choose one set of model input parameters and one model output. Instead, it is important for model applications to calculate the range of possible outcomes, on the basis of the range of available parameter estimates so that the worst of what may potentially happen may be considered.

The following table (Table B5) lists the types of errors found in Analytical contaminant transport models, their implications, and hints for the auditor on items to check.

Table B5: Checklist for Analytical Contaminant Transport model Errors

Data gathering errors	Potential implication for solution	Auditor check	OK - tick	Comments
Field measurements of parameters incorporate inherent inaccuracies	These are errors are associated with human error or an instrument error used for instance in a pumping test or a tracer test. Calibration to inaccurate targets compromises model accuracy and predictions.	Have measuring errors been assessed?		
Analysis of field data. Many of the model input parameters require some analysis of the field measurements. For instance mean pore velocity relies on the analysis of pump test drawdown – time data, water level gradients, and porosity or alternatively concentration – time data from tracer tests.	Inaccurate assumptions in the analysis of field data will compromise the analysis of the parameters, and the model calibration.	Are the estimates of aquifer parameters calculated correctly from aquifer or tracer tests?		
Extrapolation of field data. Aquifer properties, such as hydraulic conductivity are different when derived from a pump test compared to a tracer test.	In a pumping test the calculated hydraulic conductivity is based on the drawdown response as water is drawn from both low and high permeability strata. In contrast, for a tracer test, hydraulic conductivity is calculated based on the time of maximum concentration at any observation point, which is related to the fastest moving groundwater (flowing through the most permeable pathway within the aquifer strata). Inappropriate extrapolation will compromise the model calibration.	Has the appropriate extrapolation of field data been used for the strata at the site?		

Data input errors	Potential implication for solution	Auditor check	OK - tick	Comments
Inconsistent parameter units - i.e. grams and metres and days.	It is important to use consistent units when modelling. Inaccuracies can occur easily if the same units are not used.	Are the model units consistent for all parameters – i.e. days and seconds, cubic metres per day etc?		
Contaminant discharge must be specified over entire transient simulation period.	Failing to define discharge rates for the full time period give inaccurate results.	Is the discharge specified correctly for the transient simulation period?		
Model assumption errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Variable or constant density assumptions	Neglecting density variations can give incorrect indications of flow field.	Are there density variations within the flow field and if so have they been accounted for?		
Inappropriate model selection given model assumptions re boundaries and initial conditions and parameterisation/ oversimplification of the problem.	It is inappropriate to attempt to define complex plume movement with an analytical model incapable of representing heterogeneity and other known hydrogeological features of a complex site, such as rivers, lakes, variable aquifer thickness or hydraulic conductivity, 3-D groundwater flow, or multiple aquifers. The rate of contaminant entering an aquifer when using a constant concentration boundary varies with pore velocity. This boundary condition is often misused for situations where a velocity independent flux is entering groundwater from the surface, i.e. in stormwater discharges etc.	Is it appropriate to use an analytical model for the problem being assessed? If it is – has the correct solution been chosen? Have the impacts of parameter heterogeneity on model plume predictions been assessed?		

Calibration errors	Potential implication for solution	Auditor check	OK - tick	Comments
Forcing questionable data to fit	Where a model has been fit to an observation bores data is sketchy and does not show a complete breakthrough curve, such that it is not possible to tell whether the peak concentration has not yet come or has passed – the predictions will be compromised by this uncertainty.	Have questionable data been forced to fit?		
Sensitivity analysis	A sensitivity analysis should be used a part of the calibration process – so that calibration efforts are targeted to the parameters which model predictions are most sensitive to.	Has a sensitivity analysis been undertaken? Which were the most sensitive parameters?		
Prediction errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Not incorporating data variability or uncertainty into the analysis	As discussed, despite our efforts, model parameters can never be precisely known. Variations in measured data are either an indication of measurement uncertainty, model bias, or the result of real physical differences. Use the range of data values that reflect data variability to give an indication of the range of possible model predictions. A conservative approach in reporting model results, recognises the uncertainty inherent in modelling and displays a firm understanding of the goals of groundwater modelling	Has the model report discussed the situations where the model predictions are most likely to be valid?		
Blind acceptance of model output	The accuracy of a model is no better than the accuracy of the data. Make sure that the model results agree with your understanding of the site hydrogeology and sound hydrogeological principles.	Do the model results agree with your understanding of the site hydrogeology and hydrogeological principles?		

Predictive uncertainty must be addressed.	Given the non-uniqueness of models, it is important the uncertainty of predictions is explored and the limiting scenario (worst case) is reported.	Has predictive uncertainty analysis been undertaken?		
The correct predictive simulations must be undertaken to fulfil model purpose		Does the model fulfil its purpose?		

7.0 Case studies

A BP Risc model example

The BP Risc model uses the contaminant package AT123D. However, while the AT123D model requires a mass flux input into a defined area to be specified, the BP Risc version requires that a groundwater source concentration over an area and depth is specified. The BP Risc version then translates the source concentration value into a mass flux entering the aquifer, which is achieved by multiplying the source concentration, by the groundwater flux, and by the cross sectional area of the source perpendicular to groundwater flow (please refer to the BP Risc users manual).

The case study used the BP Risc model to assess the potential contamination occurring from a stormwater discharge into a soak hole at a timber treatment site. An unconfined alluvial aquifer underlies the site. Note: this was a purely predictive model, i.e. no calibration.

The following model inputs were used.

Contaminants: No particular contaminants were targeted, rather the dilution rate for non decaying contaminants was considered.

Contaminant transport velocity: The contaminant transport velocity is calculated using the following equation:

$$v = (-Ki)/n$$

Where: K = hydraulic conductivity

i = hydraulic gradient

n = porosity

In this assessment a range of values for hydraulic conductivity and hydraulic gradient were used. The hydraulic conductivity (K), i.e., the horizontal hydraulic conductivity of the saturated porous medium was assumed to range between 1 and 500 m/day. The hydraulic gradient (i), or slope of the potentiometric surface, was assumed to vary between 0.001 and 0.00001. A porosity of 0.25 was assumed. This combination of input parameters gives a range of groundwater contaminant velocities of between 0.00004 m/day and 2 m/day.

These calculated velocities were considered low for the alluvial aquifers of concern where tracer tests indicated pore velocities of 5 to 200 m/day. Remember for non decaying contaminants a slower contaminant transport velocity is more conservative, i.e. the plume will migrate further with less dispersion. Consequently, the velocities used in this assessment can be considered to be conservative from a mass transport perspective.

Mass flux: Mass flux is calculated from the discharge rate of the contaminant (L^3/T) multiplied by the concentration (M/L^3):

Mass Flux = Concentration x flow rate

Although this is an apparently simple definition, the ways of calculating mass flux are many and varied, e.g., the BP Risc model and the AT123D model use differing methods. In this model, the mass flux was calculated by multiplying the concentration by the groundwater throughflow beneath the site.

The groundwater throughflow rate = K iA

Where K = Hydraulic conductivity

i = Hydraulic gradient

A = Area of groundwater contamination

Concentration

It was unclear how the source concentrations in the modelled scenarios were determined. They should represent leaching of chemicals from natural soils in addition to possible concentrations from any chemical spillages. The source input has been applied for 50 years which is a conservative approach for a stormwater discharge.

Area of contamination

The source area has been assumed to be approximately the size of the soak hole, which is understood to be 2 m (perpendicular to groundwater flow direction) by 5 m (in groundwater flow direction) in area. The source concentration is assumed to extend to a depth of 0.3 m depth. An appropriate depth and cross sectional area is difficult to assess and difficult to justify. Some mounding and spreading of the stormwater would be expected beyond the soak hole, so this area could be greater than the 5 m by 2 m estimated. Similarly, the cross sectional depth could extend more or less than the 0.3 m depth. In the absence of any data a conservative assessment should be assumed, i.e. on the basis of distance between lowest water table and the shallowest well screen depths, where a contaminant would be at its most concentrated.

Groundwater throughflow

As discussed in the groundwater velocity section, a range of differing hydraulic conductivity (K) and hydraulic gradient values (i) were used. Consequently, a range of groundwater throughflow values are used, which means that a range of differing mass fluxes are assumed to enter the aquifer. The mass flux therefore becomes greater if we assume faster moving groundwater systems. The range of mass flux entering the aquifer has been assumed to be dependant on the groundwater flow regime, rather than on the range of stormwater flows entering the aquifer, which is not consistent with the physical problem. A worst case situation would occur where a high stormwater event causing a large mass flux enters a very slow moving groundwater system.

A catchment flow analysis for the soakhole catchment would be required to assess varying stormwater flows into the soakhole. Then the mass flux could be calculated on the basis of the stormwater flows and concentrations derived from leaching tests on soils and assessments of spillage risk.

Dispersivity: The dispersivity relationship used in BP Risc is not specified. However when compared to the Neuman relationship outlined in section 4 above, the relationship used in BP Risk calculates a greater dispersivity for a distance of 20 m travel (i.e. 2.59 instead of 1.52 calculated by Neuman's relationship). A recent review of tracer tests and modelling in Canterbury (Moore and Scott, 2000) indicates that dispersivities of approximately 0.5 times lower than that calculated by the Neuman relationship are appropriate when using the constant dispersivity contaminant transport equation utilised in AT123D.

Do the Model Outputs Represent Conservative Predictions of Likely Concentrations?

In summary the assumptions that were made can be grouped as follows:

Conservative	Not Conservative
• Low transport velocity causes low dispersion • 50 year source input	• Low transport velocity causes low mass flux • Uncertainty over source concentration, which may not allow for chemical spillages • Source area is limited to the soak hole dimensions • High dispersivity values have been used

On balance, it would appear that this modelled assessment of a 133 fold dilution over 20 metres is not necessarily conservative, although there is uncertainty about some of the parameters that have been used.

For a comparison, a review of tracer tests in New Zealand gravel aquifers (Environment Canterbury report U99/84) report a dilution rate of 1-2 orders of magnitude reduction can be expected over a 100 m travel distance within this type of aquifer.

Table B6: Case study - checklist for analytical contaminant transport model errors

Data gathering errors	Potential implication for solution	Auditor check	OK - tick	Comments
Field measurements of parameters incorporate inherent inaccuracies	These are errors are associated with human error or an instrument error used for instance in a pumping test or a tracer test. Calibration to inaccurate targets compromises model accuracy and predictions.	Have measuring errors been assessed?		Not stated.
Analysis of field data. Many of the model input parameters require some analysis of the field measurements. For instance mean pore velocity relies on the analysis of pump test drawdown – time data, water level gradients, and porosity or alternatively concentration – time data from tracer tests.	Inaccurate assumptions in the analysis of field data will comprise the analysis of the parameters, and the model calibration.	Are the estimates of aquifer parameters calculated correctly from aquifer or tracer tests?	√	A range of velocities were considered. BUT the mass flux varied with velocity estimates, which is not appropriate for a storm water discharge.
Extrapolation of field data. Aquifer properties, such as hydraulic conductivity are different when derived from a pumping test compared to a tracer test.	In a pump test the calculated hydraulic conductivity is based on the drawdown response as water is drawn from both low and high permeability strata. In contrast, for a tracer test, hydraulic conductivity is calculated based on the time of maximum concentration at any observation point, which is related to the fastest moving groundwater (flowing through the most permeable pathway within the aquifer strata). Inappropriate extrapolation will comprise the model calibration.	Has the appropriate extrapolation of field data been used for the strata at the site?	√	Assumed a range of velocities.

Data input errors	Potential implication for solution	Auditor check	OK - tick	Comments
Inconsistent parameter units - i.e. grams and metres and days.	It is important to use consistent units when modelling. Inaccuracies can occur easily if the same units are not used.	Are the model units consistent for all parameters – i.e. days and seconds, cubic metres per day etc?	√	Ok
Contaminant discharge must be specified over entire transient simulation period.	Failing to define discharge rates for the full time period give inaccurate results.	Is the discharge specified correctly for the transient simulation period?	√	Ok
Model assumption errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Variable or constant density assumptions	Neglecting density variations can give incorrect indications of flow field.	Are there density variations within the flow field and if so have they been accounted for?	√	Appropriate for this setting.
Inappropriate model selection given model assumptions re boundaries and initial conditions and parameterisation/ oversimplification of the problem.	It is inappropriate to attempt to define complex plume movement with an analytical model incapable of representing heterogeneity and other known hydrogeological features of a complex site, such as rivers, lakes, variable aquifer thickness or hydraulic conductivity, 3-D groundwater flow, or multiple aquifers. The rate of contaminant entering an aquifer when using a constant concentration boundary varies with pore velocity. This boundary condition is often misused for situations where a velocity independent flux is entering groundwater from the surface, i.e. in stormwater discharges etc.	Is it appropriate to use an analytical model for the problem being assessed? If it is – has the correct solution been chosen? Have the impacts of parameter heterogeneity on model plume predictions been assessed?		**Mass flux assumptions are not appropriate for a stormwater discharge!**

Calibration errors	Potential implication for solution	Auditor check	OK - tick	Comments
Forcing questionable data to fit	Where a model has been fit to an observation bores data is sketchy and does not show a complete breakthrough curve, such that it is not possible to tell whether the peak	Have questionable data been forced to fit?		

	concentration has not yet come or has passed – the predictions will be compromised by this uncertainty.			
Sensitivity analysis	A sensitivity analysis should be used a part of the calibration process – so that calibration efforts are targeted towards the parameters to which model predictions are most sensitive.	Has a sensitivity analysis been undertaken? Which were the most sensitive parameters?		
Prediction errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Not incorporating data variability or uncertainty into the analysis	As discussed, despite our efforts, model parameters can never be precisely known. Variations in measured data are either an indication of measurement uncertainty, model bias, or the result of real physical differences. Use the range of data values that reflect data variability to give an indication of the range of possible model predictions. A conservative approach in reporting model results, recognises the uncertainty inherent in modelling and displays a firm understanding of the goals of groundwater modelling	Has the model report discussed the situations where the model predictions are most likely to be valid?	√	Range of aquifer parameters used – ensures the conservative end of the range is included in the assessment.
Blind acceptance of model output	A model's accuracy is no better than the accuracy of the data. Make sure that the model results agree with your understanding of the site hydrogeology and sound hydrogeological principles.	Do the model results agree with your understanding of the site hydrogeology and hydrogeological principles?		
Predictive uncertainty must be addressed.	Given the non-uniqueness of models, it is important the uncertainty of predictions is explored and the limiting scenario (worst case) is reported.	Has predictive uncertainty analysis been undertaken?	√	Addressed although compromised by mass flux assumptions.

The correct predictive simulations must be undertaken to fulfil model purpose		Does the model fulfil its purpose?	√	The modelling answered the questions asked – albeit potentially incorrectly.

Appendix C

Appendix C – Numerical flow model

Table of contents

Figures

Tables

1.0 Description

Numerical flow models solve the partial differential flow equations for the entire flow field of interest. To do this, the area of interest is subdivided into small areas (referred to as cells or elements) and the flow equation is approximated by algebraic equations for each cell. These algebraic equations are solved numerically through an iterative process. The two most common groups of numerical models are finite difference and finite element models. Of these, the finite difference model MODFLOW is by far the most widely used.

Numerical flow models are used where the assumptions of the more simple analytical equation are not appropriate. Numerical models allow for multiple layers and aquifer heterogeneity within an aquifer system and for as complex a combination of aquifer boundaries and stresses as is required. They are used for:

- Predicting groundwater flow in complex aquifer systems for which there is no appropriate analytical solution;
- Predicting groundwater flow for an entire aquifer system, such as when assessing aquifer management options;
- Predicting impacts on flow for complex large scale developments such as quarrying, irrigation schemes, etc, for which there is no appropriate analytical solution;
- Predicting impacts on flow where the possible magnitude of predictions needs to be as realistic as possible.

Table C1 lists the commonly available numerical codes, of which the most commonly used is MODFLOW.

Table C1: Commonly available numerical flow model codes

Code	Description
MODFLOW	3D finite difference saturated flow model
ASM	2D finite difference saturated flow model
SEEP2D	2D finite element flow model – saturated and unsaturated flow
HST3D*	3D finite difference saturated flow, heat and solute transport model.
SUTRA*	2D finite element flow and contaminant transport density driven saturated and unsaturated zone transport
FEMWATER*	3D finite element flow and contaminant transport density driven saturated and unsaturated zone transport.

*Flow and contaminant transport

The model inputs which govern groundwater flow are dependent on the following factors:

- Aquifer geological conditions, such as top and bottom elevations, and confining layers.
- Aquifer hydrological parameters such as transmissivity and storativity.
- Aquifer stresses, such as recharge from rainfall and rivers and pumping from wells.
- Aquifer flow boundaries, such as impermeable and no-flow boundaries, or drains, rivers, etc.

2.0 Numerical flow models – how do they work?

Using MODFLOW as an example of how a numerical model works, the mathematical model for three dimensional movement of groundwater of constant density through porous strata can be described by the following partial differential equation.

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

where:

K_{xx}, K_{yy} and K_{zz} = values of hydraulic conductivity along the x,y and z coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity.

h = the potentiometric head

W = a volumetric flux per unit volume and represents sources and/or sinks of water

S_s = specific storage of the porous material

t = time

This equation can be difficult to solve, particularly when all the terms in the equation can vary spatially and temporally. By dividing the area of interest (the model domain) into a mesh of model cells (or elements for finite element models), and splitting the model simulation into time steps, the equation above can be solved by a series of much simpler algebraic equations for each model cell, in each time step. Figure C1 illustrates how the model domain can be split into cells.

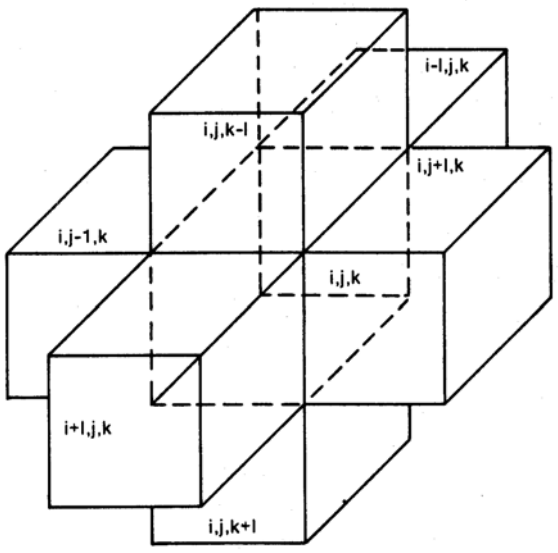

Figure C1: Discretisation of the model domain into cells aligned along three principal axes, l (rows), j (columns), and k(layers).

Where the model domain is discretised spatially into model cells, as shown in Figure C1. The algebraic equation for the balance of flow for each model cell is

$$\Sigma Q_i = S_S{}^{\Delta h}\Delta V$$

Where:

Q_i = flow rate into the cell

S_S = Specific storage (Storativity divided by aquifer thickness)

ΔV = Volume of the cell

Δh = Change in water level over a time interval of length Δt

Additional algebraic equations are used to determine the flow components (Q_i) in this equation (the specific storage and volume of the cell are defined in model inputs). The hydraulic head (i.e. the dependent variable) is calculated for each cell. The model iterates to a solution for this system of algebraic equations in each cell for each time step. The method starts by arbitrarily assigning a trial value or estimate, for the head in each cell. During each time step these estimates are altered in a step-wise fashion to produce a new set of heads which is in closer agreement with the system of equations. This procedure is repeated successively until the heads approach values which would exactly satisfy the set of equations. Each repetition of the calculation is called an iteration.

Finite difference models have ‘cells’ which make up a rectangular grid over which the spatial density of individual cells may change. Finite element models have ‘elements’ or ‘segments’ that make up a model mesh in which the length or orientation of the mesh elements is not fixed.

3.0 Calibration targets for numerical flow models

3.1 Calibration parameters

The following is a list of some parameters that are altered in the calibration of a numerical flow model. A full description of these parameters is outlined in Section 5 of this appendix.

Calibration parameters

- Hydraulic conductivity or transmissivity
- Storage coefficients
- Stream and river bed conductances
- Recharge rates
- Boundary conditions

3.2 Calibration Targets

Both qualitative and quantitative calibration criteria are used to measure the success of flow models calibration. As summarised below.

Qualitative calibration criteria (These are subjective assessment measures.)

- Comparison of drawdown curves (water level – time data)
- Assessment of the 'reasonableness' of the input parameters
- Piezometric contour patterns
- Water balance estimates
- Water level hydrographs
- Patterns of hydrograph

Quantitative calibration criteria

- Water level and flow measurements

  Statistical analysis-Mean, root mean square, standard deviations.

Quantitative measurements

The match to water levels and flow measurements, taken at specific points in space and time is measured quantitatively. This is done using a number of statistical, and mathematical measures of the difference between measured and simulated water levels and flow measurements. These differences are called model error. The objective of calibration is to minimise this error. The range of measures for the quantification of model error are called the objective function. Table C2 outlines a number of different forms of these measures of fit or objective functions.

In addition to these mathematical measures, the residuals between measured and modelled data should be random. Where there is a trend in the residuals, the model configuration may be in error and should be revisited.

Table C2: Quantitative calibration criteria. Criteria in this table are to be used only as a guide to model calibration success; they should not be used without analysis and reference to the hydrogeological basis of the model.

Description of measure	Equation	Comment
Residual	$R_i = H_i - h_i$ where: R_i = residual H_i = measured head at location i h_i = modelled head at location i	The smaller the residual the better the calibration.
Mean error (ME)	$\frac{1}{n}\sum_{i=1}^{n}(H_i - h_i)$	A mean error incorporates both negative and positive residuals. Therefore a small mean error may not indicate a good calibration.
Mean absolute error (MAE)	$\frac{1}{n}\sum_{i=1}^{n}\lvert H_i - h_i\rvert$	A small MAE indicates a good calibration.
Root mean squared error (RMS)	$\frac{1}{n}\sum_{i=1}^{n}\sqrt{(H_i - h_i)^2}$	A small RMS indicates a good calibration.
Sum of residuals	$\sum_{i=1}^{n} W_i\lvert H_i - h_i\rvert$ where: W_i = weighting from 0 to 1	Useful for comparing successive model runs. The measure is dependent on sample size. Weights are used to emphasise more or less reliable data, or change the emphasis of a specific parameter or area.
Correlation function - R	$\frac{\sum(h_i - \bar{h})(H_i - \bar{H})}{\sqrt{\sum(h_i - \bar{h})^2}\sqrt{(H_i - \bar{H})^2}}$ where: $\bar{h}$ and $\bar{H}$ are the average of the modelled and measured heads respectively	May tend to one for perfect calibrations but see note on Mean error. May be achieved by poor models.

R^2	$\frac{\sum_{i=1}^{n} W_i\left(H_i - \overline{H}\right)^2}{\sum_{i=1}^{n} W_i\left(h_i - \overline{H}\right)^2}$ where : $\overline{h}$ and $\overline{H}$ are the average of the modelled and measured heads respectively	May tend to one for perfect calibrations, but can also be achieved by poor models
Weighted least squares – S(b) – used to describe parameter estimation	$(H - h(b))^T \underline{w}(H - h(b))$ where : b = vector containing parameter estimates h(b) = matrix of modelled heads which is a function of b H = matrix of measured heads	This is a matrix function used in parameter estimation software.
Maximum likelihood –S'(b)	$(ND + NPR)\ln 2\pi - \ln\lvert\underline{w}\rvert + (H - h(b))^T \underline{w}(H - h(b))$ where : ND = number of observations NPR = number of prior information values $\lvert\underline{w}\rvert$ = determinant of the weight matrix	This is a matrix function used in parameter estimation software.

Note: Heads have been used to represent the observations for comparison with model output. However, other measurements such as flows could be used in the above equations.

4.0 Predictive uncertainty and numerical models

As discussed in Section 5 of the main report, model predictive uncertainty is related to model assumptions and parameter uncertainty. In addition, model errors may compromise model predictions. Because of this the model auditor needs to:

- Consider the degree to which the model assumptions are different from the real world and assess what the likely bias on predictions may be as a result of model assumptions.
- Consider the possible range of parameters and their natural variability or heterogeneity, measurement errors, interpretation of measurement errors, or lack of measurements. The auditor also needs to simply check that the model solutions are within a realistic realm, as some combinations of parameters, within realistic ranges, can produce unrealistic solutions
- Undertake checks for model errors.

Due to the greater number of parameters and data associated with numerical models, they entail a greater propensity to create errors than the simpler analytical models.

When addressing model uncertainty, the chief aim is to identify the limiting case for the model prediction (often called worst case). For example, if the model is being used to determine drawdown interference effects, what is the biggest drawdown interference that could occur, given the information available? Or if dewatering rates are being calculated, what is the biggest pump rate that may be required, given the available data? The model auditor needs to be satisfied that this limiting worst case has been realistically identified in such a way that it takes into account the model uncertainty.

4.1 Model assumption uncertainty

Numerical models include a whole range of model assumptions. However, unlike analytical models most of the assumptions are chosen by the modeller and therefore are model specific. The model assumptions that are likely to have the greatest effect on model predictive uncertainty are:

- model parameter zonation of hydraulic conductivity and storage coefficients,
- boundary conditions,
- discretisation of the model in space and time, and
- density variations.

4.1.1 Assumptions of parameter zonation

Numerical models allow aquifer heterogeneity to be represented by defining different zones of hydraulic conductivity and storage coefficient, within which the property has a constant value. Calibration of a numerical groundwater flow model, usually includes the specification of such zones. Geological mapping provides guidance on where these zones should be placed. However, often there is insufficient detail in the geological data. Mapping of aquifer parameters from pumping tests can also provide guidance for zone delineation.

During calibration, the parameters within these zones are modified until the discrepancies between model outputs and field measurements are acceptably minimised. Where the fit is not acceptable, additional zones are often introduced where the modeller feels they will be effective in improving the model fit to field observations. The placement of zones is therefore quite subjective and can be a laborious and time consuming process. Furthermore, the characterisation of

geological heterogeneity by zones of uniform parameters is neither consistent with the nature of alluvial material nor with fractured aquifers, both of which form the stratal framework for many aquifers in New Zealand. In many cases zonation is defensible only on the basis that it is better to employ such a zonation scheme than ignore geological heterogeneity altogether.

Note: The effects of small scale heterogeneities on model predictions are not able to be explored within zonation patterns, however this is a more significant issue for contaminant transport modelling.

Parsimony

The zonation pattern selection affects the parameterisation of the model and model predictions. As the parameter zonation becomes more complex, the parameters within the zones are estimated with an increasing degree of uncertainty. To minimise this uncertainty Hill (1998) discusses the principle of parsimony, where a model should only be as complex as needed for the system being considered. In order to achieve this Hill recommends investigating the processes and characteristics that are likely to be most dominant first and adding additional processes or complexity gradually, always testing the importance of the added complexity to the observations used as calibration targets and to the predictions of interest. A summary table of methods and guidelines to achieve this is outlined in Table C3 (from Hill 1998).

Table C3 – Method for calibration (from Hill 1998)

Guideline	Description
1. Apply the principle of parsimony	Start simple and add the complexity as warranted by the hydrogeology and the inability of the model to reproduce observations.
2. Use a broad range of information to constrain the problem	For example, in ground-water model calibration, use hydrology and hydrogeology to identify likely spatial and temporal structure in, for example, areal recharge and hydraulic conductivity, and use this structure to limit the number of parameters needed to represent the system. Do not add features to the model to attain model fit if they contradict other information about the system.
3. Maintain a well-posed, comprehensive regression problem	a) Define parameters based upon their need to represent the system, within the constraint that the regression remains well-posed. Accomplish this using composite scaled sensitivities (css_j) and parameter correlation coefficients. b) Maintain a comprehensive model in which as many aspects of the system as possible are represented by parameters, and as many parameters as possible are estimated simultaneously by regression.
4. Include many kinds of data as observations in the regression	Adding different kinds of data generally provides more information about the system. In ground-water flow model calibration, it is especially important to provide information about flows. Hydraulic heads simply do not contain enough information in many circumstances, as indicated by the frequency with which extreme values of parameter correlation coefficients occur when using only hydraulic heads.
5. Use prior information carefully	a) Begin with no prior information to determine the information content of the observations. b) Insensitive parameters (parameters with small composite scale sensitivities) can be included in regression using prior information to maintain a well posed problem, but during calibration it often is advantageous to exclude them from the regression to reduce execution time. Include these parameters for Guidelines 13 and 14. c) For sensitive parameters, do not use prior information to make unrealistic optimised parameter values realistic.

Guideline	Description
6. Assign weights which reflect measurement errors	Initially assign weights to equal $1/\sigma_i^2$, where σ_i^2 is the best available approximation of the variance of the error of the i^{th} measurement. (This is for a diagonal weight matrix; see text for full weight matrix.)
7. Encourage convergence by making the model more accurate	Even when composite scaled sensitivities and correlation coefficients indicate that the data provide sufficient information to estimate the defined parameters, nonlinear regression may not converge. Working to make the model represent the system more accurately obviously is beneficial to model development, and generally results in convergence of the nonlinear regression. Use model fit and the sensitivities to determine what to change.
8. Evaluate model fit	Use the methods discussed in the sections "Statistical Measures of Model Fit" and "Graphical Analysis of Model Fit and Related Statistics" – in Hill (1998)
9. Evaluate optimised parameter values	a) Unreasonable estimated parameter values could indicate model error. b) Identify parameter values that are mostly determined based on one or a few observations using dimensionless scaled sensitivities and influence statistics. c) Identify highly correlated parameters.
10. Test alternative models	Better models have three attributes: better fit, weighted residuals that are more randomly distributed, and more realistic optimal parameter values.
11. Evaluate potential new data	Use dimensionless scaled sensitivities, composite scaled sensitivities, parameter correlation coefficients and one-percent scaled sensitivities. These statistics do not depend on model fit or, therefore, the possible new observed values.
12. Evaluate the potential for additional estimated parameters	Use composite scaled sensitivities and parameter correlation coefficients to identify system characteristics for which the observations contain substantial information. These system characteristics probably can be represented in more detail using additional estimated parameters.
13. Use confidence and prediction intervals to indicate parameter and prediction uncertainty	a) Calculated intervals generally indicate the minimum likely uncertainty. b) Include insensitive and correlated parameters, perhaps using prior information, or test the effect of excluding them. c) Start by using the linear confidence intervals, which can be calculated easily. d) Test model linearity to determine how accurate these intervals are likely to be. e) If needed and as possible, calculate nonlinear intervals (This is not supported in the present versions of UCODE and MODFLOWP). f) Calculate prediction intervals to compare measured values to simulated results. g) Calculate simultaneous intervals if multiple values are considered or the value is not completely specified before simulation.
14. Formally reconsider the model calibration from the perspective of the desired predictions	Evaluate all parameters and alternative models relative to the desired predictions using prediction scaled sensitivities (pss_j), confidence intervals, composite scaled sensitivities, and parameter correlation coefficients.

AIC/BIC statistics

To address the issue of increasing uncertainty associated with an increasing number of estimated parameters Carrera and Neuman (1986a, b, & c) discuss the use of AIC and BIC statistics in groundwater. These statistics are originally from time series analysis (see Akaike and Kitagawa 1999). These are relative statistics only, allowing differently parameterised versions of the same model to be compared with each other. The AIC and BIC statistic is simply a measure of the goodness of the fit (represented by the objective function) plus the number of parameters used in the model. There is no absolute value these statistics should have. Rather, the model with the smaller statistic represents the more accurate model.

AIC (b') = S(b') +2 x NP

Where AIC (b') is a measure of the combined goodness of fit and the drawbacks associated with increasing the number of estimated parameters.

NP = the number of estimated parameters

S('b) = the weighted least squares objective function (as defined in table C2)

The BIC statistic was developed as a response to concern that the AIC sometimes promoted the use of more parameters than was required.

BIC = S(b') + NP x ln(ND+NPR)

Where BIC is an 'improved' measure of the combined goodness of fit and the drawbacks associated with increasing the number of estimated parameters.

NP = the number of estimated parameters

S('b) = the weighted least squares objective function

NPR = the number of prior information values

ND = the number of observations

Pilot points

One option for determining parameter zonation more 'objectively', using parameter estimation software, is described in Doherty (2002). Instead of the modeller assigning parameter zones, they assign points ('pilot points'). Parameters are estimated at these points, such that discrepancies between model outputs and field observations are minimised. The points are spatially interpolated (using kriging), so that zones are defined by the contouring of these points. The more points used the better, as the actual location of the pilot points becomes increasingly unimportant. Where there is a sound geological basis for zonation, the pilot points method can be used in conjunction with these zones.

Because the interpolation process presents areas of contoured parameter constancy wherever possible, parsimony prevails, as the model simplicity is sacrificed only to the extent required for model calibration.

4.1.2 Assumptions of model boundaries

Boundaries are one of either a specified head, specified flow or head dependent flow boundary. A numerical model allows flexibility when assigning the location and time period of a model boundary. Usually a flow system will have a mix of these boundaries and where possible real physical boundaries should be used. Where the model domain does not extend to regional physical flow boundaries two options are used; distant boundaries, or hydraulic boundaries.

Distant boundaries may be arbitrarily located far from the centre of the grid as long as the stresses to the system do not extend to the boundaries during the model simulation. For example a fixed head boundary may be chosen where a drawdown cone of depression does not reach the boundary. If the boundary is too close, the calculated drawdown will be biased by the effect of the boundary. It is not possible to define what too close is, instead each model should be checked to determine whether the flow to or from a boundary is reasonable, and is consistent with flow to and from the boundary, prior to pumping.

Hydraulic boundaries are derived from the groundwater flow net and are therefore 'artificial' boundaries set by the model designer. They can be no-flow boundaries represented by chosen stream lines (flow lines perpendicular to piezometric contours), as by definition there is no flow across a stream line. Alternatively they may be boundaries with known hydraulic head represented by equipotential lines. Hydraulic boundaries have the disadvantage of not being permanent fixtures, as they can change in time. Because of this it is important to place hydraulic boundaries far enough from the area of interest so that they do not influence the flow pattern in the area of interest.

Surface waterways must be analysed carefully before deciding what their role in a model will be. Fully penetrating streams offer a straightforward solution. If they are large enough to sustain a large groundwater withdrawal in the adjacent aquifer, they are ideal constant head boundaries. If the river is partially penetrating, and/or the groundwater withdrawal may cause the river to dry, the river cannot be set as an external boundary but instead as an internal boundary to the model.

4.1.3 GRID/TIME discretisation

Finite difference models have cells making up a rectangular grid, whereas finite element models have a mesh composed of variably oriented and length elements.

4.1.3.1 Grid

Laying out the model grid or mesh is the starting point of the computer model design. Finite difference model domains are split up into rows, columns and layers, which form cells. Finite element model domains are characterised by elements within which there is parameter homogeneity. Definition of layers is typically consistent with the presence of aquifers and aquitards. An average solution is calculated for each cell or element. The model grid or element must be sufficiently small in the area of interest or where steep hydraulic gradients will occur (i.e., around a seepage face, a drain, or pumping wells) to accurately represent local variations in soil properties, hydraulic head and groundwater concentrations. Typically the model grid or element array is aligned in the general direction of groundwater flow.

The most stable solutions are provided for uniformly spaced grids or elements. For finite difference models a change in distance between adjacent gridlines should be less than 1.5 times for model numerical stability.

4.1.3.2 Time

Smaller time steps, together with small cell sizes, allow better numerical approximations to the partial differential flow equation. So the greater the degree of temporal discretisation, the better the definition of solution. However, this needs to be balanced against the longer solution time.

Reduction of time step size is also used where there are numerical instabilities and where unrealistic and/ or oscillating solutions occur. The sensitivity of the solution to time step size and gird size should be tested.

Some guidance for approximation of time steps is given, such that the time step would be small enough to allow an explicit solution to be calculated within that time. One option de Marsily (1986) presents is to use an initial time step Δt, by $\Delta t = Sa^2/4T$,

Where:

a = grid dimension Δx or Δy for a regular grid

T = transmissivity

S = storativity

If time steps are increased, this can be done as a geometric progression of ratio 1.2 to 1.5.

4.1.4 Assumption of constant density

Most model codes assume that the density of groundwater is constant and approximately equal to 1.0 g/cm^3. This is a valid assumption for water with low concentrations of total dissolved solids or temperatures in the range of most shallow aquifers. For situations where this is not valid, then density dependent flow should be modelled, as relatively small changes in density can significantly alter the flow field water. This includes situations where water is hot (say 50°C, which changes water density to 0.988 g/cm^3), as in geothermal reservoirs; or where water has a large total dissolved solids content (TDS), such as salt water which has a TDS of around 35 000 mg/L giving it a density of 1.025 g/cm^3. Some contaminant plumes also have high a TDS content. Public domain software for density dependent codes include SUTRA (for two dimensional problems), FEMWATER (for density dependent flow) and HST3D (for three dimensional problems).

4.2 Parameters, their uncertainty and model predictive uncertainty

For numerical flow models the aquifer parameters involved are chiefly hydraulic conductivity (and transmissivity) and storage coefficients. In most cases, hydraulic conductivity is the most critical and sensitive modelling parameter.

Every attempt should be made to design a model with realistic values of hydraulic conductivity obtained in the field, preferably by pumping tests. Furthermore if using test data, the accuracy of these data should be assessed along with an estimation of how representative they are of the entire data set. Molz (1998) discusses how the variability of hydraulic conductivity measurements increases as the measurement volume decreases. Slug test measurement certainly exhibit this variability more so than pump tests. Schulze-Makuch et al. (1999) also suggest that the hydraulic conductivity measurements are scale dependent, generally increasing for increasing measurement volumes.

The modeller and auditor need to consider how representative are the hydraulic conductivity, transmissivity and storage field data being used in the model.

4.2.1 Methods to address predictive uncertainty

Non calibrated models

The range of what is possible in model predictions is large where models are not constrained by calibration. Parameter ranges are chosen on the basis of regional information, or even literature values. It is important that the modeller does not just choose one preferred set of parameters, as although reasonable, other combinations of parameters may also be reasonable. Different parameter combinations have a different impact on the model predictions. It is important to explore this range of parameter combinations possible in order to identify the range of predictions possible and the worst of these predictions.

Calibrated models

Calibration of a model constrains the possible range of model predictions by requiring that the model outputs match the observed data. However, when calibrating a model it is usually found that the parameter estimates are not unique, i.e.

different combinations of parameter estimates match the field observations equally well. Parameter non uniqueness is partly caused by the complexity of many real systems coupled with the lack of sufficient data. However, in addition to this, the bias that model assumptions impart on model parameterisation also contributes to parameter uncertainty. Because of this non uniqueness there is a range of possible model predictions that are equally valid, given the available data. Even though this range is significantly less than for an un-calibrated model. Predictive uncertainty is assessed by running predictive simulations on the possible range of calibrated models. Obviously this is a time consuming task.

In Hill's 'Methods and Guidelines for Effective Model Calibration' (1998) the use of parameter estimation software is strongly advocated. However, despite the clear advantages of using this software, it is not commonly used, with trial and error calibration still being much more the common practice. This is partly because of the problems of instability, non-uniqueness (as discussed above) and instability. Insensitivity occurs when there is simply not enough observation information to support the estimation of parameters. Instability occurs when slight changes in parameter values or observations create large changes in the model results. However, model calibration by trial and error also incorporates these problems, but the modeller is less likely to be aware of them. Parameter estimation software essentially allows modellers to understand their models and data better by undertaking all the steps involved in multiple model calibrations far more quickly than the modeller can achieve by trial and error.

Hill (1998) states: *'The benefits of inverse modelling include (1) clear determination of parameter values that produce the best possible fit to the available observations; (2) diagnostic statistics that quantify (a) quality of calibration, (b) data shortcomings and needs, (3) inferential statistics that quantify reliability of parameter estimates and predictions; and (4) identification of issues that are easily overlooked during non-automated calibration.'*

Flow model predictions are typically most sensitive to hydraulic conductivity parameterisation. Because of this Kresic (1997) recommends adjusting all other calibration avenues, such as boundary locations and conditions and stresses, and only then engage in changing the distribution of hydraulic conductivity.

Methods that allow a very clear identification of a worst case include 'predictive analysis' (Doherty 2000), discussed in Section 5.2 of the main report, or response functions , where the relative rather than the absolute magnitude of predictions is of concern.

5.0 Data requirements for numerical flow models

Typical numerical model inputs are described in this section. These inputs can be based on site specific information if a site specific prediction is required, or general regional flow data if the model is being used for exploration of a general case or literature values for a theoretical assessment. Judgement is required in determining if the data is adequate to simulate the system accurately. The following text boxes describe the parameters required in a numerical model, and give examples or ranges of values

Parameter	Model domain
Description	The model domain is the extent of the model. It is surrounded by boundaries that describe the relationship between the model domain and the rest of the world. The extent of the model, or the model domain is selected so that it is large enough both to encompass the area of interest and so that the selected boundary conditions do not significantly influence model results. Where possible natural boundaries are used such as rivers, lakes, wetlands, bedrock outcrops or a water table ridge (groundwater divide).

Parameter	Model boundaries
Description	Model boundaries are one of three types. A no-flow boundary is a boundary along which no flow leaves or enters the aquifer. Examples of this are a groundwater divide or geologic boundary. A flow boundary is a boundary along which there is known flow into or out of an aquifer. Examples of this are rainfall recharge, evapotranspiration, or seepage from another aquifer or stream leakage. A head-dependent flow boundary is a boundary along which the flow into or out of the aquifer is dependent on the difference in head between the aquifer and the boundary. These boundaries are sometimes called constant head boundaries, or if a conductance term limits the connection between the aquifer and boundary – they may be called a general head boundary. Rivers and drains also form head-dependent boundaries where the leakage or drain flows are dependent on the difference between the head in the aquifer and in the river or drain. When calibrating to piezometric contours a model needs at least one head-dependent boundary. NOTE: A river or stream can form two of these three boundaries.

Parameter	Model grid/mesh - rows, columns and layers/ elements
Description	The model domain is split up into a grid of rows, columns and layers. This produces model cells within which an average solution is calculated for each cell. Alternatively the model domain can be split up into irregular shaped elements (for finite element models) and the solution is calculated for each element. The model grid must be sufficiently small in the area of interest or where steep hydraulic gradients will occur (e.g. around a seepage face, a drain, or pumping wells) to accurately represent local variations in soil properties, hydraulic head and groundwater concentrations. Typically the model grid is aligned in the general direction of groundwater flow. The top and bottom elevations of each layer need to be defined with respect to a datum are also used for water level measurements (unless the aquifer is confined).

Parameter	Time parameters
Description	• Time parameters are specified for time dependent (transient) conditions. They include: • Time unit, i.e., Seconds, minutes, days, etc • Stress period - Most numerical codes allow the simulation period to be divided into blocks of variable time, known as stress periods. The option of stress periods allow the aquifer stresses to be altered while the simulation is in process. During each stress period all model parameters associated with boundary conditions and stresses remain constant. Having more stress periods allows these stress and boundary parameters to change in time. For example a pumping well can change its pumping rate in different stress periods, and the river stage can vary according to seasons. The modeller must decide which length of stress period is required for the modelling problem, and how many stress periods are required. • Time steps - A stress period is further divided into time steps, allowing changes in say hydraulic head to be analysed within the stress period. Time steps do not have to be of equal length. In addition, time steps can then be defined separately for different stress periods. The smaller the time step the more accurate the iterative computations.

Parameter	**Hydraulic conductivity (K)**
Units	m/day
Description	The hydraulic conductivity is defined as the volume of water that will move through a porous medium, in unit time, under a unit hydraulic gradient, through a unit area measured at right angles to the direction of flow. The hydraulic conductivity parameter contains properties of the fluid (water) and of the saturated porous medium (the aquifer). It is defined as: $K = \frac{k\rho_{water} g}{\mu}$ Where: k = intrinsic permeability of the strata g = acceleration due to gravity ρ_{water} = density of water μ = viscosity of water Hydraulic conductivity can vary in differing directions and this feature is called anisotropy. **Anisotropy** especially occurs in all sediments which are stratified, giving them a greater conductivity in the direction of flow. The major axes of hydraulic conductivity are defined as K_{xx}, K_{yy} and K_{zz}. Anisotropy is usually represented on a layer by layer basis in numerical models, where the magnitude of the anisotropy and its principal direction are defined. Hydraulic conductivity also varies spatially from one point in the aquifer to another, this property is called **heterogeneity**. Heterogeneity can be represented in a numerical model by having different zones of hydraulic conductivity. Both heterogeneity and anisotropy affect groundwater flow.
Typical values (m/day) <u>*Sedimentary*</u> Gravel Coarse sand Medium sand	Values taken from Domenico and Schwartz (1990) $3 \times 10^{-4} - 3 \times 10^{-2}$ $9 \times 10^{-7} - 6 \times 10^{-3}$ $9 \times 10^{-7} - 5 \times 10^{-4}$

Fine sand	$2 \times 10^{-7} - 2 \times 10^{-4}$
Silt, Loess	$1 \times 10^{-9} - 2 \times 10^{-5}$
Till	$1 \times 10^{-12} - 2 \times 10^{-6}$
Clay	$1 \times 10^{-11} - 4.7 \times 10^{-9}$
Un-weathered marine clay	$8 \times 10^{-13} - 2 \times 10^{-9}$
Sedimentary rocks	
Karstified and reef limestone	$1 \times 10^{-6} - 2 \times 10^{-2}$
Limestone, dolostone	$1 \times 10^{-9} - 6 \times 10^{-6}$
Sandstone	$3 \times 10^{-10} - 6 \times 10^{-6}$
Siltstone	$1 \times 10^{-11} - 1.4 \times 10^{-8}$
Salt	$1 \times 10^{-12} - 1 \times 10^{-10}$
Anhydrite	$4 \times 10^{-13} - 2 \times 10^{-8}$
Shale	$1 \times 10^{-13} - 2 \times 10^{-9}$
Crystalline rocks	
Permeable basalt	$4 \times 10^{-7} - 2 \times 10^{-2}$
Fractured igneous and metamorphic rock	$8 \times 10^{-9} - 3 \times 10^{-4}$
Weathered granite	$3.3 \times 10^{-6} - 5.2 \times 10^{-5}$
Weathered gabbro	$5.5 \times 10^{-7} - 3.8 \times 10^{-6}$
Basalt	$2 \times 10^{-11} - 4.2 \times 10^{-7}$
Massive (un-fractured) igneous and metamorphic rocks	$3 \times 10^{-14} - 2 \times 10^{-10}$

Parameter	**Transmissivity (T)**
Typical Units	m^2/day
Description	Transmissivity is defined as the hydraulic conductivity multiplied by the saturated thickness of the aquifer. For confined aquifers, the transmissivity of the aquifer is constant, whereas for unconfined aquifers, transmissivity varies with water level fluctuations. Heterogeneity of hydraulic conductivity can be represented in a numerical model by zones of differing transmissivity.

Parameter	**Specific storage, (S_s), Storage Coefficient (S) and Specific yield (S_y)**
Units	dimensionless
Description	The storage coefficient (S), of the aquifer is the volume of water released per unit surface area of aquifer, for each unit decline in the piezometric surface. The specific storage, (S_s), is defined as the storage coefficient divided by the saturated thickness of the aquifer. As with hydraulic conductivity, storativity also varies spatially from one point in the aquifer to another (heterogeneity). Heterogeneity can be represented in a numerical model by having different zones of storativity. In confined aquifers, when the head is lowered, the aquifer remains fully saturated, and the water released is volumetrically equivalent to the expansion of the water and the contraction of the pore space. These expansion and contraction processes also occur in unconfined aquifers, but the volumes of water associated with them are negligible compared to that from the actual drainage of the pores. The storativity under unconfined conditions is referred to as the specific yield, (S_y).
Aquifer type Confined aquifers Unconfined aquifers	Typical values taken from Freeze and Cherry (1979) 0.005 – 0.00005 0.01 – 0.3

Parameter	**Well locations, pumping rate and duration (Q)**
Typical Units	m^3/day or L/s
Description	The location of each well in terms of the model layer, row and column is defined. Usually negative values of a pumping rate indicate a withdrawal well, while positive values indicate a recharging well. When simulating several wells that fall within one cell area, the user must sum the individual pumping rates. The pumping rate for each well needs to be determined for each stress period. The duration of the pumping rate therefore determines the length of a stress period. Where wells abstract from more than one layer, this is represented by having a separate well in each layer, and a proportion of the pumping rate is attributed to each layer.

Parameter	Rivers and streams
Description	The flow between an aquifer and a surface water body can be represented in numerical models. In MODFLOW this is via the river or stream package where the rate of flow is calculated as proportional to the difference in the river or stream water level (stage height) and the water level in the aquifer. The area of the river bed in contact with the aquifer, and a river bed conductance term are also specified. The MODFLOW software package dealing with rivers assumes that the head in the river remains constant (at least for each stress period), whereas the stream package also considers the flow within the stream and limits the flow between the aquifer and stream accordingly.

Parameter	Recharge and evapotranspiration
Description	The recharge software portion of MODFLOW is used to simulate infiltration from precipitation or irrigation. The evapotranspiration package is used for simulating the effects of plant water uptake.

Parameter	Initial conditions
Typical Units	m/day
Description	Initial conditions are values of hydraulic head for each active cell in the model. They must be higher than the elevation of the cell bottom and are necessary for the start of the iterative model calculations. In transient simulations the initial conditions should closely resemble the field measurements. Initial conditions are less important for steady state conditions but still need to be determined. When a model is calibrated, the head distribution for the calibrated model often becomes the initial head distribution for the prediction phase.

6.0 Errors

Errors can be generated through inappropriate model design, selection of conditions, lack of information and oversimplification. Some errors are therefore the application of inappropriate model assumptions or parameterisation, as discussed in Section 4. There are also errors of simple carelessness.

Table C4 provides a checklist which model auditors can use as they examine the validity of the predictions of a model. Meeting all the requirements outlined in the checklist does not guarantee good model predictions, but will assist an auditor to make an assessment.

Table C4: Checklist for numerical flow model errors

Data gathering errors	Potential implication for solution	Auditor check	OK - tick	Comments
Field measurements of parameters incorporate inherent inaccuracies	These are errors are associated with human error or an instrument error used for instance in a pumping test. Calibration to inaccurate targets compromises model accuracy and predictions.	Have measuring errors been assessed?		
Analysis of field data. Many of the model input parameters require some analysis of the field measurements. For instance hydraulic conductivity relies on the analysis of pump test drawdown – time data, or concentration – time data from tracer tests.	The analysis requires that assumptions are made, such as whether the aquifer is leaky, confined or unconfined. Inaccurate assumptions will compromise the analysis of the parameters, and the model calibration.	Are the estimates of aquifer parameters calculated correctly from aquifer or slug tests?		
Extrapolation of field data. Aquifer properties, such as hydraulic conductivity and porosity, are measured as some type of average over a representative elementary volume (REV).	Measurements of each of these properties is typically variable, particularly where small aquifer volumes are being sampled. Consequently, the field measurement of hydraulic conductivity should differ depending on whether K is to be used in a water supply or a contaminant transport problem. Slug tests are unlikely to be sufficient unless there are many tests undertaken throughout the area of interest. Whereas long term pump tests results represent an average aquifer property for a much larger area. Inappropriate extrapolation will compromise the model calibration.	Is the variability of the strata understood and has it been represented in the model? Was there sufficient data available for the model construction, given the predictions being made?		
Lack of far field data	The model domain must be large enough so that boundary conditions do not distort aquifer response to stress in the area of interest. However there should be some basis for specifying boundary conditions at a distance. If there are no far field data the effect of the assumed model boundary on model response should be evaluated.	Are there data for calibration across the extent of the model domain?		

Data input errors	Potential implication for solution	Auditor check	OK - tick	Comments
Inconsistent parameter units - i.e. days and seconds, gallons per minute and cubic feet per day.	It is important to use consistent units when modelling. Inaccuracies can occur if the same units are not used. For example, days are selected for your time unit and metres for the length unit, then recharge and hydraulic conductivity must be in metres per day, pumping rates must be in cubic metres per day, constant head boundaries and grid dimensions must be in metres, etc.	Are the model units consistent for all parameters – i.e. days and seconds, cubic metres per day etc?		
Incorrect sign for pumping or recharge.	It is common practice to express pumping rates as a negative value, injection and recharge as positive values in groundwater modelling programs	Are the correct signs for pumping and recharge used?		
Aquifer stresses (pumping, recharge, evapotranspiration, etc.) must be specified over entire transient simulation period	Failing to define pumping rates, recharge rates, river stages, etc. for the full time period give inaccurate results.	Are the aquifer stresses (pumping, recharge, evapotranspiration, etc) specified correctly for the transient simulation period?		
Well not specified correctly	The well parameters must be specified, especially screen length, for accurate modelling. In a case where no screen has been defined the model may be very distorted in order to get the model to 'work properly'. Pumping rates need to be specified to represent the actual conditions.	Have the well location, screen depths and pumping rates been specified correctly?		
Use a broad range of data to constrain the problem	The more data used to constrain a model calibration, the more accurate the model. (e.g.: river or drain flow data can be used as well as depth to water level measurements, where possible).	Has the model been calibrated to a broad range of data to constrain the model?		

Model assumption errors	Potential implication for solution	Auditor check	OK - tick	Comments
Variable or constant density assumptions	Neglecting density variations can give incorrect indications of flow field.	Are there density variations within the flow field and if so have they been accounted for?		
Selection of boundary conditions - inappropriate (particularly placing boundaries too close to the area of interest)	Model boundaries can inhibit the aquifer response to model stresses in the area of interest, where they are inappropriate or too close to the area of interest.	What are the boundary conditions around the perimeter of the model domain and is the hydrogeological or geochemical basis accurate?		
		Are the boundary conditions distant enough from the area of interest? Have their effect on the model simulations been assessed? (It is not possible to quantify what 'too close' is, but the auditor should check the reasonableness of the flow through any boundary zone).		
Discretisation in space and time	Incorrect time and space discretisation (time steps, and grid sizes) can cause numerical instabilities if too large or of the difference in adjacent cell sizes is too great. The model calculates average heads for the entire cell. If the head at a specific well is in question, the smaller the cell sizes around this well the more accurate the solution will be.	Are the cell sizes detailed enough in the area of interest?		
		Are the time step and cell sizes small enough to provide numerical accuracy?		
		Is the difference between adjacent cell sizes less than 1.5 times? Are conductance terms varied where there are different sized cells?		

Parameter zonation	As zonation becomes more complex, parameter estimates become more uncertain and the predictive uncertainty increases.	Is the parameter zonation more complex than it needs to be? Have the impacts of parameter zonation on predictions been assessed?		
Calibration errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Forcing questionable data to fit	If a potentiometric contour is forced to make a sharp turn to fit an observation at a single well, that observation may not be accurate. Similarly, if early-time aquifer test data do not fit a curve, perhaps the pump had not settled down, there was some well bore storage, or something similar that caused the discrepancy.	Have questionable data been forced to fit?		
Flow budget discrepancies and misinterpretation	The flow budget report includes statistics on the percent discrepancy between water added to the model and water removed from the model. The solver within the model will always attempt to minimise this discrepancy. Thus this is an indicator of solver accuracy for the specified model inputs. These discrepancies should be less than 1%. Larger discrepancies indicate an unstable solution. Sometimes the mass balance is misinterpreted as a measure of how well the model replicates the hydrogeological characteristics of the site.	Are the flow budget discrepancies less than 1%? Has this been interpreted correctly as an indication of solver stability?		
Using interpolated data distribution rather than point data	If the data are interpolated in time or space, this introduces a potential inaccuracy into the data and may compromise calibration and predictions.	Are the model calibration targets interpolated or point data?		
Target wells clustered in a small portion of the model – i.e. lack of far field calibration data.	Target wells must be distributed over the model domain in order for the calibration statistics to be meaningful to the entire model.	Are the target wells clustered in a small portion of the model? Is there a lack of far field data in the area of interest?		

Target wells too close to, or within, specified head boundaries	If a target well is too close to, or within, specified head boundaries, the aquifer's response at the well to stresses will be artificially limited by the boundary. Target wells should be distributed over the model domain and generally away from the constraints of specified head boundaries.	Are the target wells too close to, or within specified head boundaries?		
Sensitivity analysis	A sensitivity analysis should be used a part of the calibration process – so that calibration efforts are targeted to the parameters to which model predictions are most sensitive.	Has a sensitivity analysis been undertaken? Which were the most sensitive parameters?		
Forcing a fit by using unrealistic data values or over-discretising an aquifer or aquitard layer.	If the model can only achieve reasonable calibration statistics using unreasonable data values or by artificially assigning numerous zones of hydraulic conductivity, recharge etc, the hydrogeology of the site has not been fully understood. Proper characterisation of the site in and near the area of interest is necessary.	Is the parameter zonation more complex than it needs to be?		
		Have the impacts of parameter zonation on predictions been assessed?		

Prediction errors	Potential implication for solution	Auditor check	OK - tick	Comments
Omitting results inconsistent with your preconceptions	Wrong final answer and uncertainty	Review data used and results obtained		
Not incorporating data variability or uncertainty into the analysis	As discussed, despite our efforts, model parameters can never be precisely known. Variations in measured data are either an indication of measurement uncertainty, model bias, or the result of real physical differences. Use the range of data values that reflect data variability to give an indication of the range of possible model predictions. A conservative approach in reporting model results, recognises the uncertainty inherent in modelling and displays a firm understanding of the goals of groundwater modelling	Has the model report discussed the situations where the model predictions are most likely to be valid?		
Blind acceptance of model output	A model's accuracy is no better than the accuracy of the data. Make sure that the model results agree with your understanding of the site hydrogeology and sound hydrogeological principles.	Do the model results agree with your understanding of the site hydrogeology and hydrogeological principles?		
Predictive uncertainty must be addressed.	Given the non-uniqueness of models, it is important the uncertainty of predictions is explored and the limiting scenario (worst case) is reported.	Has predictive uncertainty analysis been undertaken?		
The correct predictive simulations must be undertaken to fulfil model purpose		Does the model fulfil its purpose?		

7.0 Case study

7.1 Case study

A number of model projects were reviewed for this report, to check whether issues have been addressed. This case study was chosen because of the relatively high number of model errors it contained.

7.1.1 Model purpose

The groundwater flow model, MODFLOW, was used to assess dewatering rates for excavations in a valley infilled with alluvial gravels. The auditor's check list was filled out for this case study in Table C5.

7.1.2 Model components

Layers

The model area was modelled as three layers: Layers 1 and 2 represent a younger and an older alluvial gravel sequence. Layer 3 represents basement strata comprised of clay and silt-rich, fine to coarse sand with minor gravel. Layer 1 is modelled as unconfined, layers 2 & 3, as confined. The degree of connection between layers has been defined by MODFLOW vertical conductivity (VCONT) arrays, assuming a vertical hydraulic conductivity as one tenth of the horizontal hydraulic conductivity. This is an appropriate assumption given that there are no test data to confirm this.

Boundaries

The model external boundaries are two general head boundaries and no flow boundaries on the valley sides where the basement strata outcrops on the valley sides. There is also an internal river boundary.

The general head boundaries (GHB) were used to represent the upstream and downstream hydraulic boundaries. These GHB's have been set based on small water level ranges at the top end of the valley, which suggests that the use of GHB's is a reasonable representation of this part of the groundwater flow system.

For the river, stage heights have been based on survey data. River bed conductances were approximated using the standard equation in the MODFLOW manual, – however the basis of this approximation was not specified in terms of the river bed hydraulic conductivity, river bed width and river bed thickness. Therefore it was not possible to judge whether the values are physically realistic.

Grid set up

The area of the model domain is 1920 m by 3400 m, represented by 356 rows and 220 columns.

The cell sizes in some adjacent cells vary by more than 50%, this can lead to numerical instability. This could be remedied by altering cell widths and heights.

7.1.3 Model calibration

Steady State calibration

A steady state model was calibrated to one-off depth measurements taken when exploratory bores were drilled. While this is not a true piezometric surface as the water levels were not recorded at the same time – it is the only data available at present. The steady state model approximately reproduced these water levels. Given that the water level data did not represent any actual piezometric surface, the steady state calibration match was as good as could realistically be expected.

The model assumes that the hydraulic conductivity of layers 2 and 3 are both two orders of magnitude less than in layer 1. This is based on anecdotal evidence regarding the seepage rates into the lower strata. It may be appropriate to test

the hydraulic conductivity of the second layer, to allow refinement of the model. However at present this assumption is reasonable.

Transient calibration

The model was then calibrated to a pump test undertaken at the site. The calibration utilised a constant head boundary close to the pumping and observation wells (Refer to Figure C2). However the constant head boundary is removed in the subsequent simulations. It appears that in order to calibrate the model to the pump test data, the constant head cells were placed around the wells to provide a flat background water level, on which the pump test response could be identified. However, the constant head cells were placed too close to the pumping well and caused lower water level drawdown response to the pump test than would occur typically with the aquifer parameters chosen. This is an artificial constraint within the model that does not represent actual conditions within the groundwater system. Because of its dampening effect, a low hydraulic conductivity was used to achieve the drawdown response in the monitoring wells. Without these constant head cells, a much higher hydraulic conductivity is required to achieve similarly small drawdown effects.

The main concern when auditing this model was that the model calibration, constrained by the constant head cells, meant that the hydraulic conductivities and storativity values arrived at, were likely to be too low to represent the hydrogeological conditions that have been indicated by the monitoring data, including the pumping test.

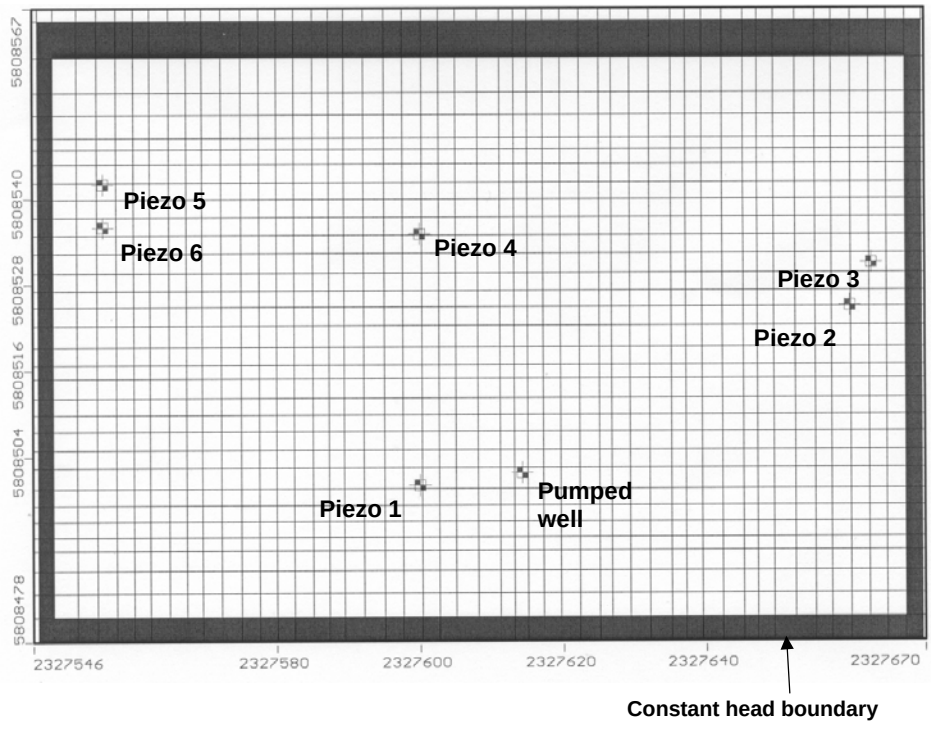

Figure C2 : Example of Visual Modflow screen showing data input

Budget discrepancies/ model solver

Large model budget discrepancies of up to 7% occurred in the transient model calibration. As a rule, flow budget discrepancies should not be greater than 1%. If larger errors occur, the model solution cannot be considered reliable. In this particular case, as a result of the model audit a change in the model solver helped to eliminate large budget

discrepancies. The reduction of the budget errors had a marked effect on the numerical solutions in this model and significantly affected the transient model calibration and the subsequent simulations.

VOLUMETRIC BUDGET FOR ENTIRE MODEL AT END OF TIME STEP 10 IN STRESS PERIOD 2

CUMULATIVE VOLUMES L**3 RATES FOR THIS TIME STEP L**3/T

IN:		**IN:**	
STORAGE =	632.09	STORAGE =	11.12
CONSTANT HEAD =	0.0	CONSTANT HEAD =	0.0
WELLS =	4320.0	WELLS =	0.0
RIVER LEAKAGE =	47738.2	RIVER LEAKAGE =	37532.8
TOTAL IN =	52690.3	TOTAL IN =	37543.9
OUT:		**OUT:**	
STORAGE =	54264.2	STORAGE =	26261.7
CONSTANT HEAD =	0.0	CONSTANT HEAD =	0.0
WELLS =	0.0	WELLS =	0.0
RIVER LEAKAGE =	1626.9	RIVER LEAKAGE =	0.0
TOTAL OUT =	55891.1	TOTAL OUT =	26261.7
IN - OUT =	-3200.8	**IN - OUT** =	11282.2
PERCENT DISCREPANCY =	**-5.90**	**PERCENT DISCREPANCY =**	**35.36**

7.1.4 Sensitivity Analysis

A sensitivity analysis for the original model was undertaken by varying the hydraulic conductivity in layer 1 from 50 m/day to 100 m/day, compared to the calibrated model of 65 m/day. As expected, the sensitivity analysis indicated that the estimates of excavation inflows are highly sensitive to selection of hydraulic conductivity values. Consequently efforts to understand the variability of this parameter will have the greatest impact on model predictive uncertainties.

7.1.5 Model predictions

The predictive simulations comprised three stress periods. Drains were included in the model to represent the excavations. The first two stress periods did not utilise the drain cells and in the third stress period, the drain cells become active. The purpose of the initial two stress periods is to achieve a reasonable background water level pattern.

The drain cells were located in Layer 1, however the elevations in some of these cells are set below the base of Layer 1, and should have been assigned to Layer 2. This occurred in at least 25 – 30 cells and results in underestimates of the

dewatering rates. By assigning the drain cells to both Layer 1 and Layer 2, allows the drain cells to operate if their invert was below Layer 1 and also allows the drain cells to continue to operate if the Layer 1 cells go dry.

7.1.6 Model uniqueness and predictive uncertainty

Once the model errors are corrected, the accuracy of the estimates in the simulations is still limited by the accuracy of the field data that have been collected. In addition while the model parameters may allow the model to match the field data it does not represent a unique solution i.e., another combination of aquifer transmissivity and storage and aquifer boundary characteristics could be used to reproduce the measured water levels and pump test response. Consequently predictive analysis should have been undertaken.

7.1.7 Summary

The main points from the audit of the original model can be summarised as follows.

1. Data. The model predictions would have been improved by more data, in particular hydraulic conductivity values as the sensitivity analysis indicated that this was the most sensitive parameter.
2. Model conceptualisation - The general conceptual characterisation of the aquifer was reasonable. However, there are aspects of the model calibration and set-up, which need refinement to allow the likely range of dewatering estimates to be determined with greater certainty.
3. The steady state model calibration to the measured background water levels was reasonable, although the accuracy of the field data is less than desirable (data having been measured at a variety of different times).
4. The transient model calibration to the pump test data was flawed in two main ways; the presence of the constant head cells too close to the pumping area; large model budget discrepancies giving unreliable solutions.
5. The sensitivity analysis approach is reasonable, but again was hampered by using the transient calibration parameters as a starting point.
6. The simulations were carried out in a reasonable manner, but were hampered by using the aquifer parameters from the transient calibration, and the drain elevations were not always assigned to the correct layer, potentially underestimating dewatering rates.

The combination of the above meant that the calculated dewatering rates did not cover the full range of variables, in particular hydraulic conductivity, that could realistically occur at this site.

Table C5: Case study - checklist for numerical flow model errors

Data gathering errors	Potential implication for solution	Auditor check	OK – tick	Comments
Field measurements of parameters incorporate inherent inaccuracies	These are errors are associated with human error or an instrument error used for instance in a pumping test. Calibration to inaccurate targets compromises model accuracy and predictions.	Have measuring errors been assessed?		
Analysis of field data. Many of the model input parameters require some analysis of the field measurements. For instance hydraulic conductivity relies on the analysis of pump test drawdown – time data, or concentration – time data from tracer tests.	The analysis requires that assumptions are made, such as whether the aquifer is leaky, confined or unconfined. Inaccurate assumptions will compromise the analysis of the parameters, and the model calibration.	Are the estimates of aquifer parameters calculated correctly from aquifer or slug tests?		The initial values of hydraulic conductivity in steady state model were based on a pump test –however the effect of the recharging river was not accounted for, consequently the initial estimates of hydraulic conductivity were overestimated. However, during calibration the values were lowered.

Extrapolation of field data. Aquifer properties, such as hydraulic conductivity and porosity, are measured as some type of average over a representative volume (REV).	Measurements of each of these properties is typically variable, particularly where small aquifer volumes are being sampled. Consequently, the field measurement of hydraulic conductivity should differ depending on whether K is to be used in a water supply or a contaminant transport problem. Slug tests are unlikely to be sufficient unless there are many tests undertaken throughout the area of interest; whereas long term pump test results represent an average aquifer property for a much larger area. Inappropriate extrapolation will compromise the model calibration.	Is the variability of the strata understood and has it been represented in the model?		
		Were there sufficient data available for the model construction, given the predictions being made?		Transient data insufficient.
Lack of far field data	The model domain must be large enough so that boundary conditions do not distort aquifer response to stress in the area of interest. However there should be some basis for specifying boundary conditions at a distant. If there are no far field data the effect of the assumed model boundary on model response should be evaluated.	Are there data for calibration across the extent of the model domain?		Insufficient data for transient simulation.
Data input errors	**Potential implication for solution**	**Auditor check**	**OK – tick**	**Comments**
Inconsistent parameter units - i.e. days and seconds, gallons per minute and cubic feet per day.	It is important to use consistent units when modelling. Inaccuracies can occur easily if the same units are not used. (e.g.: if days are selected for time unit and feet for length unit, then recharge and hydraulic conductivity must be in feet per day, pumping rates must be in cubic feet per day, constant head boundaries and grid dimensions must be in feet, etc.	Are the model units consistent for all parameters – i.e. days and seconds, cubic metres per day etc?	√	

Incorrect sign for pumping or recharge.	It is common practice to express pumping rates as a negative value, injection and recharge as positive values in groundwater modelling programs	Are the correct signs for pumping and recharge used?	√	
Aquifer stresses (pumping, recharge, evapotranspiration, etc.) must be specified over entire transient simulation period	Failing to define pumping rates, recharge rates, river stages, etc. for the full time period give inaccurate results.	Are the aquifer stresses (pumping, recharge, evapotranspiration, etc) specified correctly for the transient simulation period?	√	
Well not specified correctly	The well parameters must be specified, especially screen length, for accurate modelling. In a case where no screen has been defined the model may be very distorted in order to get the model to "work properly'. Pumping rates need to be specified to represent the actual conditions.	Have the well location, screen depths and pumping rates been specified correctly?	√	
Use a broad range of data to constrain the problem	The more data used to constrain a model calibration, the more accurate the model is likely to be. For instance river or drain flow data can be used as well as depth to water level measurements where possible.	Has the model been calibrated to a broad range of data to constrain the model?		
Model assumption errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Variable or constant density assumptions	Neglecting density variations can give incorrect indications of flow field.	Are there density variations within the flow field and if so have they been accounted for?	√	
Selection of boundary conditions - inappropriate (particularly placing boundaries too close to the area of interest)	Model boundaries can inhibit the aquifer response to model stresses in the area of interest, where they are inappropriate or too close to the area of interest.	What are the boundary conditions around the perimeter of the model domain and is the hydrogeological or geochemical basis accurate?	√	The external boundary conditions were appropriate.

		Are the boundary conditions distant enough from the area of interest? Have their effect on the model simulations been assessed? (It is not possible to quantify what 'too close' is, but the auditor should check the reasonableness of the flow through any boundary zone).		The internal boundaries used in the transient simulation were too close to the area of interest.
Discretisation in space and time	Incorrect time and space discretisation (time steps, and grid sizes) can cause numerical instabilities if too large or if the difference in adjacent cell sizes is too great. The model calculates average heads for the entire cell. If the head at a specific well is in question, the smaller the cell sizes around this well the more accurate the solution will be.	Are the cell sizes detailed enough in the area of interest?	√	
		Are the time step and cell sizes small enough to provide numerical accuracy?	√	
		Is the difference between adjacent cell sizes less than 1.5 times?		
Parameter zonation	As zonation becomes more complex, parameter estimates become more uncertain and the predictive uncertainty increases.	Is the parameter zonation more complex than it needs to be?	√	There was a single zone for each layer. Very parsimonious!
		Have the impacts of parameter zonation on predictions been assessed?		
Calibration errors	**Potential implication for solution**	**Auditor check**	**OK – tick**	**Comments**
Forcing questionable data to fit	If a potentiometric contour is forced to make a sharp turn to fit an observation at a single well, that observation may not be accurate. Similarly, if early-time aquifer test data do not fit a curve, perhaps the pump had not settled down, there was some well bore storage, or	Have questionable data been forced to fit?	√	

	something similar that caused the discrepancy.			
Flow budget discrepancies and misinterpretation	The flow budget report includes statistics on the percent discrepancy between water added to the model and water removed from the model. The solver within the model will always attempt to minimise this discrepancy. Thus this is an indicator of solver accuracy for the specified model inputs. These discrepancies should be less than 1%. Larger discrepancies indicate an unstable solution. Sometimes the mass balance is misinterpreted as a measure of how well the model replicates the hydrogeological characteristics of the site.	Are the flow budget discrepancies less than 1%? Has this been interpreted correctly as an indication of solver stability?		Large flow budget terms indicating numerical instability.
Using interpolated data distribution rather than point data	If the data are interpolated in time or space, this introduces a potential inaccuracy into the data and may compromise calibration and predictions.	Are the model calibration targets interpolated or point data?		There was no actual piezometric survey for steady state calibration, only the initial water levels of a number of drill holes, which were interpolated in time to approximate one piezometric surface.
Target wells clustered in a small portion of the model – i.e. lack of far field calibration data.	Target wells must be distributed over the model domain in order for the calibration statistics to be meaningful to the entire model.	Are the target wells clustered in a small portion of the model? Is there a lack of far field data in the area of interest?		Target wells were clustered in a very small portion of the model for the transient simulation.
Target wells too close to, or within, specified head boundaries	If a target well is too close to, or within, specified head boundaries, the response of the aquifer at the well to stresses will be	Are the target wells too close to, or within specified head boundaries?		Definitely too close.

	artificially limited by the boundary. Target wells should be distributed over the model domain and generally away from the constraints of specified head boundaries.			
Sensitivity analysis	A sensitivity analysis should be used a part of the calibration process – so that calibration efforts are targeted to the parameters to which model predictions are most sensitive.	Has a sensitivity analysis been undertaken? Which were the most sensitive parameters?	√	This was carried out correctly.
Forcing a fit by using unrealistic data values or over-discretising an aquifer or aquitard layer.	If the model can only achieve reasonable calibration statistics using unreasonable data values or by artificially assigning numerous zones of hydraulic conductivity, recharge etc, the hydrogeology of the site has not been fully understood. Proper characterisation of the site in and near the area of interest is necessary.	Is the parameter zonation more complex than it needs to be? Have the impacts of parameter zonation on predictions been assessed?	√	There was a single zone for each layer. Very parsimonious!
Prediction errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Omitting results inconsistent with your preconceptions	Wrong answer or uncertainty	Check data used ad results obtained		
Not incorporating data variability or uncertainty into the analysis	As discussed, despite our efforts, model parameters can never be precisely known. Variations in measured data are either an indication of measurement uncertainty, model bias, or the result of real physical differences. Use the range of data values that reflect data variability to give an indication of the range of possible model predictions. A conservative approach in reporting model results, recognises the uncertainty inherent in modelling and displays a firm understanding of the goals of groundwater modelling	Has the model report discussed the situations where the model predictions are most likely to be valid?		

Blind acceptance of model output	The accuracy of a model is no better than the accuracy of the data. Make sure that the model results agree with your understanding of the site hydrogeology and sound hydrogeological principles.	Do the model results agree with your understanding of the site hydrogeology and hydrogeological principles?		
Predictive uncertainty must be addressed.	Given the non-uniqueness of models, it is important the uncertainty of predictions is explored and the limiting scenario (worst case) is reported.	Has predictive uncertainty analysis been undertaken?		This was not addressed at all.
The correct predictive simulations must be undertaken to fulfil model purpose		Does the model fulfil its purpose?	√	The correct simulations were undertaken.

Appendix D

Appendix D – Numerical Contaminant Transport Model

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Figures

Tables

1.0 Description

Numerical contaminant transport models solve the partial differential advection dispersion equations for the entire flow field of interest. The area of interest is subdivided into small areas (referred to as cells or elements) allowing the advection dispersion equation to be replaced by a simple algebraic equation which is solved for each cell and time step. These algebraic equations are solved numerically through an iterative process – thus the term numeric models. The two most common groups of numerical models are: finite difference and finite element models. Some of the numerical contaminant transport models (MT3D, RT3D) are integrated with the numerical flow model MODFLOW. FEMWATER, a finite element model, is an example of an integrated flow and contaminant transport model.

Contaminant movement in naturally fractured and heterogeneous porous aquifers is highly complex, due to strongly varying velocity fields. The chief advantage of numerical contaminant transport models over analytical versions is that they allow the variability of flow and transport parameters, which dominate contaminant movement, to be represented. It is this flexibility that allows the simulation of the complex plume shapes that often develop in natural systems. Analytical models can not account for this variability in transport parameters. The parameters that vary in heterogeneous aquifers include hydraulic conductivity, porosity, dispersivity and cation exhange capacity.

However, even with numerical modelling tools it is virtually impossible to observe or predict local concentrations absolutely accurately, because of:

- the physical inaccessibility of subsurface systems complicating the measurement of their local properties, and
- the variability of transport parameters,
- errors and uncertainties of measurements.

Consequently, prediction of concentration values and contaminant flows is inherently uncertain. Because of this stochastic modelling methods are being employed to explore this predictive uncertainty. These stochastic methods use geostatistical tools to represent the hydrogeological variability that is beyond what is able to be measured, as discussed in Carle and Fogg (1997) and Jones et al. (2002).

Numerical contaminant transport models are used in two typical situations.

- When designing monitoring, management and remediation systems for sites where groundwater contamination is occurring. To do this it is important to be able to predict these complex plume shapes requiring a considerable amount of data.
- In some situations the model stresses or boundary conditions or aquifers are too complex to be represented by an analytical model and so a numerical model is used.

As numerical models are more complex, operator errors may be more frequent. Model assumptions, parameter uncertainties and model error as they relate to contaminant transport numerical models, are discussed in Section 4 of this appendix.

Table D1: Commonly available numerical contaminant transport codes.

Code	Description
MT3D	3D finite difference saturated contaminant transport model
RT3D	2D finite difference saturated contaminant transport model
CTRANS	2D finite element saturated contaminant transport model
SUTRA	3D finite element flow and contaminant transport density driven saturated and unsaturated zone transport
HST3D	3D finite difference flow and heat and solute transport in saturated strata.
FEMWATER	3D finite element flow and contaminant transport density driven saturated and unsaturated zone transport.

2.0 Numerical contaminant transport models – how do they work?

Contaminant transport

As groundwater moves through an aquifer it does so at a range of differing velocities, as shown in Figure D1.

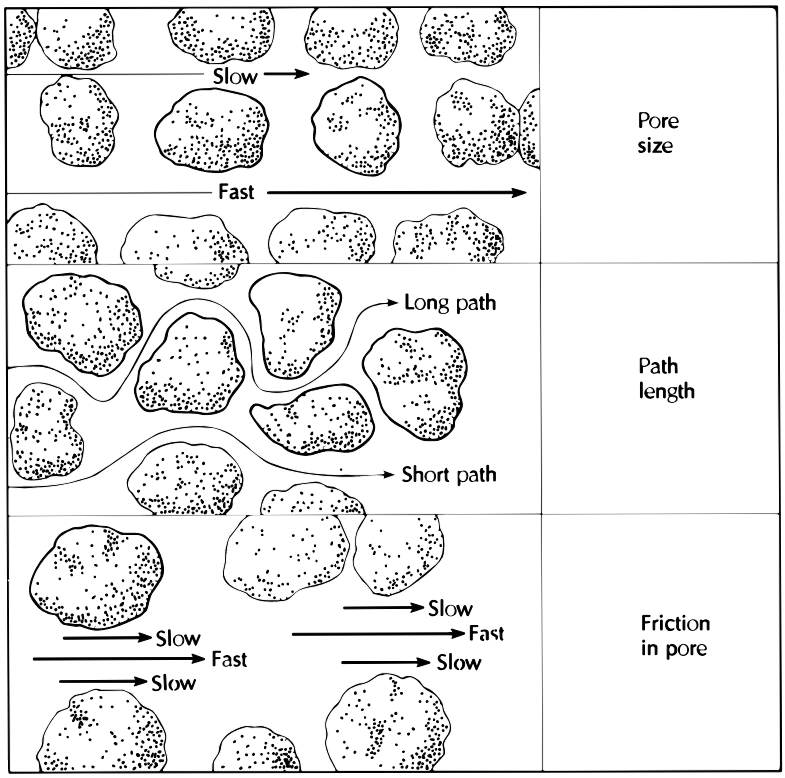

Figure D1. Factors causing pore velocity variations (Fetter 1994).

In contaminant transport problems this variation in pore velocity is addressed by using a mean groundwater pore velocity plus a mechanical dispersion term. Mechanical dispersion describes the mixing that occurs as a consequence of the local variations in pore velocity around some mean pore velocity.

A composite 'dispersion' term is made up of both mechanical dispersion and chemical diffusion. However diffusion is usually negligible compared to mechanical dispersion except in very slow moving groundwater systems.

Contaminant migration is attenuated by chemical reactions taking place during transport. These reactions can occur between the contaminant mass and the soil or rock particles, or the contaminant mass and pore fluids. In addition contaminants can decay biologically or radioactively, reducing the active contaminant mass with time.

Numerical contaminant transport models

Using MT3D as an example of how a numerical model works, the mathematical model for three dimensional movement of a contaminant in groundwater of constant density through porous strata can be described by the following partial differential equation.

$$\frac{\partial C}{\partial t} = \frac{\partial\left(D_{ij}\frac{\partial C}{\partial xj}\right)}{\partial x_i} - \frac{\partial(v_i C)}{\partial x_i} + \frac{q_s}{\theta}C_s + \sum_{k=1}^{N} R_k$$

C is the concentration of contaminants dissolved in groundwater, ML^{-3};

t is time, T;

X_{ij} is the distance along the respective Cartesian coordinate axis, L;

D_{ij} is the hydrodynamic dispersion coefficient, L^2T^{-1};

v_j is the seepage or linear pore water velocity, LT^{-1};

q_s is the volumetric flux of water per unit volume of aquifer representing sources (positive) and sinks (negative), T^{-1};

C_s is the concentration of the sources or sinks, ML^{-3};

θ is the porosity of the porous medium, dimensionless;

$\sum_{k=1}^{N} R_k$ is a chemical reaction term, $ML^{-3}T^{-1}$.

Numerical contaminant transport models are usually coupled with flow models, and the velocity term in the equation above is derived from the model. This equation can be difficult to solve, particularly when all the terms in the equation can vary spatially and temporally. Two types of models, finite-difference (grids), and finite element (element mesh) are used by dividing the area of interest (the model domain) into a mesh of model cells (or elements for finite element models)., By splitting the model simulation into time steps, the equation can be solved by a series of much simpler algebraic equations for each model cell, in each time step. Figure D2 illustrates how the model domain can be split into cells.

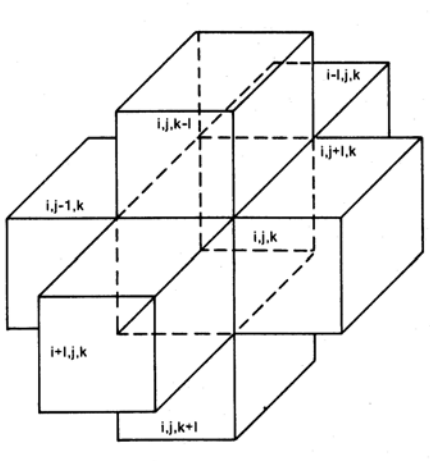

Figure D2: Discretisation of the model domain into cells aligned along three principal axes, I (rows), j (columns), and k(layers).

The model iterates to a solution for this system of algebraic equations in each cell for each time step. The method starts by arbitrarily assigning a trial value or estimate, for the head in each cell. During each time step these estimates are altered in a step-wise fashion to produce a new set of heads which is in closer agreement with the system of equations. This procedure is repeated successively until the heads approach values which would exactly satisfy the set of equations. Each repetition of the calculation is called an iteration.

3.0 Calibration

3.1 Calibration parameters

The following is a list of parameters that are altered in the calibration of a contaminant transport model. A full description of these parameters is outlined in Section 5 of this appendix.

Calibration parameters

- Mean pore velocity (if coupled with a flow model – this will already be determined)
- Heterogeneity (if coupled with a flow model – this will already be determined)
- Dispersivity
- Diffusion coefficient
- Adsorption coefficient
- Degradation rate
- Source locations
- Source history

3.2 Calibration Targets

Both qualitative and quantitative calibration criteria are used to measure the success of the calibration of a contaminant transport model. These criteria are summarised below.

Qualitative calibration criteria

- Comparison of general patterns; plume patterns; breakthrough curves
- Assessment of the 'reasonableness' of the input parameters
- Mass budgets (estimate of the source mass released into the aquifer, the mass adsorbed by the aquifer, or released into streams, wells, the coast etc)

These are subjective assessment measures.

Quantitative calibration criteria

- Calculation of concentration residuals

  Mean, root mean square, standard deviations etc (for statistics as outlined in Table D2 below)

- Correlation of residuals

  Scattergrams, Residual contours

Quantitative measurements

The match to concentrations, taken at specific points in space and time is measured quantitatively. This is done using a number of statistical, and mathematical measures of the difference between measured and simulated concentrations. These differences are called model error. The objective of calibration is to minimise this error. The range of measures for the quantification of model error are called the objective function. Table D2 outlines a number of different forms of these measures of fit or objective functions.

In addition to these mathematical measures, the residuals between measured and modelled data should be random. Where there is a trend in the residuals, the model configuration may be in error and should be revisited. The analytical model configuration may be too simple and a numerical model may be required.

Table D2: Quantitative calibration criteria. Criteria in this table are to be used only as a guide to model calibration success; they should not be used without analysis and reference to the hydrogeological basis of the model.

Description	Equation	Comment
Residual	$R_i = C_i - c_i$ where: R_i = residual C_i = measured head at location i c_i = modelled head at location i	The smaller the residual the more likely the calibration is correct.
Mean error (ME)	$\frac{1}{n}\sum_{i=1}^{n}(C_i - c_i)$	A mean error incorporates both negative and positive residuals. Therefore a small mean error may not indicate a good calibration.
Mean absolute error (MAE)	$\frac{1}{n}\sum_{i=1}^{n}\lvert C_i - c_i\rvert$	A small MAE may indicate a good calibration.
Root mean squared error (RMS)	$\frac{1}{n}\sum_{i=1}^{n}\sqrt{(C_i - c_i)^2}$	A small RMS may indicate a good calibration.
Sum of residuals	$\sum_{i=1}^{n} W_i\lvert C_i - c_i\rvert$ where: W_i = weighting from 0 to 1	Useful for comparing successive model runs. The measure is dependent on sample size. Weights are used to emphasize more or less reliable data , or change the emphasis of a specific parameter or area.

Table D2: Quantitative calibration criteria (continued)

Correlation function - R	$\frac{\sum (c_i - \bar{c})(C_i - \bar{C})}{\sqrt{\sum (c_i - \bar{c})^2}\sqrt{(C_i - \bar{C})^2}}$ where : $\bar{c}$ and $\bar{C}$ are the average of the modelled and measured concentrations respectively	May tend to one for perfect calibrations, may be close to one for poor models.
R^2	$\frac{\sum_{i=1}^{n} W_i \left(C_i - \bar{C}\right)^2}{\sum_{i=1}^{n} W_i \left(c_i - \bar{C}\right)^2}$ where : $\bar{c}$ and $\bar{C}$ are the average of the modelled and measured concentrations respectively	May tend to one for perfect calibrations, may be close to one for poor models.
Weighted least squares – S(b) – used to describe parameter estimation	$(C - c(b))^T \underline{w} (C - c(b))$ where : b = vector containing parameter estimates c(b) = matrix of modelled concentrations which is a function of b C = matrix of measured concentrations	This is a matrix function, is used in parameter estimation software.
Maximum likelihood –S'(b)	$(ND + NPR)\ln 2\pi - \ln\lvert\underline{w}\rvert + (C - c(b))^T \underline{w} (C - c(b))$ where : ND = number of observations NPR = number of prior information values $\lvert\underline{w}\rvert$ = determinant of the weight matrix	This is a matrix function, is used in parameter estimation software.

Note: Concentrations have been used to represent the observations for comparison with model output. However other measurements, such as flows could be used in the equations listed in Table D2.

4.0 Predictive uncertainty and numerical models

As discussed in Section 5 of the main report, model predictive uncertainty is related to model assumptions and parameter uncertainty. In addition, model errors clearly also compromise model predictions. As a result the model auditor needs to:

- Consider the degree to which the model assumptions are different from the real world and assess what the likely bias on predictions may be as a result of model assumptions.
- Consider the possible range of parameters and their natural variability or heterogeneity, measurement errors, interpretation of measurement errors, or lack of measurements. The auditor also needs to simply check that the model solutions are within a realistic realm, as some combinations of parameters, within realistic ranges, can produce unrealistic solutions
- Undertake checks for model errors.

Due to the greater number of parameters and associated data associated, numerical models are inherently more likely to induce errors than the simpler analytical models.

When addressing model uncertainty, the chief aim is to identify the limiting case for the model prediction (often called worst case). For example, if the model is being used to determine the distance at which a threshold concentration may occur, what is the largest distance given the information available? Or, if the concentration at a well is being estimated, what is the greatest concentration that may occur, given the available data? The model auditor needs to be satisfied that this limiting worst case has been realistically identified in such a way that it takes into account the model uncertainty.

4.1 Model assumption uncertainty

Numerical models include a whole range of model assumptions. However, unlike analytical models most of the assumptions are chosen by the modeller and therefore are model specific. The model assumptions in numerical contaminant transport models that are likely to have the greatest effect on predictive uncertainty are:

- How aquifer heterogeneities are represented,
- Boundary conditions,
- Discretisation of the model in space and time,
- Density variations, and
- Biological and chemical reactions – decay , and equilibrium and non equilibrium adsorption and solute pore fluid reactions.

As a contaminant model often uses a flow model to determine the velocity field, reference should also be made to Appendix C as appropriate.

4.1.1 Aquifer heterogeneity representation

When migrating through a heterogeneous aquifer, groundwater moves through zones of varying permeabilities with associated differing mean flow velocities. Because of this a contaminant mass in groundwater is distributed over a range of different permeability zones and migrates away from its source at differing velocities. Contaminant transport is dominated by these preferential flow paths. The realistic quantification of this movement is difficult because of the uncertainty in characterization of aquifer properties.

The generally accepted approach is to attempt to resolve (describe) the hydraulic conductivity (or velocity) field at a sufficiently high level and apply a numerical code which allows for the representation of the aquifer by the definition of zones, within which the property has a constant value. Geological mapping provides guidance on where these zones should be placed. Similarly, mapping of aquifer parameters from pumping tests can also provide guidance for zone delineation. However often there is insufficient detail in the geological data.

During calibration, the parameters within these zones are adjusted until the fit between model outcomes and field observations is acceptable. Where the fit is not acceptable, additional zones are often introduced where the modeller feels they will be effective in improving the model fit to field observations. The placement of zones is therefore quite subjective.

Furthermore the characterisation of geological heterogeneity by zones of piecewise uniformity is not consistent with the nature of alluvial material, which is the stratal framework for much of the aquifers in New Zealand. The effect of small scale heterogeneities on model predictions are not even able to be explored within zonation patterns, rather the zonation represents an average parameterisation. Even highly discretized systems (e.g., with block sizes of the order of 10 cubic metres in large aquifers) have not adequately captured the migration patterns, as unresolved heterogeneities of a fractal type also exist at these relatively small scales. The presence of this very fine scale variation, which cannot be measured, and neither can be inferred by the calibration process, does affect contaminant flow and so contributes to predictive uncertainty.

To address this heterogeneity associated chaotic uncertainty, stochastic methods are being advocated for contaminant fate and transport problems. These stochastic approaches, represent these small scale variabilities using geostatistical terms, or where there is no measurement information as completely random parameter fields (Carle and Fogg 1997).

One common stochastic technique, is the Monte Carlo method. In this method a number of different hydraulic property fields are derived from site measurements such that they all satisfy geostatistical and calibration constraints. The model predictive simulations are then run with each of the equally valid models, so that a measure of the predictive uncertainty can be determined.

Another method is the small perturbation approximation. In this approach flow parameters, such as hydraulic conductivity are replaced in the governing equation by a mean plus a zero mean perturbation term. The statistical mean and standard deviation of the predictions are then reported.

Similarly the continuous time random walk approach uses a probability density function (pdf) which describes each particle transition over a distance and direction over a number of time steps. The mean and standard deviation of this pdf describes the movement and spread of the plume.

It is generally agreed that stochastic methods are important in addressing the predictive uncertainty in contaminant transport modelling. However these methods are still very much the domain of academic research and are not yet commonplace in modelling.

4.1.2 Assumptions of model boundaries

Compared to analytical models, the numerical modeller has much greater choice in the combination and location of simplifying assumptions. In terms of flow boundaries this flexibility allows the situations such as the contaminant flux into a stream or at a beach foreshore to be examined. For more discussion on flow boundaries refer to Appendix C. Contaminant boundaries occur in the model where the dissolved concentrations are leaving or entering the model domain. Boundaries are typically defined as either a specified concentration in groundwater, or as a concentration of a flux which enters or leaves the aquifer.

4.2 GRID/TIME discretisation

The advection dispersion equation is difficult to solve even with numerical solutions. A phenomenon known as numerical dispersion can occur where errors associated with the discretisation of the model in time and space give unreliable solutions. Numerical dispersion is more common for advective dominated transport. There are a number of grid size or time step stability criteria as outlined below.

Stability control criteria

Grid size

Peclet number is less than or equal to one.

where Pe = $\Delta l/\alpha$, where Δl is the characteristic grid spacing, and α is the characteristic dispersivity

Time step

Courant number is less than or equal to one (where C = $v\Delta t/\Delta l$, where v = velocity, Δt = time step size). That is the time step size should be less than the time it takes to move across a cell.

For decaying contaminants, $\Delta t \leq 1/$ decay rate – for the lowest decay rate.

4.2.1 Density dependence

Most model codes assume that the density of groundwater is constant and approximately equal to 1.0 g/cm^3. This is a valid assumption for water with low concentrations of total dissolved solids or temperatures in the range of most shallow aquifers. For situations where this is not valid, then density dependent flow should be modelled, as relatively small changes in density can significantly alter the flow field water. This includes situations where water is hot (say 50°C, which changes water density to 0.988 g/cm^3), as in geothermal reservoirs and aquifer heat storage systems; or where water has a large total dissolved solids content (TDS), such as salt water which has a TDS of around 35 000 mg/L giving it a density of 1.025 g/cm^3. Some contaminant plumes also have high a TDS content. Public domain software for density dependent codes include SUTRA (for two dimensional problems) and HST3D (for three dimensional problems).

4.2.2 Chemical

Assumptions of chemical and biological reactions, such as sorption onto particles in the aquifer matrix, decay are relatively simple to include in both numerical and analytical models where required and most numerical contaminant transport codes provide for these reactions. Sometimes non-equilibrium reactions need to be considered. Interactions between solutes can also be important to consider, however these are more rare, and often the data required for such models are not available without running field tracer tests.

It is commonly assumed that reactions in contaminant transport models have reached equilibrium. However where transport of a contaminant is faster than its sorption reaction, chemical non-equilibrium will occur. Similarly, non-equilibrium conditions occur due to aquifer heterogeneity, where zones of comparatively mobile and immobile water occur.

4.3 Parameters, their uncertainty and model predictive uncertainty

For numerical contaminant transport models the model parameters of principal importance are the determination of mass flux, the velocity field and dispersion.

4.3.1 Methods to address predictive uncertainty

Non calibrated models

The range of what is possible in model predictions is large where models are not constrained by calibration. Parameter ranges are chosen on the basis of regional information, or even literature values. It is important that the modeller does not just choose one preferred set of parameters, as although reasonable, other combinations of parameters will also be reasonable. Different parameter combinations have a different impact on the model predictions. It is important to explore this range of possible parameter combinations in order to identify the range and the worst of these predictions.

Calibrated models

Calibration of a model constrains the possible range of model predictions by requiring that the model outputs match the observed data. However, when calibrating a model it is usually found that the parameter estimates are non-unique, i.e. different combinations of parameter estimates match the field observations equally well. Parameter non-uniqueness is partly caused by the complexity of many real systems coupled with the relative lack of data sets. In addition to this, the bias that model assumptions impart on model parameterisation also contributes to parameter uncertainty. Because of this non-uniqueness there is a range of possible model predictions that are equally valid, given the available data. Even though this range is significantly less than for an un-calibrated model. Predictive uncertainty is assessed by running predictive simulations on the possible range of calibrated models. This is a time consuming task.

The high variability of aquifer parameters that cannot be determined in the calibration process can be explored using stochastic methods. While this is not common practice at present, it is recommended that these methods be used as they become more generally available.

In Hill's 'Methods and Guidelines for Effective Model Calibration' (1998) the use of parameter estimation software is strongly advocated. However, despite the clear advantages of using this software, it is not commonly used, with trial and error calibration still being much more the common practice. This is partly because of the problems of instability, non-uniqueness (as discussed above) and instability. Insensitivity occurs when there is simply not enough observation information to support the estimation of parameters. Instability occurs when slight changes in parameter values or observations create large changes in the model results. However, model calibration by trial and error also incorporates these problems, but the modeller is less likely to be aware of them. Parameter estimation software essentially allows modellers to understand their models and data better by undertaking all the steps involved in multiple model calibrations far more quickly than the modeller can achieve by trial and error.

Hill (1998) states: *'The benefits of inverse modelling include (1) clear determination of parameter values that produce the best possible fit to the available observations; (2) diagnostic statistics that quantify (a) quality of calibration, (b) data shortcomings and needs, (3) inferential statistics that quantify reliability of parameter estimates and predictions; and (4) identification of issues that are easily overlooked during non-automated calibration.'*

Methods that allow a very clear identification of a worst case include 'predictive analysis' (Doherty 2000), as discussed in Section 5.1 of the main report, or response functions , where the relative rather than the absolute magnitude of predictions is of concern.

Mass flux

In some modelling problems, the determination of the mass flux can require a large number of assumptions. In some cases the mass flux is determined by running another model, which estimates the flux moving through unsaturated strata before it reaches the water table. The assumptions used in determining a mass flux can be flawed. A model auditor should examine the assessment of mass flux, to ensure the assumptions are valid and appropriate for the modelling problem being investigated.

5.0 Data requirements

Typical numerical model inputs are described in this section. These inputs can be based on site specific information if a site specific prediction is required, or general regional flow data if the model is being used for exploration of a general case or literature values for a theoretical assessment. Judgement is required in determining if the data are adequate to simulate the system accurately. Where a flow model is used to determine velocities, refer to Appendix C. The following text boxes list, describe and include discussion of parameters that may be required in a numerical contaminant transport model

Parameter	**Model domain - layer extent, and top and bottom elevations**
Description	The extent of the model, or the model domain, is selected so that it is large enough to encompass the area of interest and to ensure that the selected boundary conditions do not significantly influence model results. Where possible, natural boundaries are used, such as rivers, lakes, wetlands, bedrock outcrops or a water table ridge (groundwater divide). The top and bottom elevations of each layer need to be defined with respect to a datum which will also be used for water level measurements (unless the aquifer is confined). The model is defined in three dimensions, using a system or rows, columns and layers.

Parameter	**Model grid / element mesh**
Description	The model domain is split up into cells or elements, as required, given that an average solution is calculated for each cell or element. The model grid must be sufficiently small in the area of interest or where steep hydraulic gradients will occur (i.e. around a seepage face, a drain, or pumping wells) to accurately represent local variations in soil properties, hydraulic head and groundwater concentrations. Typically the model grid is aligned to the general direction of groundwater flow. The most stable solutions are provided for uniformly spaced grids (for finite difference models a change in distance between adjacent gridlines should be less than 1.5 times for model stability). Smaller time steps, together with small cell sizes, allow better numerical approximations to the partial differential flow equation. So the greater the degree of spatial discretisation, the better the definition of the solution. However this needs to be balanced against the longer solution time. The sensitivity of the solution to time step size and grid size should be tested.

Parameter	Time steps
Description	Smaller time steps, together with small cell sizes, allow better numerical approximations to the partial differential flow equation. So the greater the degree of temporal discretisation, the better the definition of solution. However these need to be balanced against the longer solution time. Reduction of time step size is also used where there are numerical instabilities – where unrealistic oscillating solutions occur. The sensitivity of the solution to time step size and gird size should be tested. Some guidance for approximation of time steps is given such that the time step would be small enough to allow an explicit solution to be calculated within that time. One option de Marsily (1986) presents is to use an initial time step Δt, by $\Delta t = Sa^2/4T$, Where: a = grid dimension Δx or Δy for a regular grid T = transmissivity S = storativity Time steps are typically increased as a geometric progression of ratio 1.2 to 1.5.

Parameter	Stress periods
Description	Most numerical codes allow the simulation period to be divided into blocks of variable time, known as stress periods. The option of stress periods allow the stresses to be altered while the simulation is in process. In addition, time steps can then be defined separately for different stress periods.

Parameter	Groundwater pore velocities
Units	m/day
Description	The volume of water that will move through a porous medium in unit time under a unit hydraulic gradient through a unit area measured at right angles to the direction of flow. Hydraulic conductivity parameter contains factors accounting for the properties of the fluid (water) and of the saturated porous medium. It is defined as: $$K = \frac{k\rho_{water} g}{\mu}$$ Where: k = intrinsic permeability of the strata

	g = acceleration due to gravity ρ_{water} = density of water μ = viscosity of water Hydraulic conductivity can vary depending on the direction when measured at one point and this feature is called anisotropy. This is especially for sediments, which are often stratified and have a greater conductivity in the direction of depositional flow. Because of this the major axes of hydraulic conductivity are defined as K_{xx}, K_{yy} and K_{zz}. Anisotropy is usually represented on a layer by layer basis in numerical models, where the magnitude of the anisotropy and the principal direction are defined. Hydraulic conductivity also varies spatially from one point in the aquifer to another (heterogeneity). Heterogeneity can be represented in a numerical model by having different zones of hydraulic conductivity. Both heterogeneity and anisotropy affect groundwater flow.

Parameter	**Well locations, pumping rate and duration (Q)**
Typical Units	m^3/day or L/s
Description	The location of each well in terms of the model layer, row and column (or element) is defined. Usually negative values of a pumping rate indicate a withdrawal well, while positive values indicate a recharging well. When simulating several wells that fall within one cell area, the user must sum the individual pumping rates. The pumping rate for each well needs to be determined for each stress period. The duration of the pumping rate therefore determines the length of a stress period. Where wells abstract from more than one layer, this is represented by having a separate well in each layer, and the proportion of the pumping rate is attributed to each layer.

Parameter	**Initial conditions**
Typical Units	kg/m^3 or mg/L
Description	Initial conditions are values of concentration for each active cell in the model.

Parameter	**Input Mass/Mass Flux**
Units	kg or Numbers or kg/day or numbers/day
Description	The mass flux entering the groundwater at either a point, along a line or over an area (the most conservative assumption is that the mass enters groundwater at a point). If the source is instantaneous an input mass is entered. Where the source is continuous the mass entering groundwater each day is entered, and this is called the mass flux.
Discussion	Although this is an apparently simple definition when the concentration and flow rate are defined, the ways of calculating mass flux where one of these parameters is not defined are many and varied. The following discussion identifies some factors, which may need to be considered.

Contaminant mass is discharged to unsaturated strata before percolating to groundwater

A conservative and sometimes unrealistic mass flux assumes that there is no attenuation in unsaturated strata. This assumption is realistically conservative if the groundwater table occurs in very shallow gravel strata. A worst-case assumption is often made that the mass flux is directly entering groundwater, rather than first travelling through the unsaturated zone. Because this approach ignores processes in the unsaturated zone, such as adsorption, volatilisation and biodegradation, it will tend to overestimate mass flux.

If groundwater is deep, this assumption becomes unrealistic, particularly for decaying contaminants. It is important that the greater degree of groundwater protection associated with a greater depth to the groundwater is reflected in the mass flux value.

Neither the contaminant concentration nor the flow rate are defined

In some situations, neither the contaminant mass nor the flow rate is well defined. This can be the case where a contaminant is being leached from contaminated soil, either by infiltrating rainwater or groundwater throughflow.

Flow rate is not defined

In these situations the flow rate is estimated by considering either the rainfall infiltration rate (if leaching is occurring via rainfall infiltration) or by groundwater throughflow (if groundwater is in contact with contaminated soil).

For rainfall infiltration through contaminated soil consideration of the area of contaminated soil and rainfall infiltration is necessary, e.g. for a fuel spillage adsorbed onto soil in the unsaturated strata above a water table.

Where contaminated soil is in contact with groundwater, the mass flux can then be calculated by assessing the groundwater flow through the contaminated strata. This may be necessary where free phase hydrocarbon product is sitting on top of the water table, contaminated soil is inundated by high groundwater levels, or in a landfill where high groundwater levels inundate the base of the landfill.

To consider the relevant groundwater flow rate, we need to determine the following; the thickness of the flow zone; the depth over which the waste is in contact with groundwater flow or the smear zone of hydrocarbons caused by a fluctuating water table; and finally the width of the contaminated zone. We can calculate the mass flux by multiplying the concentration by the groundwater throughflow beneath the site, using the following equation:

Groundwater throughflow rate = K i A

where:

K = Hydraulic conductivity,

i = Hydraulic gradient, and

A = Area of groundwater contamination.

Determining concentration in water when the soil concentration is known

The concentration of contaminants in leachate or groundwater throughflow can be related to the soil contaminant concentration by considering the distribution coefficient for the contaminant.

$C_{soil} = K_d C_{water}$

where:

K_d = distribution coefficient,

C_{soil} = concentration of contaminant in soil, and

	C_{water} = concentration of contaminant in water. This calculation assumes equilibrium conditions between the soil and water partitioning. The mass flux is then calculated knowing the rainfall recharge rate and the leachate concentration. Note: Some contaminants are present in soil in a number of phases. For example hydrocarbons can be present in the sorbed phase, a soluble phase, a vapour phase and an immiscible (free) phase. ***Determining concentrations in water where there are no soil concentrations*** We often do not know the concentration of a contaminant in the contaminated soil or in the groundwater source. Sometimes the concentration in leachate or in the contaminated groundwater must be measured, or literature values can be referred to. A few approaches used to estimate the source concentration of contaminated soil or groundwater are discussed below. *Using groundwater monitoring data*. Where we have actual groundwater monitoring data, we can use this to calibrate a model to determine the mass flux (i.e. back calculate the mass flux using a groundwater contaminant model). *Leachate tests (laboratory).* A sample of the contaminated soil or landfill is collected and tested. There are many methods available including: *Column test*. The sample is packed into a column and a solution (e.g. local rainwater) is poured onto the column and the concentration of the leachate collected at the bottom of the column is analysed. *Tumble test.* The sample is mixed with a solution in a container and then tumbled for several hours. The solution is then poured off and analysed. *Lysimeter measurement*s. A lysimeter allows the collection of in situ soil water in the unsaturated zone (much like a piezometer allows the collection of groundwater). *Literature values.* There are many papers available that cite concentrations of elements in landfill leachate and stormwater. In the absence of any field data, these literature concentrations can be used to estimate mass flux. Alternatively, physical relationships cited in the literature, such as the solubility of an element and the partitioning of an element between soil and water (K_d), and the limits to the partitioning (Raoult's Law) can be used to estimate a mass flux. 'Raoult's Law' determines the maximum solubility of a hydrocarbon as: $C_{wmax} = x_i S_i$ where: C_{wmax} = maximum concentration in water x_i = mole fraction of compound, (e.g. mole fraction of benzene/gasolene = 0.03) S_i = solubility of compound, (e.g. solubility of benzene in water = 1800 mg/L)

Boundary Condition	**Instantaneous or Continuous or Fixed Duration Mass Input**
Description	Instantaneous source - a slug of contamination is instantaneously injected into the aquifer. In reality nothing can be introduced instantaneously, it always takes some time. However sources which are introduced quickly into an aquifer, compared to the time frame of interest, can be considered to be introduced instantaneously. For example, this would be the case for a spill which may enter groundwater over an hour period, and the nearest point of concern is approximately 3 days travel distance away. Continuous source – a contaminant is continuously injected into an aquifer at a constant rate. Check –

	most models use a daily time frame. Any mass input that is constant on a daily basis can be considered a continuous source. A domestic waste water discharging every day to ground can be considered to be a continuous source. Fixed duration sources – a contaminant is injected into an aquifer at a specified rate for a specified amount of time. Irrigation of wastewater to land over a summer irrigation period could be considered a fixed duration source. Model contaminant boundaries are either: Constant concentration in groundwater, or Concentration of a recharge flux.

Parameter	**Effective porosity (σ or n)**			
Units	m^3/m^3			
Description	The dimensionless ratio of the volume of interconnected voids to the bulk volume of the aquifer matrix. Note that "total porosity" is the ratio of all voids (including non-connected voids) to the bulk volume of the aquifer matrix. The difference between total and effective porosity reflects lithological controls on pore structure.			
Typical values for alluvial aquifers	Porosity	**Method of Measurement**	**Location**	**Reference**
	0.25	Field density tests	Heretaunga Plains	Thorpe et al. (1982)
	0.2	Repacked aquifer material in laboratory column	Templeton	Sinton et al. (1997)
	0.19	Repacked aquifer material in laboratory column	Burnham	Pang and Close (1999)
	0.2 – 0.3	Resistivity results	McLeans Island	Broadbent and Callander (1991)
	0.25 – 0.35	Seismic results	Canterbury Plains Quaternary sediments	Broadbent (1978)
Typical values for other types of strata	Values taken from Domenico and Schwartz (1990):			
Rock type	Range of porosities			
SEDIMENTARY				
Gravel, coarse	0.24 – 0.36			
Gravel, fine	0.25 – 0.38			
Sand, coarse	0.31 – 0.46			
Sand, fine	0.26 – 0.53			

Silt	0.34 – 0.61
Clay	0.34 – 0.60
SEDIMENTARY ROCKS	
Sandstone	0.05 – 0.30
Siltstone	0.21 – 0.41
Limestone, dolostone	0 – 0.20
Karstified and reef limestone	0.05 – 0.50
Shale	0 – 0.10
CRYSTALLINE (igneous and metamorphic) ROCKS	
Fractured crystalline rock	0 – 0.10
Dense crystalline rock	0 – 0.05
Basalt	0.03 – 0.35
Weathered granite	0.34 – 0.57
Weathered gabbro	0.42 –0.45

Parameter	**Pore Velocity (v)**
Units	m/day
Description	The pore velocity, v, (also known as the contaminant transport velocity) is calculated as follows: v = (-Ki)/n where: n = porosity i = hydraulic gradient K = hydraulic conductivity Note 1: Beware, in heterogeneous aquifers pore velocities determined from tracer tests are quite different to those calculated from pumping test results see below. Note 2: Beware the term 'velocity' is also used to describe the flux velocity, so be sure you know which one you are dealing with! The flux velocity is the volumetric flow rate (or flux) divided by the cross-sectional area normal to flow. U = -Ki

Guidance on selection of pore velocity	Because of aquifer heterogeneity, there is often a discrepancy between the mean groundwater pore velocities often apparent from tracer test studies and those calculated from pump test data (for estimates of K and n) and piezometric maps. For example, using typical hydraulic conductivity values derived from pump test results in alluvial gravel aquifers (ranging from 10 m/d to 200 m/d), hydraulic gradients from piezometric contour maps (ranging from 0.01 to 0.001) and a typical porosity for gravel strata (ranging between 0.2 and 0.4), gives velocities from less than 1 m/day up to 10 m/day. However, tracer tests in Canterbury alluvial aquifers indicate much faster pore velocities ranging from 5 to 200 m/day. The likely explanation for this difference is that in a pump test the calculated hydraulic conductivity is based on the drawdown response as water is drawn from both low and high permeability strata. In contrast, for a tracer test, hydraulic conductivity is calculated based on the time of maximum concentration at any observation point, which is related to the fastest moving groundwater (flowing through the most permeable pathway within the aquifer strata). The following approach for choosing reasonable ranges of pore velocity estimates is advocated: • For heterogeneous strata, such as alluvial gravels, pore velocity estimates should be based on tracer test data. Where there is no data available in a specific area, reference should be made to the data available in the literature for similar strata. In alluvial gravel aquifers, tracer tests at Burnham, Templeton and Heretaunga Plains studies, as described by Sinton et al. (1997) and Pang and Close (1999) and Thorpe et al. (1982) respectively indicate peak concentration velocities of between 60 – 140 m/day. On the basis of these velocities it may be necessary to recognise that the maximum pore velocity could be as high as 200 m/day. • For homogeneous strata such as sand or beach gravels calculated pore velocity (v) estimates from pump test data are likely to be appropriate, using the equation v = (Ki)/n.

Parameter	**Dispersivity** **Longitudinal dispersivity α_L** **Transverse dispersivity, α_T** **Vertical dispersivity, α_V** **Longitudinal scale dispersivity, E_1** **Transverse scale dispersivity, E_2** **Vertical scale dispersivity, E_3**
Units	m
Description	Dispersion refers to the process whereby a plume will spread out in a longitudinal direction (along the direction of groundwater flow), transversely (perpendicular to groundwater flow), and vertically downwards due to mechanical mixing in the aquifer and chemical diffusion. Dispersion occurs as a result of two processes - chemical diffusion and mechanical dispersion. Diffusion originates from mixing caused by random molecular motions due to the kinetic energy of the contaminant. Mechanical dispersion is mixing that occurs as a consequence of local variations in velocity around some mean velocity. Dispersivity is defined in three dimensions, in the direction of groundwater flow – longitudinal dispersivity (α_L), perpendicular to the direction of groundwater flow – transverse dispersivity (α_T), and with depth(α_V) vertical dispersivity. Dispersivity values increase with scale; i.e. the further away from a source, the greater the contaminant is dispersed. More recently, scale dispersivity terms have been defined (Hunt, 1998) as follows: (α_L), = E_1x, where (α_L), is the longitudinal dispersivity, x is the distance from source, and E_1, is the longitudinal dispersivity dimensionless coefficient.

	Similarly, (α_T) = E_2x, where (α_T), is the transverse dispersivity, x is the distance from source, and E_2, is the transverse dispersivity dimensionless coefficient, and (α_V) = E_3x, where (α_V) is the vertical dispersivity, x is the distance from source, and E_3, is the vertical dispersivity dimensionless coefficient.

Parameter	**Hydraulic conductivity (K)**
Units	m/day
Description	The hydraulic conductivity is defined as the volume of water that will move through a porous medium, in unit time, under a unit hydraulic gradient, through a unit area measured at right angles to the direction of flow. The hydraulic conductivity parameter contains properties of the fluid (water) and of the saturated porous medium (the aquifer). It is defined as: $K = \frac{k\rho_{water} g}{\mu}$ Where: k = intrinsic permeability of the strata g = acceleration due to gravity ρ_{water} = density of water μ = viscosity of water Hydraulic conductivity can vary in differing directions and this feature is called anisotropy. **Anisotropy** especially occurs in water laid sediments which are often stratified and have a greater conductivity in the direction of flow. The major axes of hydraulic conductivity are defined as K_{xx}, K_{yy} and K_{zz}. Anisotropy is usually represented on a layer by layer basis in numerical models, where the magnitude of the anisotropy and its principal direction are defined. Hydraulic conductivity also varies spatially from one point in the aquifer to another, this property is called **heterogeneity**. Heterogeneity can be represented in a numerical model by having different zones of hydraulic conductivity. Both heterogeneity and anisotropy affect groundwater flow.
Typical values	Values taken from Domenico and Schwartz (1990)
<u>*Sedimentary*</u>	
Gravel	$3 \times 10^{-4} - 3 \times 10^{-2}$
Coarse sand	$9 \times 10^{-7} - 6 \times 10^{-3}$
Medium sand	$9 \times 10^{-7} - 5 \times 10^{-4}$
Fine sand	$2 \times 10^{-7} - 2 \times 10^{-4}$

Silt, Loess	$1 \times 10^{-9} – 2 \times 10^{-5}$
Till	$1 \times 10^{-12} – 2 \times 10^{-6}$
Clay	$1 \times 10^{-11} – 4.7 \times 10^{-9}$
Un-weathered marine clay	$8 \times 10^{-13} – 2 \times 10^{-9}$
Sedimentary rocks	
Karstified and reef limestone	$1 \times 10^{-6} – 2 \times 10^{-2}$
Limestone, dolostone	$1 \times 10^{-9} – 6 \times 10^{-6}$
Sandstone	$3 \times 10^{-10} – 6 \times 10^{-6}$
Siltstone	$1 \times 10^{-11} – 1.4 \times 10^{-8}$
Salt	$1 \times 10^{-12} – 1 \times 10^{-10}$
Anhydrite	$4 \times 10^{-13} – 2 \times 10^{-8}$
Shale	$1 \times 10^{-13} – 2 \times 10^{-9}$
Crystalline (igneous and metamorphic) rocks	
Fractured basalt	$4 \times 10^{-7} – 2 \times 10^{-2}$
Fractured igneous and metamorphic rock	$8 \times 10^{-9} – 3 \times 10^{-4}$
Weathered granite	$3.3 \times 10^{-6} – 5.2 \times 10^{-5}$
Weathered gabbro	$5.5 \times 10^{-7} – 3.8 \times 10^{-6}$
Basalt	$2 \times 10^{-11} – 4.2 \times 10^{-7}$
Massive (un-fractured) igneous and metamorphic rocks	$3 \times 10^{-14} – 2 \times 10^{-10}$

Parameter	Hydraulic Gradient (i)
Units	(m/m)
Description	The slope of the potentiometric surface. In unconfined aquifers, this is equivalent to the slope of the water table. The hydraulic gradient is typically calculated by constructing potentiometric surface maps using static water level data from monitoring wells and estimating the slope of the potentiometric surface. Typically it can range from 0.01 - 0.0001.

5.1 Chemical or biological processes

Parameter	Decay Coefficient (λ)			
Units	1/day			
Description	The decay coefficient is used to represent both radioactive decay and biological die-off of the source. In both cases the initial concentration of a contaminant is continually decreasing as follows; $N(t) = N_0 e^{-\lambda t}$ Where, N is the number of elements in the contaminant source (i.e. faecal coliforms, atoms, etc.), t is time and λ is the rate constant for decay. $T_{1/2} = 0.693/\lambda$, where $T_{1/2}$ is the half life and $T_{90} = 2.303/\lambda$, where T_{90} is the time where 90% die off has occurred.			
Discussion	*Chemicals.* Decay rates are usually derived from laboratory experiments. There are many references which list decay rates for many substances, e.g. Howard et al. (1991) list environmental decay rates for soil, water and air environments for a comprehensive range of chemicals *Microbes.* For microbes, the decay rates appear to vary significantly depending on the environment they are in. This is at least partly because the measured decay rates for microbes assessed through tracer tests also account for other removal processes dependent on aquifer strata such as filtration, sedimentation and adsorption (Sinton, 1997). As with any data derived from model calibration to test data, the decay rates that are obtained are very unlikely to be a unique solution. Some decay rates for microbial tracer tests in Canterbury are discussed in Appendix B, Section 5.4 and below. NOTE: If a decay rate derived from model calibration to tracer test data is used, then it is important that a model with similar assumptions is used, i.e. with the same model bias.			
Some examples of decay rates	Contaminant	λ (day^{-1})	T_{50} (half –life)	T_{90}
	Benzene	$0.07 – 9.5 \times 10^{-4}$	10 days to 24 months	33 days – 2424 days
	Toluene	0.1 – 0.025	7 days to 4 weeks	23 days – 92 days
	Ethylbenzene	$0.12 – 3.0 \times 10^{-3}$	6 days to 228 days	19 days – 768 days
	Xylene	0.05 – 1.9×10^{-3}	2 - weeks to 12 months	46 days – 1212 days

	Faecal coliforms Oxidation pond effluent	0.37	1.8 days	6.2 days

	Faecal coliforms Septic tank effluent	$\lambda = 0.8$	0.87 days	T90 = 2.9 days,

Parameter	**Kd = distribution coefficient (used for Adsorption assessments)**
Units	mL/g
Description	The coefficient that describes the degree of sorption of contaminants to the solid aquifer matrix. The degree of sorption depends on both aquifer and constituent properties. Increasing Kd values are indicative of a greater tendency for sorption. Usually estimated from soil and chemical data using variables described below; Koc = organic carbon-water partition coefficient, foc = fraction organic content on uncontaminated soil where Kd = Koc x foc Also derived from batch experiments.

Parameter	**Organic Carbon Partition Coefficient (Koc)**
Units	(mg/kg) (L/kg) (mg /L) or (mL/g)
Description	Chemical-specific partition coefficient between soil organic carbon and the aqueous phase. Larger values indicate greater affinity of contaminants for the organic carbon fraction of soil. This value is chemical specific and can be found in chemical reference books. Note there is a wide range of reported values for Koc in chemical reference literature, listing relationships between Koc and solubility of Koc and the octanol-water partition coefficient (Kow). Some typical examples are: Benzene 38 L/kg Toluene 135 L/kg Ethylbenzene 95 L/kg Xylene 240 L/kg

Parameter	**Fraction Organic Carbon (foc)**
Units	Unitless
Description	Fraction of the aquifer soil matrix comprised of natural organic carbon in uncontaminated areas. More natural organic carbon means higher adsorption of organic constituents on the aquifer matrix. Typical Values

	range from 0.0002 - 0.03. The fraction organic carbon value should be measured if possible by collecting a sample of aquifer material from an uncontaminated zone and performing a laboratory analysis (e.g. ASTM method 2974-87 or equivalent).

6.0 Errors

Errors can be generated through the following:

- inappropriate models design;
- selection of conditions;
- lack of information and oversimplification.

Some errors are also due to the application of inappropriate model assumptions, as discussed in Section 4 of this appendix. There are also errors caused by carelessness.

Table D3 provides a check list which model auditors can use as they consider the validity of the predictions of a model. Meeting all the requirements outlined in the checklist does not guarantee good model predictions, but will assist an auditor to make an assessment.

Table D3: Checklist for numerical contaminant transport model errors

Data gathering errors	Potential implication for solution	Auditor check	OK - tick	Comments
Field measurements of parameters incorporate inherent inaccuracies	These are errors are associated with human error or an instrument error used for instance in a pumping test or a tracer test. Calibration to inaccurate targets compromises model accuracy and predictions.	Have measuring errors been assessed?		
Analysis of field data. Many of the model input parameters require some analysis of the field measurements. For instance mean pore velocity relies on the analysis of pump test drawdown – time data, water level gradients, and porosity or alternatively, concentration – time data from tracer tests.	Inaccurate assumptions in the analysis of field data will compromise the analysis of the parameters, and the model calibration.	Are the estimates of aquifer parameters calculated correctly from aquifer or tracer tests?		
Extrapolation of field data. Aquifer properties, such as hydraulic conductivity are different when derived from a pump test compared to a tracer test.	In a pump test the calculated hydraulic conductivity is based on the drawdown response as water is drawn from both low and high permeability strata. In contrast, for a tracer test, hydraulic conductivity is calculated based on the time of maximum concentration at any observation point, which is related to the fastest moving groundwater (flowing through the most permeable pathway within the aquifer strata). Inappropriate extrapolation will compromise the model calibration.	Has the appropriate extrapolation of field data been used for the strata at the site.		

Data input errors	Potential implication for solution	Auditor check	OK - tick	Comments
Inconsistent parameter units - i.e. grams and metres and days.	It is important to use consistent units when modelling. Inaccuracies can occur easily if the same units are not used.	Are the model units consistent for all parameters – i.e. days and seconds, cubic metres per day etc?		
Incorrect sign for pumping or recharge.	It is common practice to express pumping rates as a negative value, injection and recharge as positive values in groundwater modelling programs	Are the correct signs for pumping and recharge used?		
Contaminant discharge must be specified over entire transient simulation period.	Failing to define discharge rates for the full time period give inaccurate results.	Is the discharge specified correctly for the transient simulation period?		

Model assumption errors	Potential implication for solution	Auditor check	OK – tick	Comments
Variable or constant density assumptions	Neglecting density variations can give incorrect indications of flow field.	Are there density variations within the flow field and if so have they been accounted for?		
Selection of contaminant boundary conditions – inappropriate	The rate of contaminant entering an aquifer when using a constant concentration boundary varies with pore velocity. This boundary condition is often misused for situations where a velocity independent flux is entering groundwater from the surface, i.e. in stormwater discharges etc.	What are the contaminant boundary conditions and is the hydrogeological or geochemical basis accurate?		
Discretisation in space and time	Incorrect time and space discretisation (time steps, and grid sizes) can cause numerical instabilities if too large or if the difference in adjacent cell sizes is too great. The model calculates average concentration values for the entire cell.	Are the cell sizes detailed enough in the area of interest?		
		Are the time step and cell sizes small enough to provide numerical accuracy?		

Parameter heterogeneity	Where accurate delineation of plume migration patterns is important to the modelling question, parameter heterogeneity needs to be accounted for. Stochastic methodologies are increasingly advocated – but as yet are not commonplace.	Have the impacts of parameter heterogeneity on model plume predictions been assessed?		
Calibration errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Forcing questionable data to fit	Where a model has been fitted to incomplete observation bore data and does not show a complete breakthrough curve, such that it is not possible to tell whether the peak concentration has not yet come or has passed – the predictions will be compromised by this uncertainty.	Has questionable data been forced to fit?		
Sensitivity analysis	A sensitivity analysis should be used a part of the calibration process – so that calibration efforts are targeted to the parameters for which model predictions are most sensitive.	Has a sensitivity analysis been undertaken? Which were the most sensitive parameters?		
Prediction errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Not incorporating data variability or uncertainty into the analysis	As discussed, despite our efforts, model parameters can never be precisely known. Variations in measured data are either an indication of measurement uncertainty, model bias, or the result of real physical differences. Use the range of data values that reflect data variability to give an indication of the range of possible model predictions. A conservative approach in reporting model results, recognises the uncertainty inherent in modelling and displays a firm understanding of the goals of groundwater modelling	Has the model report discussed the situations where the model predictions are most likely to be valid?		
Blind acceptance of model output	A model's accuracy is no better than the accuracy of the data. Make sure that the model results agree with your understanding of the site hydrogeology and sound hydrogeological principles.			

Predictive uncertainty must be addressed.	Given the non-uniqueness of models, it is important the uncertainty of predictions is explored and the limiting scenario (worst case) is reported.	Has predictive uncertainty analysis been undertaken?		
The correct predictive simulations must be undertaken to fulfil model purpose		Does the model fulfil its purpose?		

7.0 Case study

7.1.1 Model purpose

The finite element saturated and unsaturated flow model SEEP/W and the integrated contaminant transport model CTRANS/W were used to determine whether ammonia leaching from a landfill would have concentrations at the coast below the threshold values as follows:

ANZECC (2000) guidelines - marine water quality guidelines 0.4 - 5.3 g/m^3, and

ANZECC (2000) guidelines - recreational water quality guidelines 0.15 - 15 g/m^3

7.1.2 Model components

Layers

The area was modelled as a cross section of four layers: Layers 1 – the landfill, Layers 2 – 4 comprise the natural strata.

Boundaries

The left and right hand model external boundaries are two constant head boundaries, representing the coast and the inland throughflow from the aquifer. A recharge boundary above ground represented rainfall recharge. No flow boundary occurs beneath layer 4.

Grid set up

The area of the model domain is 1.2 km long and 50 thick. The cell sizes were a uniform 10 m length and 11m breadth.

7.1.3 Model calibration

A transient flow model was calibrated over a 16 year time period, to measured heads, using qualitative assessment of the residual head differences between observed and calculated heads at each location. Using the velocity field from the flow model, the contaminant transport model was then used to explore the range of dispersion, diffusion and adsorption that would allow the concentrations encountered in the observation bores.

No further details of model calibration were provided in the model report.

The main concern when auditing this model was whether the full range of parameter combinations, that allowed model calibration, had been explored. In addition, although a sensitivity analysis was alluded to, there were also no details provided of this. Similarly no model output files were provided to allow checks for errors. This makes the model difficult to audit.

7.1.4 Model predictions

The predictive simulations where run for a 50 year period and indicated the threshold concentrations would be met.

7.1.5 Model uniqueness and predictive uncertainty

While the model parameters may allow the model to match the field data (although this was not documented) it still does not represent a unique solution i.e., another combination of aquifer transmissivity and storage and aquifer boundary characteristics could be used to reproduce the measured water levels and measured contaminant concentrations. Consequently predictive analysis should have been undertaken.

7.1.6 Summary

The audit of this model was compromised by lack of details in the model report.

Table D4: Case study - check list for numerical contaminant transport models

Data gathering errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Field measurements of parameters incorporate inherent inaccuracies	These are errors are associated with human error or an instrument error used for instance in a pumping test or a tracer test. Calibration to inaccurate targets compromises model accuracy and predictions.	Have measuring errors been assessed?		**None stated.**
Analysis of field data. Many of the model input parameters require some analysis of the field measurements. For instance mean pore velocity relies on the analysis of pump test drawdown – time data, water level gradients, and porosity or alternatively concentration – time data from tracer tests.	Inaccurate assumptions in the analysis of field data will compromise the analysis of the parameters, and the model calibration.	Are the estimates of aquifer parameters calculated correctly from aquifer or tracer tests?		**Not reported.**
Extrapolation of field data. Aquifer properties, such as hydraulic conductivity are different when derived from a pump test compared to a tracer test.	In a pump test the calculated hydraulic conductivity is based on the drawdown response as water is drawn from both low and high permeability strata. In contrast, for a tracer test, hydraulic conductivity is calculated based on the time of maximum concentration at any observation point, which is related to the fastest moving groundwater (flowing through the most permeable pathway within the aquifer strata). Inappropriate extrapolation will compromise the model calibration.	Has the appropriate extrapolation of field data been used for the strata at the site.		**Report states calibration is to field measurements – but no details are provided to assess whether this has been done correctly.**
Data input errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Inconsistent parameter units - i.e. grams and metres and days.	It is important to use consistent units when modelling. Inaccuracies can occur easily if the same units are not used.	Are the model units consistent for all parameters – i.e. days and seconds, cubic metres per day, etc?		No details provided.
Incorrect sign for pumping or recharge.	It is common practice to express pumping rates as a negative	Are the correct signs for		No details provided.

	value, injection and recharge as positive values in groundwater modelling programs	pumping and recharge used?		
Contaminant discharge must be specified over entire transient simulation period.	Failing to define discharge rates for the full time period give inaccurate results.	Is the discharge specified correctly for the transient simulation period?		No details provided.
Model assumption errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Variable or constant density assumptions	Neglecting density variations can give incorrect indications of flow field.	Are there density variations within the flow field and if so have they been accounted for?		
Selection of contaminant boundary conditions - inappropriate	The rate of contaminant entering an aquifer when using a constant concentration boundary varies with pore velocity. This boundary condition is often misused for situations where a velocity independent flux is entering groundwater from the surface, i.e. in stormwater discharges etc.	What are the contaminant boundary conditions and is the hydrogeological or geochemical basis accurate?	√	Considered reasonable for this setting.
Discretisation in space and time	Incorrect time and space discretisation (time steps, and grid sizes) can cause numerical instabilities if too large or if the difference in adjacent cell sizes is too great. The model calculates average concentration values for the entire cell.	Are the cell sizes detailed enough in the area of interest?	√	Reasonable.
		Are the time step and cell sizes small enough to provide numerical accuracy?	√	
Parameter heterogeneity	Where accurate delineation of plume migration patterns is important to the modelling question, parameter heterogeneity needs to be accounted for. Stochastic methodologies are increasingly advocated – but as yet are not commonplace.	Have the impacts of parameter heterogeneity on model plume predictions been assessed?		It has been stated that the solution is not unique – however predictive analysis not carried out.
Calibration errors	**Potential implication for solution**	**Auditor check**	**OK -**	**Comments**

			tick	
Forcing questionable data to fit	Where a model has been fitted to incomplete data from observation bores and does not show a complete breakthrough curve, such that it is not possible to tell whether the peak concentration has not yet come or has passed – the predictions will be compromised by this uncertainty.	Have questionable data been forced to fit?		Not enough information to assess this. No model inputs or outputs provided or calibration matches provided.
Sensitivity analysis	A sensitivity analysis should be used a part of the calibration process – so that calibration efforts are targeted to the parameters for which model predictions are most sensitive.	Has a sensitivity analysis been undertaken? Which were the most sensitive parameters?		Alluded to – but no details provided.
Prediction errors	**Potential implication for solution**	**Auditor check**	**OK - tick**	**Comments**
Not incorporating data variability or uncertainty into the analysis	As discussed, despite our efforts, model parameters can never be precisely known. Variations in measured data are either an indication of measurement uncertainty, model bias, or the result of real physical differences. Use the range of data values that reflect data variability to give an indication of the range of possible model predictions. A conservative approach in reporting model results, recognises the uncertainty inherent in modelling and displays a firm understanding of the goals of groundwater modelling	Has the model report discussed the situations where the model predictions are most likely to be valid?		Exploration of variability not stated.
Blind acceptance of model output	A model's accuracy is no better than the accuracy of the data. Make sure that the model results agree with your understanding of the site hydrogeology and sound hydrogeological principles.	Do the model results agree with your understanding of the site hydrogeology and hydrogeological principles?	√	The report has noted some model assumptions which may not be reasonable – but has not explored the impact of these on predictions.
Predictive uncertainty must be addressed.	Given the non-uniqueness of models, it is important the uncertainty of predictions is explored and the limiting scenario (worst case) is reported.	Has predictive uncertainty analysis been undertaken?		Should be undertaken.

The correct predictive simulations must be undertaken to fulfil model purpose		Does the model fulfil its purpose?	√	Simulations did answer the model question – but worst case may not have been identified.