Guide to Good Practice for the Development of Conceptual Models and the Selection and Application of Mathematical Models of Contaminant Transport Processes in the Subsurface

National Groundwater & Contaminated Land Centre report NC/99/38/2

Guide to Good Practice for the Development of Conceptual Models and the Selection and Application of Mathematical Models of Contaminant Transport Processes in the Subsurface

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Statement of Use
This document provides guidance to Environment Agency staff on the development of conceptual models and the use of contaminant fate and transport models in the subsurface. This document forms one of a set of three reports produced under this project.

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Glossary

Absorption	The incorporation of a chemical (due to diffusion) into the structure of a porous particle where it sorbs onto an internal surface.
Adsorption	The attachment of a chemical to the surface of a solid or liquid.
Advection	Mass transport caused by the bulk movement of flowing groundwater.
Analytical model	Exact mathematical solutions of the flow and/or transport equation for all points in time and space. In order to produce these exact solutions, the flow/transport equations have to be simplified (e.g. very limited, if any, representation of the spatial and temporal variation of the real system).
Aquifer	A permeable geological stratum or formation that is capable of both storing and transmitting water in significant amounts.
Attenuation	Reduction in contaminant concentration through biological, chemical and physical processes as it passes through a medium.
Biodegradation	The transformation of a chemical by micro-organisms, resulting in a change in chemical mass within the environment.
Conceptual model	A simplified representation of how the real system is believed to behave based on a qualitative analysis of field data. A quantitative conceptual model includes preliminary calculations for key processes.
Compliance point	Location where a target concentration must be achieved.
Conservative pollutants	Pollutants which can move through the aquifer and which are unaffected by biodegradation or interaction with the rock matrix (e.g. chloride).
Controlled waters	Defined by Water Resources Act 1991, Part III, Section 104. All rivers, canals, lakes, ground waters, estuaries and coastal waters to three nautical miles from the shore.
Deterministic model	A model where all elements and parameters of the model are assigned unique values.
Diffusion	Movement of chemicals at the molecular scale from areas of higher concentration to areas of lower concentration, due to random atomic scale motion of atoms and molecules.
Dilution	Reduction in concentration brought about by the addition or mixing with water.

Dispersion	Irregular spreading of solutes due to aquifer heterogeneities at pore-grain scale (mechanical dispersion) or at field scale (macroscopic dispersion).
Dispersivity	A property that quantifies the physical dispersion of a solute being transported in a porous medium. [L]
Finite difference model	Numerical model where the equations describing groundwater and contaminant movement are solved using finite difference methods.
Finite element model	Numerical model where the equations describing groundwater and contaminant movement are solved using finite element methods.
Groundwater	All water which is below the surface of the ground, in the saturation zone, and in direct contact with the ground or subsoil (Groundwater Directive 80/68/EEC).
Ground waters	Any waters contained in underground strata (Water Resources Act, 1991).
Hydraulic conductivity	A coefficient of proportionality describing the rate at which water can move through a permeable medium. [L]/[T]
Hydraulic gradient	The rate change in total hydraulic head with change in distance in a given direction. (dimensionless)
Hydraulic head	The sum of the elevation head, the pressure head, and the velocity head at a given point in the aquifer. [L]
Intergranular	Occurring between the grains of a rock or soil.
Mathematical model	Mathematical expression(s) or governing equations which approximate the observed relationships between the input parameters (recharge, abstractions, transmissivity etc) and the outputs (groundwater head, river flows, etc). These governing equations may be solved using *analytical or numerical* techniques.
Model	A simplification of reality in order to aid in the understanding of and/or predict the outcomes of the real system. In this report the term 'model' is used to describe the code or equations plus the data.
Non-aqueous phase liquid (NAPL)	Liquids whose miscibility with water is limited (and are present at concentrations above their solubility limit).
Numerical model	Solution of the flow and/or transport equation using numerical approximations, i.e. inputs are specified at certain points in time and space which allows for a more realistic variation of parameters than in *analytical models.* However, outputs are also produced only at these same specified points in time and space.

Parameter	Physical or chemical property of the flow or transport system under investigation.
Partition coefficient	Describes how a chemical will distribute between different media (e.g. partitioning of a chemical between soil and water) (dimensionless)
Pathway	A route along which a particle of water, substance or contaminant moves through the environment and comes into contact with or otherwise affects a receptor.
Permeability	General term referring to the ability of a medium to transmit a fluid.
Pollution of groundwater	The discharge by man, directly or indirectly, of substances or energy (e.g. heat) into groundwater, the results of which are such as to endanger human health or water supplies, harm living resources and the aquatic ecosystem or interface with other legitimate uses of water (Groundwater Directive, 80/68/EEC)
Pollution	Pollution of the environment due to the release (into any environmental medium) from any process of substances which are capable of causing harm to man or any other living organism supported by the environment (Environmental Protection Act, 1990).
Porosity	The ratio of the volume of void spaces in a rock or sediment to the total volume of the rock or sediment. (dimensionless)
Probabilistic model	An aggregation of model realisations, where the input parameters to each realisation are characterised by probability distributions.
Receptor	An entity (e.g. human, animal, controlled water, plants, building, air) which is vulnerable to the adverse effects of a hazardous substance or agent.
Recharge	The quantity of water of near surface origin (may include meteoric water and, for example, water mains leakage) that reaches the water table.
Remedial target	The goal of remedial activity set for the site; may take the form of a maximum or minimum permitted concentration in the soil or groundwater.
Retardation	A measure of the reduction in solute velocity relative to the velocity of the advecting groundwater caused by processes such as adsorption. (dimensionless)
Risk	A term used to denote the probability of suffering harm or pollution from a hazard and which embodies both likelihood and consequence.

Saturated zone	The zone in which the voids of the rock or soil are filled with water at a pressure equal to or greater than atmospheric. The water table is the top of the saturated zone in an unconfined aquifer.
Source	A region where a hazardous substance or agent (e.g. a contaminant that is capable of causing harm) may enter the natural system.
Source Protection Zone (SPZ)	An area designated around a groundwater source, the maximum extent of which is the catchment area for the source and within which the Environment Agency seeks to limit the processes and activities that can occur within that area.
Sorption	Absorption and adsorption considered jointly.
Target concentration	Maximum or minimum acceptable chemical concentration at compliance point.
Transport porosity	Porosity that is involved in the movement or advection of groundwater. The transport porosity is usually less than the total porosity and is also referred to as kinematic or effective porosity.
Unsaturated zone	The zone between the land surface and the water table. It includes the soil zone, unsaturated rock, 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 within the unsaturated zone. Also called zone of aeration or vadose zone.
Validation	The process of determining that a model is an adequate representation of reality for the purposes required.
Verification	The process of determining that a model produces correct outputs given the inputs.
Uncertainty	The degree to which a well-defined and located parameter (e.g. the horizontal hydraulic conductivity of a 1 cm cube of rock at a defined location) is unknown.

Executive Summary

Risk assessments undertaken to determine the risks to the subsurface environment often involve the use of quantitative contaminant fate and transport models. This document aims to provide guidance on good practice in the development of conceptual models which should form the basis for such assessments and on the application of mathematical models to contaminant transport problems.

The key stages in carrying out a modelling study are described including:

- Scoping study, comprising review of existing information and consultation with relevant parties, to define the objectives of the study and the scope and programme of work, i.e. why are we and how are we going to do the work;
- Development of a conceptual model of the system behaviour and how we can represent this using a mathematical model;
- Selection of the mathematical modelling approach;
- Construction of the mathematical model and assessment of the model results against historic data (i.e. can we be confident that the model provides a credible representation of the system behaviour);
- Sensitivity analysis to determine which parameters have the most significant influence on the model results;
- Uncertainty analysis to take account of uncertainty in the conceptual model, parameter measurement, and natural variability of parameters;
- Predictions and assessment of results (i.e. application of the model);
- Reporting and presentation;
- Consultation with regulators: clarification of legal requirements and policy constraints for the risk assessment, which should be an on going process throughout the study.

The development of a conceptual model is emphasised and this must identify and consider all the relevant aspects of the flow system and the contaminant transport processes, including the source of contamination, the pathways of flow and transport and all of the potential receptors. Clear graphical presentation of the conceptual model is recommended.

The conceptual model and the mathematical model should be continually challenged and updated throughout the modelling exercise.

The development of a conceptual model will involve a number of assumptions regarding system behaviour. The assessment must take these assumptions and uncertainties into account and decide whether these are important, i.e. it may be acceptable to adopt a relatively simple mathematical model of contaminant transport, or alternatively our understanding and definition of the system behaviour may be so poor that development of a mathematical model is inappropriate, and the first priority should be to obtain further site-specific data.

A phased approach in using mathematical models is recommended, moving from simple calculations, to analytical models, and finally to numerical models (if appropriate). In each case the selection of the modelling approach should be justified and appropriate to the available data and understanding of the system behaviour. A model should not be used as an alternative to obtaining site-specific data.

Data collection should be an iterative process and linked to the development and refinement of the conceptual model and the mathematical model. Site-specific data should be obtained wherever possible and for certain parameters site-specific data are essential. Literature values may need to be used for some parameters, and will need to be justified.

The results of the mathematical model will need to be checked against historic data to provide assurance that the model provides a credible and acceptable representation of system behaviour. If this cannot be achieved, the conceptual model and adopted mathematical model should be re-assessed and additional site-specific information collected.

Reporting of modelling studies must be clear and concise but also include information and justification for all assumptions and decisions made and parameters used. All stages of the process should be reported and be auditable.

Consultation with the Environment Agency (the Agency) should begin at an early stage in any project and continue through to final decision making. Agreement on key decisions and model inputs saves time and effort for all parties concerned.

Key words

Conceptual model, risk assessment, groundwater, fate and transport, exposure modelling.

1. Introduction

1.1 Background

The Environment Agency (the Agency) has duties (i.e. obligations) and powers (i.e. ability and discretion) to ensure the protection of groundwater and the remediation of contaminated land and groundwater. The Agency employs the principle of risk assessment (the risk of a contaminant source causing harm or pollution via a given pathway at an identified receptor) to assist with decision making for problems involving contaminant transport and also encourages external bodies to adopt a risk assessment philosophy.

The use of models to assess the risk to the subsurface environment from contaminants is becoming increasingly popular and a wide range of modelling software is readily available. Models may be used to determine the risks to receptors from land contamination or from other specific activities, such as landfilling. Output may include travel times to receptors and concentrations of contamination likely to reach receptors. These models can also be used to design or test remediation strategies once an unacceptable risk to the environment or other receptor has been identified.

In the context of this report, a model is defined in the broadest sense as a mathematical representation of reality in the form of equations and values of parameters (i.e. computer code or equations plus data). The report deals specifically with model codes/equations which simulate the transport of aqueous-phase contaminants in the subsurface, which includes the unsaturated and saturated zones, and models used for determining impacts on groundwater and surface water receptors, but does not include surface water or vapour transport models.

The selection and application of a mathematical model must be based on a conceptual model. The conceptual model is a simplification of reality which aims to identify the **key** processes that affect the contaminant transport behaviour. The conceptual model should also consider how these processes should be translated into a mathematical model. The conceptual model should also describe any uncertainties in understanding or representing the system behaviour, and whether these allow a mathematical model to be adopted.

Environmental professionals carrying out contaminant transport modelling have a diverse range of qualifications and experience. Specific expertise and experience are required because of the highly complex nature of contaminant fate and transport problems and the increasing complexity of models. The lack of such expertise and experience can result in the inappropriate use of these types of models. Problems can occur at any stage in the process from data collection through to interpretation of model results and liaison with regulatory authorities. Inconsistent and inappropriate approaches to modelling and the use of models can make them difficult to assess and may render their results invalid. Problems can arise at different stages of a project due to:

- (Mis)interpretation of legislative requirements and constraints;
- Poor sampling and analysis;
- Inadequate conceptual model;
- Inappropriate model selection;
- Use of inappropriate data sources (literature);

- (Mis)interpretation/use of results.

1.2 Purpose of document

The purpose of this document is to provide guidance on a generic ‘good practice’ approach to contaminant fate and transport modelling from setting objectives to interpretation of results and validation, that will help avoid the above problems. It highlights the issues that need to be considered and tackled and points to existing guidance or recognised standards and key references. It is not intended as a step-by-step recipe book for how to set up and run models.

1.3 Target audience

The document is aimed at hydrogeologists and environmental professionals both internal and external to the Agency, who understand the concepts and processes of groundwater flow and transport in the subsurface. It is specifically targeted at improving the general standard of contaminant fate and transport modelling and the presentation of modelling projects.

It is applicable to fate and transport simulation undertaken to determine both the likely risks associated with the presence of pollutants in the subsurface and determination of site-specific remedial objectives as described in Agency R&D Publication 20 (EA, 1999).

1.4 Definition of key terms

This section defines some of the key terms used in this document. These key terms are used frequently throughout the text and always refer to the definitions given below. These key terms and other technical terms used in the document are also listed in the glossary.

Key Definitions:	
Model	A simplification of reality in order to aid in the understanding of and/or predict the outcomes of the real system. In this report the term ‘model’ is used to describe the code or equations plus the data.
Analytical model	Exact mathematical solutions of the flow and/or transport equation for all points in time and space. In order to produce these exact solutions, the flow/transport equations have to be simplified (e.g. very limited, if any, representation of the spatial and temporal variation of the real system).
Conceptual model	A simplified representation of how the real system is believed to behave based on a qualitative analysis of field data. A quantitative conceptual model includes preliminary calculations for key processes.
Numerical model	Solution of the flow and/or transport equation using numerical approximations, i.e. inputs are specified at certain points in time and space which allows for a more realistic variation of parameters than in *analytical models.* However, outputs are also produced only at these same specified points in time and space.
Probabilistic model	An aggregation of model realisations, where the input parameters to each realisation are characterised by probability distributions.
Deterministic model	A model where all elements and parameters of the model are assigned unique values.

1.5 Relationship to other guidance

This report is one of a number of technical guidance documents produced by the Environment Agency's National Groundwater and Contaminated Land Centre and is aimed at improving understanding and capability, both inside and outside the Agency, in modelling contaminant fate and transport. This document is one of a series of three technical guidance notes produced on the subject of contaminant fate and transport modelling in the subsurface. The other two documents in this series are:

- *Guidance on the Assessment and Interrogation of Subsurface Analytical Contaminant Fate and Transport Models* (Environment Agency 2001a).
- *Guidance on Assigning Values to Uncertain Parameters in Subsurface Analytical Contaminant Fate and Transport Modelling* (Environment Agency 2001b).

These documents are intended to be used in conjunction with the DETR's *Guidelines for environmental risk assessment and management* (DETR *et al*, 2000) and more specifically the Environment Agency report *Methodology for the Derivation of Remedial Targets for Soil and Groundwater to Protect Water Resources* (Environment Agency, 1999a) which presents a framework for deriving remedial targets for soil and groundwater to protect water resources. The Agency has also prepared guidance on groundwater flow models as part of its developing Strategic Review of Groundwater Modelling, (Environment Agency, 2001c).

This document is also intended for use with other Agency risk assessment tools such as *LandSim* and *ConSim.*

The process of collecting site-specific data, which is used to characterise a site and define input into a contaminant transport or risk assessment model, is critical to the quality of the data and hence the quality of the model and results. The Agency and other authoritative bodies have produced a number of guidance documents on data collection procedures. These include:

- BSI, (1999) BS5930: Code of Practice for Site Investigations;
- BSI, (2001) BS10175: Investigation of potentially contaminated sites – Code of Practice;
- Secondary Model Procedures for the Development of Appropriate Soil Sampling Strategies for Land Contamination. Environment Agency R&D Technical Report P5-066/TR (EA, 2001d);
- Technical aspects of site investigation. Environment Agency R&D Technical Report P5-065/TR (EA, 2001e);
- Remedial Treatment for Contaminated Land, Volume III - Site Investigation and Assessment (CIRIA, 1995);
- Sampling Strategies for Contaminated Land CLR4. Department of the Environment, 1994;
- Contaminated Land Research Report CLR11. Model Procedures for the Management of Contaminated Land (DETR & Environment Agency, in prep);
- Guidance on the Assessment and Monitoring of Natural Attenuation of Contaminants in Groundwater. (Environment Agency, 2000b).

1.6 Key steps in contaminant fate and transport modelling

A flow chart showing the key stages in developing a contaminant fate and transport model is shown in Figure 1.1. The initial stages of data collection and the development of a sound conceptual model are required regardless of whether it is decided that a numerical model is appropriate for the objectives of the study. It must be emphasised that modelling is an iterative process and should involve consultation with the Agency and other regulatory bodies where appropriate.

1.7 Document layout

Chapter 2 gives an overview of the basic principles and approach, including the types of mathematical model. It looks at setting objectives, appropriate use of models and details the key stages in model development.

Chapter 3 looks at the development of the conceptual model, which is the most important step in a modelling exercise. This chapter discusses the processes that need to be considered in a conceptual model, data requirements and key steps in defining sources, pathways and receptors.

Data collection, collation and review is discussed in Chapter 4, which looks at data requirements for modelling, sources of data, data quality issues and data management.

Chapter 5 provides an overview of the factors that need to be taken into account in selecting a mathematical model. Chapter 6 discusses analytical models in detail including analytical techniques, data requirements for analytical models. Chapter 7 gives similar details for numerical models.

Chapter 8 looks at design and construction of a contaminant transport model, and outlines the approach to refining and checking the model against historical data.

The application of models is outlined in Chapter 9, which covers the interpretation of model results, and summarises the factors that need to be reviewed in order to complete a model and determine whether further work needs to be considered.

Chapter 10 looks at reporting modelling projects. There is discussion on the requirements of a well constructed modelling report and what other records may be appropriate for auditing and QA. Recommendations for liaison and consultation with the Agency are also presented.

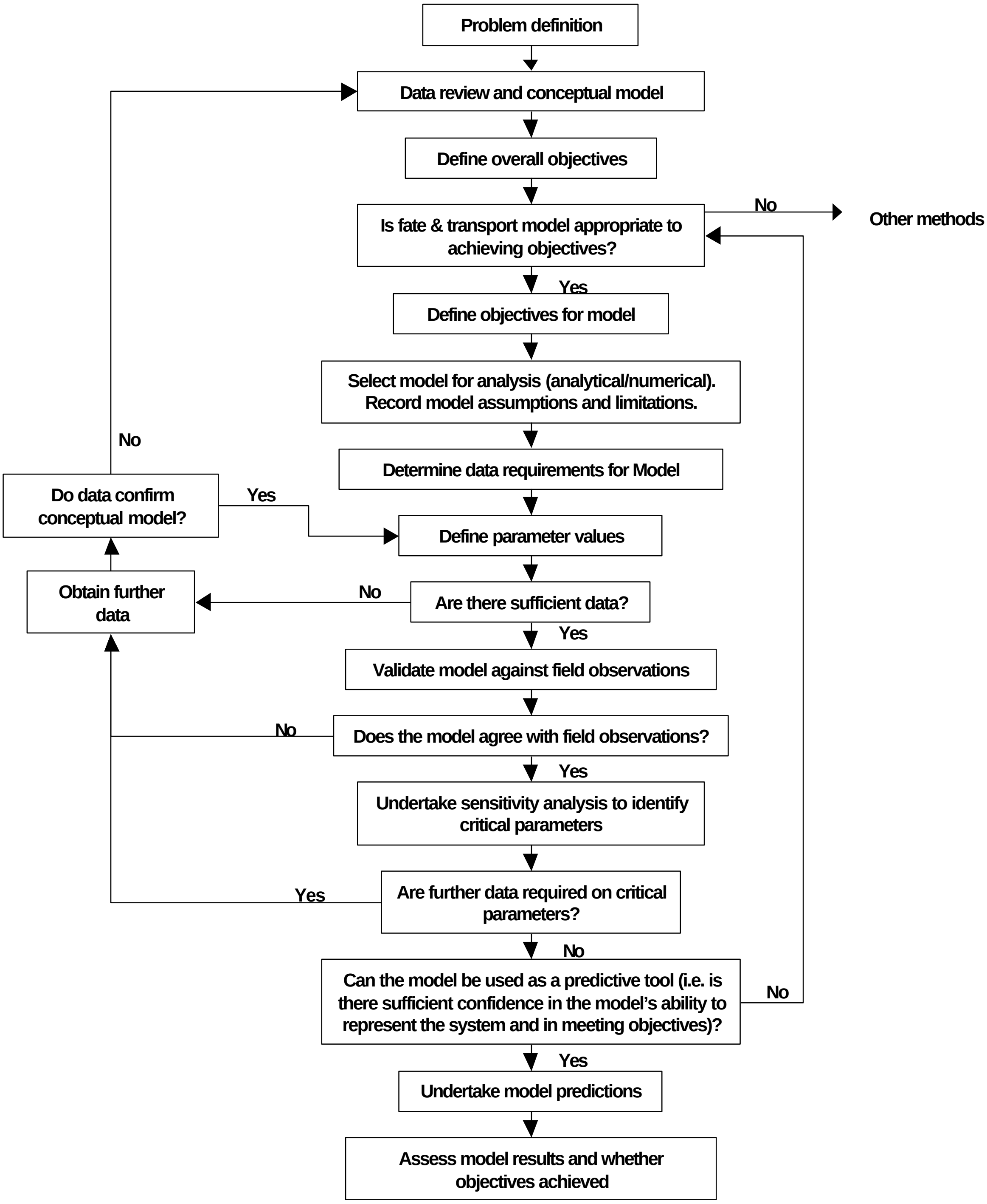


Figure 1.1 Basic Steps in the Application of a Fate and Transport Model

2. Overall Approach

2.1 Introduction

Fate and transport models provide a tool in the assessment of contamination problems. However, the danger in the use of all models is their inappropriate application to hydrogeological situations such that the results may be misleading.

A model should be used only when it is clear why and how it is to be used. The modelling approach must be determined by the objectives of the study, the availability of data and the complexity of the system and transport processes. A model should not just be used for the sake of it.

The next step is to formulate and document our understanding of how the system operates and to test these ideas quantitatively. This conceptual model should identify which elements of the system are important and how these could be represented using a mathematical model.

The conceptual model will involve a number of hypotheses, simplifications and assumptions which should be challenged continually throughout the modelling project by quantitative testing and comparison with field observations. This quantitative testing is one of the main purposes of any mathematical modelling

Box 2.1 Example

Consider the following example of a petrol spillage to ground. A review of the available data has identified that the site is underlain by a sand and gravel aquifer and that a groundwater abstraction borehole is located down gradient of the site, with the potential for this source to become polluted. An initial conceptual model has been formulated (based on experience of other sites) with biodegradation as a key factor controlling the fate of organics migrating through the sand and gravel. A mathematical model has been used to predict the concentrations of organics along the groundwater flow path (taking account of biodegradation) and ultimately to assess whether contaminant breakthrough would be expected at the borehole. The degradation of organics is represented in the model as a first order reaction. This example incorporates a number of assumptions/simplifications including:

- Biodegradation is occurring at the site (e.g. based on experience of other sites);
- Biodegradation can be represented as a first order reaction, which will have required some estimate of the rate of the reaction;

Whilst these assumptions may be valid, they are not based on site-specific information and could therefore lead to incorrect conclusions. For example, biodegradation may not be occurring at this site as the geochemical environment may inhibit this process, or degradation may be inhibited at high contaminant concentrations such that the assumption of first order reaction may be incorrect.

The collection of site-specific data allows these different assumptions to be tested and the conceptual model and modelling approach to be revised accordingly.

The development of a conceptual model and mathematical modelling approach must be iterative and linked. Typically the modelling approach will start with relatively simple calculations or models moving through to more complicated analytical or numerical models if these are required to meet the objectives of the study. In some cases, it may be appropriate to use simple calculations only, if this can be justified in the context of the project.

2.2 Appropriate use of mathematical models

It is essential that any modelling study has well defined objectives from the start and that the mathematical model itself will meet the objectives and provide the necessary results to enable decisions to be made. There are two basic questions to be addressed:

1. Is a modelling approach appropriate? Modelling contaminant transport is an order of magnitude more complex than modelling groundwater flow and the equations used are far less defensible.
2. What modelling approach should be used?

In deciding whether a modelling approach is appropriate, some of the questions that need to be considered are:

- Why are we modelling and what are its benefits. For example, the mathematical model may help in the decision making process by quantifying the potential impact on a receptor, and therefore the need to take some action to protect this receptor;
- Can the mathematical model provide reliable answers? For example is the system too complex to be adequately represented by the available modelling resources, in which case the application of a model would be pointless;
- Do we understand the system sufficiently to warrant the use of the mathematical model;
- Are sufficient data available to define the system? A mathematical model should not be used as an alternative to obtaining site-specific data, although if used appropriately a model could be used to help guide further data acquisition.

The decision to adopt a modelling approach will be subjective and largely based on experience, but must be fully documented and justified.

Box 2.2 Example

For example, in the assessment of whether an accidental spillage of a contaminant poses a risk to an identified receptor, the first step is to develop a conceptual model of the system (based on site information) and determine whether there is a plausible linkage from the source to any receptor(s). If a potential linkage is identified, then a mathematical model could be used to evaluate the risk. This exercise may, however, conclude that the site is poorly understood (e.g. there is uncertainty whether a sand and gravel aquifer extends between the site and an abstraction borehole which is the potential receptor). In this case, further borehole drilling should be undertaken to characterise the geology of the site, prior to consideration of the need for a mathematical model.

The potential disadvantages and problems in using a model are:

- The tendency to believe that a model is correct or to imply an unrealistic level of accuracy/precision to model predictions. In undertaking any modelling exercise a number of simplifications and assumptions will have been made, these must not be ignored when making decisions based on the model results;

- Decisions and action are delayed whilst a model is being developed. Some mathematical models can take several months or years to construct and validate;
- Site-specific data are not obtained as undue emphasis has been based on a mathematical model; this must never happen;
- Modelling issues may result in the work being driven by the capabilities and limitations of the modelling tool, rather than by the problem to be solved. For example:
  - A mathematical model has been selected that is too sophisticated for the problem;
  - The system (i.e. fractured flow aquifer) and processes which affect the contaminant (degradation, sorption) are not adequately or correctly represented by the model;
  - The system has been over-simplified in constructing the conceptual model and in translating the conceptual model to the mathematical model.

  A common error is to persist with the mathematical model rather than reject it when it is found to be inadequate.
- The limitations and uncertainties in the model have been overlooked in applying the results from the model.

The danger in using an inappropriate model is that erroneous conclusions may be drawn leading to poor decision-making.

In assessing whether a modelling approach is appropriate the following factors should be considered:

- Does the model allow the key sources, processes and pathways (as identified in the conceptual model) to be represented?;
- Do simplifications in using the mathematical model to represent the system invalidate the use of the model? (for example assumption that sorption can be described by a linear isotherm);
- Does the model allow field observations to be simulated? (Clearly a model that fails to match field observations is inappropriate);
- Has any variability and uncertainty in parameter values been taken into account (e.g. if parameter values are known to vary in space and time this should be taken into account in the modelling approach through the use of probabilistic models or sensitivity analysis)?;
- Is the model over-complicated or too simplified for the problem. In many situations, particularly when the sensitivity of the environment is low, it is inappropriate and unnecessary to develop anything more than a simple calculation? (e.g. where travel time is extremely long, it may be evident that no action is required);
- Does the model provide the required output?

2.3 Key steps in fate and transport modelling

The general approach in using a fate and transport model is summarised in Figure 1.1. The main steps are outlined below:

i) **Scoping study**

The scoping study should comprise a review of existing information and liaison with relevant parties and should define the overall purpose and specific objectives of the study and the scope and programme of work. The study should also document and assess the availability of existing information and outline the current understanding of the problem (initial conceptual model). Guidance on the information that should be reviewed as part of any initial exercise is given in Environment Agency (2000a and 2000d).

This exercise may identify that a range of environmental issues need to be addressed (e.g. a risk to controlled waters and to human health), and should detail how the interface between different environmental issues should be addressed.

The scoping study may also identify the need for further site investigation and should consider whether a mathematical modelling approach is likely to be appropriate.

ii) **Development, presentation and documentation of conceptual model** (including recommendations for use and design of an appropriate mathematical modelling tool or tools) (Chapter 3).

The conceptual model is a simplification of reality that aims to identify the **key** processes that control and affect contaminant fate, transport and behaviour. It is also a collection of hypotheses and assumptions: "A conceptual model is the set of assumptions that represent our simplifies perception of the real system which is to be mathematically modelled" (Bear & Verruijt, 1987). The conceptual model should be based on a sound understanding of the groundwater flow system in order to represent properly the advective component of contaminant transport and it should identify all source-pathway-receptor linkages. The conceptual model should also consider how these processes could be translated into a mathematical model. The conceptual model should also describe the uncertainties in understanding and list the assumptions made about the behaviour of the real system.

The decision to adopt a modelling approach in order to meet the objectives of the study should be clearly justified. It is essential that throughout the modelling process, the fate and transport model should be continually referred back to the conceptual model and vice versa.

iii) **Selection of modelling approach and verification of code** (Chapter 5)

Selection of approach should be based on the objectives for the study, the conceptual model (e.g. complexity of the hydrogeological system and processes that need to be represented) and data availability. A phased approach should be adopted, starting with simple calculations and moving through to more sophisticated numerical model codes, if necessary.

The model code should be verified to determine its outputs are correct given known inputs, i.e. there are no programming or calculation errors.

iv) **Construction of model and assessment against historical data** (Chapters 8 and 9)

The model should be constructed to represent the conceptual model as closely as necessary to meet objectives. This will include definition of the domain to be represented, processes operating, model boundary conditions and model parameter values. Any simplifications made in constructing the model should be documented and justified.

Model results should be compared with any field data to test the validity of the model and determine whether or not the model is a satisfactory representation of the real system. This exercise will normally involve adjustment of the model parameters within a credible range. This may help improve the match between the model results and the field data, but its main purpose is to test the conceptual model quantitatively and systematically. The model and the model parameters should then be examined to determine if they are both still credible i.e. given the acceptable parameter ranges and spatial distributions. If the model does not provide a credible fit to field conditions, then the appropriateness of the model, the need for further data, and the conceptual model should be reviewed.

v) **Sensitivity and uncertainty analysis** (Chapter 9)

Uncertainty arises from five main sources: field and laboratory sampling and measurement error, conceptual uncertainty, mathematical representation, model input parameters and predictive uncertainty. This subject is considered in detail in Environment Agency, 2001b.

A sensitivity analysis should be undertaken to examine the effect on the model results of changing any particular parameter, and in identifying which parameters are most important in describing the system behaviour as represented by the model.

A probabilistic analysis is also recommended as a method of taking account of the variability of a parameter value and/or uncertainty in the measurement of parameter values.

vi) **Presentation and reporting** (Chapter 10)

The study should be supported by documentation that sets out the objectives for the model; the conceptual model on which the model is based; description of and justification for the model assumptions and model parameters; and results of model validation. The report should also clearly document any uncertainties in the conceptual model and any simplifications that have been made. This report should provide the basis for agreeing the validity of the modelling approach, and the use of the model as a predictive tool. The report should also include proposals for any predictive model runs.

vii) **Predictions and assessment of results** (Chapter 9)

When we have confidence that the model is representing the historical behaviour of the real system adequately, it can be used as a predictive tool. The predictive runs should be defined and agreed with relevant parties. The predictive runs should take account of key uncertainties, together with the results of any sensitivity analysis (i.e. if a previous sensitivity analyses had identified that the rate of biodegradation was a key parameter, then any predictive model runs should consider the possible range in this parameter).

The results from the modelling exercise should be assessed to determine whether they are plausible. Decisions that are made based on the model results must take account of the assumptions made in the model and any uncertainties in how the system has been described.

viii) **Final reporting** (Chapter 10)

The results of the modelling exercise should be fully documented (including results of predictive runs), together with any decisions that have been made based on these results. The mathematical model and relevant input and output files should be made available to relevant parties.

ix) **Consultation** (Chapter 10.3)

The need for consultation with regulatory bodies, principally the Environment Agency, throughout the development of a model is emphasised to ensure acceptability of the modelling approach in terms of the type of model and the parameter values to be used in the modelling exercise. The consultation serves two main purposes:

- It ensures that all issues of concern to the Agency are addressed;
- Unnecessary site investigation and modelling work is avoided as agreement is obtained at key stages of the project rather than waiting until the work is completed, only to then identify that there are key areas of disagreement.

The development and application of a model should be inseparable from the:

- Objectives of the study and purpose of the model;
- Conceptual model. The analytical or numerical model should be continually checked against observed data and the hypotheses in the conceptual model tested. Similarly, the conceptual model should continually be updated in the light of the model results to ensure compatibility between understanding and representation of the system;
- Data collection including site investigation. The model may assist in determining the key information that needs to be obtained (i.e. which are the most sensitive model parameters). Throughout the modelling process, a key question should be 'is there adequate information to support the model'.

The conceptual model and the mathematical model should be continually challenged and updated throughout the modelling exercise.

2.4 Types of model

A brief description of the different types of mathematical models is given in Box 2.3.

Box 2.3 Description of Mathematical Models

Analytical models (Chapter 6) use exact solutions to the equations which describe the migration of contaminants. In order to produce these exact solutions the flow/transport equations have to be considerably simplified such that they are typically only applicable to simple flow and contaminant transport systems. Analytical models can be simple formulae, spreadsheets or even sequences of calculations packaged up in a piece of software (for example LandSim and ConSim).

The advantages of these models are that they are simple and quick and have limited data requirements. They are particularly useful as an initial modelling tool in understanding the system behaviour. Analytical models can also be easily combined with probabilistic analysis (Monte Carlo) techniques to provide a powerful modelling tool.

Semi-analytical models are used to refer to a range of modelling approaches. Examples include:

- Models that require numerical solutions to solve equations;
- Models that combine an analytical and numerical approach, e.g. numerical particle tracking on an analytical flowfield;
- Models that allow superimposition of a number of analytical equations;

LandSim and ConSim qualify as semi-analytical models.

Numerical models (Chapter 7) use approximate numerical solutions to the governing equations of groundwater flow and/or contaminant transport. Parameter values are specified at certain points in space and time, and provide for a more realistic representation of the variation of parameters than analytical models. The use of a numerical model will require technical expertise in groundwater and contaminant movement, together with specialist and detailed investigations to define the flow regime and contaminant transport processes. Numerical models can range from relatively simple one dimensional steady-state transport models to three dimensional time-variant models and may consider any or all of advection, dispersion and retardation, biodegradation, multiphase flow and density driven flow.

The data requirements are significantly greater than for analytical models, and can include spatial variation in aquifer properties plus time variation of inflows (recharge) and outflows (abstraction).

Deterministic models

Deterministic models require a single value to be defined for each model parameter at any point, and the result is a single value. Commonly a range of input parameters are used to determine the range in possible model results.

Probabilistic models

For probabilistic models, the parameter values are defined by a distribution (log normal for example) usually referred to as a probability distribution or probability density function, and the model result will be described by a range of values. Probabilistic models are used to take account of the uncertainty in defining or measuring parameter values (e.g. due to sampling or analytical errors), or represent the intrinsic variability of a parameter (for example the variation of hydraulic conductivity in a heterogeneous aquifer).

Box 2.3 (Continued)

Probabilistic models do not allow for uncertainty in the definition of the system behaviour. For example, there may be uncertainty as to whether biodegradation could be described by a first order reaction or as a rate limited reaction (availability of oxygen). A probabilistic model cannot be used to deal with this type of uncertainty, but could be used to evaluate uncertainty in oxygen availability.

Monte Carlo simulation is the most widely used stochastic technique. In general the method involves:

i) Definition of a probability distribution for each model parameter;

ii) Repeated solution of the model (for example, the Ogata Banks analytical transport equation) with parameter sets chosen from the probability distributions;

iii) Analysis of the model results to describe the likelihood of a certain result being obtained.

Steady state models or time variant models

Mathematical models can be described as steady state or time variant. In a steady state model, the input parameters and solution are independent of time. For a time variant model, input parameter values can be specified as a function of time, and the solution is dependent on this.

3. Development of a Conceptual Model

3.1 Introduction

The most important stage in a contaminant transport modelling study is the development of a conceptual understanding or characterisation of the flow and transport processes operating on and around a project site area.

The conceptual model must identify the crucial factors influencing groundwater flow and contaminant transport, whether the observed behaviour appears to be predictable (i.e. is there a consistent trend); and whether mathematical approximations can be used to describe its behaviour. Hard thinking is required to determine:

- what is known and understood about the area;
- what is not known or not understood;
- what are the key physical and chemical processes and how can they be represented;
- any assumptions made and;
- anything we are prepared to ignore or simplify in order to come up with pragmatic answers to our questions.

Confidence in any conceptual model increases via testing. Hence a conceptual model must be more than simply a qualitative description of our understanding of the system but should include some quantitative assessment to gain an initial view of which assumptions are wrong and the significance of different processes. Preliminary testing should be carried out by using lumped water balance and mass balance calculations, and simple analytical relationships.

The conceptual model should also cover the uncertainties in defining the system behaviour and how this is dealt with in defining parameter values and processes that affect contaminant transport. This ‘conceptual model’ will provide the basis for determining further data requirements and the type of mathematical model which is appropriate. Figures 3.1 to 3.3 illustrate various aspects of a conceptual model in terms of data used to construct the model, our understanding of the system, uncertainties in this understanding, and how it can be represented mathematically. These figures are indicative only and in practice greater detail will need to be provided as part of the conceptual model.

The development of the conceptual model must be an iterative process, continually being updated as new data become available or as the understanding of the system is improved. If there is no quantitative testing of the conceptual model, the model produced is unlikely to be representative of the system and the results of the simulation will be meaningless. It is important to avoid both over-simplification, which results in a model which is incapable of simulating observed conditions adequately, and under-simplification, which results in a model which is too complex to be a useful tool for a relatively simple problem.

It is important to recognise that any conceptual model will be imperfect (it is, after all, a simplified representation), and may even be wrong. This recognises that:

- The information used to define a problem will always be incomplete;

- Assumptions will have been made in developing the conceptual model (e.g. can it be assumed that a sand and gravel deposit identified in three investigation boreholes extends laterally below the whole of the site, or have three separate sand and gravel lenses been penetrated?);
- The available information may be conflicting (e.g. laboratory leaching test results indicate that a given contaminant should be leached from a contaminated soil, whereas no evidence for this contaminant is found from groundwater sampling);
- The processes occurring may be poorly understood.

The conceptual model is a simplified representation or working description of our understanding of the physical and chemical processes operating in a specific study area. These simplifications and assumptions should be clearly documented and supporting information provided to provide justification that any assumptions are reasonable. It is important to be aware of the implications of these and to be able to justify the decisions that are made. It is important to consider whether simplifications are likely to be conservative or otherwise.

This chapter is intended to give an overview of the information and processes that need to be considered in constructing a conceptual model for a contaminant transport model and to give pointers to key references. Zheng and Bennett (1995) give useful guidance on developing conceptual models for contaminant transport modelling. Anderson and Woessner (1992), and Environment Agency (2001c) provide guidance on conceptual models for groundwater flow modelling.

3.2 Data requirements

A conceptual model should include consideration of the topics listed in Table A1.1, Appendix A. All the existing data on the flow system and transport processes should be incorporated and quantified wherever possible. All assumptions and qualitative interpretations made due to lack of data should be clearly recorded. The area covered by the conceptual model should include, but not be restricted to, the area of the contamination source, all potential pathways and all potential receptors. Many projects involving soil or groundwater contamination concentrate on a specific site, but an understanding of the wider area around the site is essential and in some cases the whole groundwater catchment may need to be included. The importance of spatial and temporal variability in parameters and processes must also be considered as part of the conceptual model development.

The basic data identified in Table A1.1 may be adequate to develop an initial conceptual model, but data requirements will vary significantly for different models and at different stages in the modelling process. Currently available data are rarely sufficient for contaminant transport modelling purposes and additional or more detailed data are likely to be required to, for example, construct and test a mathematical model. The complexity of the problem and data availability should be the driver for the mathematical model used. The data requirements for a complex problem that requires a large numerical model will be huge compared with those for a more straightforward problem that can be solved with a simple analytical spreadsheet. Further discussion on data requirements for modelling is included in Chapter 4.

For risk assessment purposes it is also useful to consider the conceptual model in terms of source, pathway and receptor. The following sections deal with this in more detail.

Data Sources (examples)
Site Plans.

Interviews with site personnel.

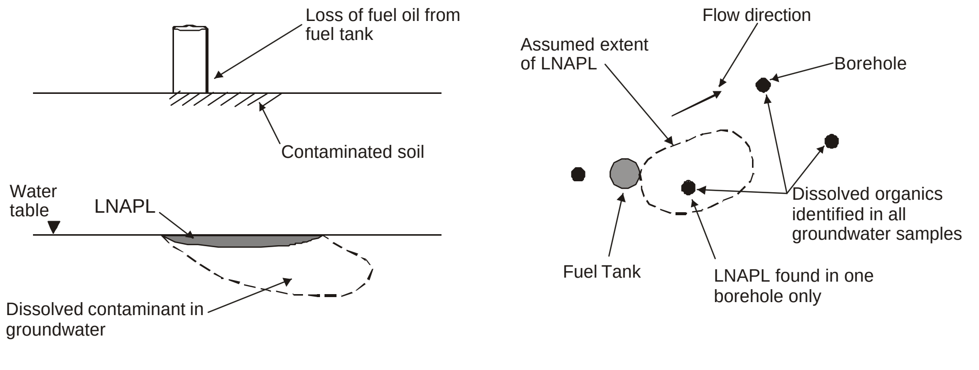
Stock records.

Site Investigation(s)
- boreholes/ trial pits
- analysis of soil and groundwater samples

Data Gaps (examples)
Date of leakage.

Volume lost.

Section **Plan**



Uncertainties
Period of leakage and volume lost.

Extent of LNAPL plume and dissolved plume. Is LNAPL plume moving?

Significance of volatilisation, degradation.

Description of Problem
Loss of fuel oil identified following review of stock records. Subsequent site investigation identified contamination of soils, presence of LNAPL at water table and dissolved contaminant concentrations in groundwater.

Conceptual Model
Three potential sources of contamination identified (soil, LNAPL, groundwater).

Site records indicate contaminant loss occurred sometime between 1995 and 1997, with between 1500 and 4000 litres loss.

Chemical analysis indicate benzene, xylene, toluene, are main contaminants of concern. Borehole drilling found (LNAPL in borehole only and dissolved contaminants in three down gradient boreholes.

Initial calculations indicate that solution of free phase by groundwater is main process for migration of contaminants.

Site measurements provide some evidence of volatilisation and degradation, but not quantified.

Translation to Mathematical Model
Contaminant source represented as constant source term, with contaminant concentration calculated from solution of free phase to dissolved phase (using Raolts Law).

Approach considered to be conservative estimate of source term, but analysis to check calculated mass does not exceed estimate of contaminant loss.

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Figure 3.1 Conceptual Model - Source Term

Data Source (examples)
Geological investigation results from adjacent site.

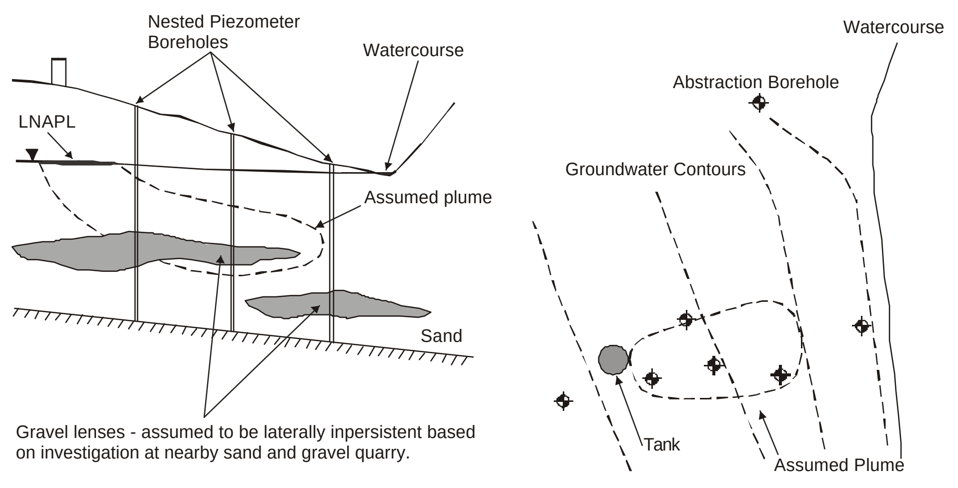
Site investigation (boreholes).

Routine monitoring (water levels, water quality).

Laboratory analysis (foc, psd).

Field tests (falling head test for hydraulic conductivity).

Section **Plan**



Uncertainties
Lateral persistence of gravel lenses.

Scale of heterogeneity.

Geometry of contaminant plume.

Conceptual Model Description
Movement through the unsaturated zone considered to be via vertical migration to the water table. LNAPL present at water table. No significant artificial pathways (drains) identified from review records.
Groundwater flow and discharge to surface watercourse.
Site underlain by sand and gravel aquifer, and gravel lenses present which will provide more permeable pathways.
Groundwater down gradient of site and watercourse identified as receptors. Abstraction not at risk based on observed extent of contamination, but needs to be reviewed based on on-going monitoring.

Translation to Mathematical Model
Assessment to be initially undertaken using values of hydraulic conductivity for gravel lenses. Preliminary calculations indicate this over estimates the extent of the plume compared with the observed contaminant distribution, although note that groundwater flow and consquently dilution will also be overestimated.

02449-01.S026

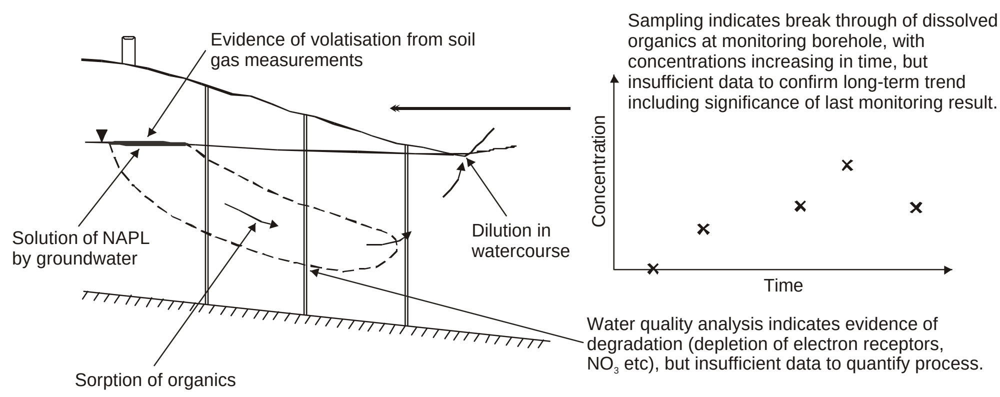
Figure 3.2 Conceptual Model - Pathway and Receptors

Data Source (examples)
Water quality sampling with time. Organic contaminants, NO_3 SO_4 Fe, alkalinity, chloride, etc.

Laboratory analysis (foc).

Soil gas monitoring.

Field measurement of pH, redox, dissolved oxygen, temperature.



Uncertainties
Is apparent discrepancy between calculated extent of plume and observed extent, function of attenuation or values of hydraulic conductivity used in calculation

Conceptual Model Description
Processes affecting contaminant migration:
- solution of NAPL by groundwater
- advection and dispersion
- sorption of contaminants (based on experience from other sites)
- biodegradation (depletion of electron acceptors within contaminant plume)

Initial calculations assumes advection, dispersion, sorption indicate plume expected to have migrated further than the observed contaminant distribution.

Translation to Mathematical Model
Sorption of organics represented by linear isotherm, with retardation calculated as:

$$R = I + \frac{foc.\ koc.}{n}\ p$$

Parameter values derived from:
- Fraction of organic (foc) from analysis of soil samples
- Density (p) from soil analysis
- Porosity (n) from literature values but checked against moisture content measurements
- Partition coefficient (koc) taken from literature values

Values based on arithmatic average of samples but sensitivity analysis undertaken to define key parameters.

Contaminate to be assumed as non-degradeable (conservative assumption) as insufficient information to demonstrate biodegradation.

02449-01.S027

Figure 3.3 Conceptual Model - Processes

3.3 Defining the source term

Definition of the source term will require a number of factors to be considered (Table A1, Appendix A and as illustrated by Figure 3.1), such as:

- Type of source;
- Source geometry;
- Contaminant substances, contaminant phases and concentrations;
- Contaminant load (large or small spill);
- Inputs/outputs to/from other media;
- History of contamination and timing of release;
- Processes that affect the source and changes in the source with time.

Definition of the source term will initially be based on a review of all the relevant site history including historical maps and plans, planning information, records of incoming and outgoing chemicals (to estimate possible contaminant loss), details of site processes and the knowledge and experience of workers or local residents. Knowledge of the activities, processes and incidents on a site is important as it leads to an understanding of the likely history of release, source geometry, release mechanism and likely contaminants.

Site investigation data are essential for understanding the source term as they give an indication of the distributions (laterally and vertically) and the concentrations of the contaminants over the period of monitoring.

Generally there will be incomplete information available on many of these aspects and, if further data collection is not possible, assumptions will need to be made, particularly in relation to the history of contaminant release or total load released.

3.3.1 Types of source

The nature of the source should be defined. Examples of contaminant sources are:

- Contaminated soil caused by historical spills, disposals or discharges. The mechanisms by which this contamination can migrate include leaching of contaminants as water percolates through the soil or due to a rise in the water table;
- Contaminated groundwater itself may act as a source for an expanding plume. Contamination may have degraded or been removed from overlying soils but remain as a plume in the groundwater below;
- Landfills and lined areas. Source terms for landfills must also consider the liner system and the operation of the site (i.e. leachate control systems) must also be taken into account;
- Discharge of contaminated water to soakaways, boreholes and unlined drains;
- Floating LNAPL. If a pool of LNAPL has formed on the water table of an aquifer, the LNAPL may move and directly transport contaminant but it will also act as a source, dissolving contaminant into the groundwater beneath;
- DNAPL which has migrated down gradient and accumulated at an impermeable boundary below the water table may act as a source of contamination to groundwater;
- NAPLs at residual saturation are immobile, but will maintain high concentrations in surrounding groundwater;
- Leaching from coal mines as water reinvades workings.

The conceptual model should consider whether the mass and nature of the source changes with time, i.e. can it be assumed to be constant or will it change. The current source concentrations do not necessarily represent the historical or future situation. For example dissolution, volatilisation and degradation of the contaminant source will result in a decrease in mass with time whereas the generation or release of additional pollutants will increase it. Chemical conditions at the source (e.g. redox, pH) may also change over time resulting in changes to contaminant behaviour.

Historical sources of contamination in soil or groundwater are generally more difficult to identify, particularly when original structures have been removed or there have been several different historical uses of a site. In these instances, it is important to obtain as much relevant historical information as possible for a site. It is also possible that the source of contamination lies on an adjacent site or has migrated off the site.

3.3.2 History of contamination and timing of release

It is important to understand the history of contaminant release for a site and whether it has occurred over days, years or tens of years. However, detailed information on the history of the contamination of a site and the timing of contaminant release is rarely available. For example a site operator may have identified that a release of diesel occurred from a fractured pipeline, but be uncertain as to how much diesel was lost and over what period.

It will commonly be necessary to make assumptions about the history and timing of contaminant release and these will often be 'worst case' assumptions. However, it is occasionally possible to carry out broad reality checks ('contaminant mass balances') on the assumptions made. The estimated volume of contaminant released to groundwater is related to:

- The volume of contaminant estimated to be currently in the ground, including sorbed, dissolved or free phase (taking account of likely mechanisms of degradation or transport off site). Estimates can be made from concentrations of the different phases measured in soil and groundwater samples during site investigations across the area of contamination;
- The total volume of the contaminant estimated to be used at the facility. Records may exist of the volumes of chemicals supplied to or, chemicals or products output from a facility and a mass balance calculation may be possible.

The purpose is to ensure that estimates of contaminants in the ground are sensible and realistic given the likely volume of the contaminant supplied to the facility, the method by which it was used or disposed and the length and period of time over which the facility operated. The assessment should aim to determine whether the contaminant source is likely to be constant or whether it will decrease in strength with time.

3.3.3 Types of contaminant

Desk study information will often give an indication of the types of contamination likely to be found on a specific site; if not, an initial screening for a wide range of contaminants in both soil and groundwater samples is required at the site investigation stage. Useful references of the likely contaminants for different sites are given in DOE industry profiles (DOE, 1995) and CLR11 (Environment Agency, 2000a).

Laboratory analyses plus a knowledge of the contaminant properties will indicate the contaminating substances and their phases:

- Solid phase - particles of contaminant;
- Sorbed phase – contaminants sorbed onto soil particles;
- Free phase – contaminants present in soil and/or porosity as non-aqueous phase liquid (NAPL). (Maybe in the unsaturated or saturated zone);
- Vapour phase - contaminants present as vapour in the soil;
- Dissolved phase – contaminants dissolved in groundwater. Likely to be associated with all of the above phases.

The identification of the specific contaminants (including speciation of mixtures) and the phases in which they are present on a site is essential if its fate and transport in the subsurface is to be predicted. The behaviour of the contaminant within the subsurface will depend on both the properties of the contaminant, the phase in which it is present and the presence of other contaminants. Key physical properties of contaminants are:

- Solubility;

- Density;
- Viscosity;
- Volatility;
- Leachability (determined by solubility and partition coefficient into water phase).

In some instances, chemical properties and other data may not be available for specific compounds and data from similar compounds may need to be used for modelling. However, this approach will introduce additional uncertainty into the model.

The conceptual model must consider both the initial contaminant and any compounds which may result from its degradation. Breakdown pathways of organic compounds, for example, may be complex and will include substances which have different properties from the original contaminant and may even be more toxic.

3.3.4 Source geometry

The 3D geometry (area, depth) of the source should be incorporated into the conceptual model. The majority of modelling studies are carried out for contamination which occurs at a specific location (point source), but some forms of contamination, such as those arising from agricultural application of nitrates, are widespread and are referred to as diffuse sources.

The geometry of a point source of contaminated soil can be difficult to define and will probably have varied over time as the contaminant spread laterally and vertically. Site investigation, sampling and analysis of soil and groundwater are required to determine the extent of contamination in the unsaturated and saturated zones. Concentrations of contaminants and the proportion of contaminant in each phase (free phase, sorbed, dissolved phase) will vary laterally and vertically depending on, for example, the properties of the lithology, the contaminant, the processes controlling migration. Site-specific data are likely to be obtained at discrete points on the site and the conceptual model will therefore include assumptions and interpolation between data points.

3.3.5 Translation of the source term to the mathematical model

In translating the source term to a mathematical model it will normally be necessary to define:

- Dimensions of contaminant source (length, width, depth). Many analytical models require the assumption of a simple source geometry, i.e. a linear source term;
- Contaminant concentration;
- Change in contaminant concentration with time. This is typically represented as either a continuous or a declining source. The former usually results in the model overestimating the volume of contaminant released. The latter is usually represented by a first order decay term.

This process will require a number of simplifications. For example, the observed contaminant concentrations may vary across the volume of affected soil or groundwater. It may not be possible to represent this variation within the mathematical model and instead a single contaminant source concentration will need to be assumed. The modeller will then need to decide whether to use the maximum or average concentration recorded in the field data. This also takes no account of the fact that the site investigation may have missed the area of highest contaminant concentrations. This illustrates that in developing a conceptual model and associated mathematical model, it is relatively easy to construct a model that could inadequately describe the contaminant source. The appropriate use of probabilistic methods (Environment Agency 2001b) may allow uncertainty in the definition of the source term to be taken into account, for example by the use of a range of values for the source contaminant concentration.

A useful check when evaluating the results from a mathematical model is to compare the mass calculated by the model to the estimated contaminant mass to give an indication of whether the model is over or under conservative.

3.4 Defining the pathway

The conceptual model should aim to define the pathways or routes by which contaminants can migrate through the subsurface from a potential source to a potential receptor. Pathways for vapour transport are not considered in this guidance, but will still need to be considered as part of the overall risk assessment. The soil zone, the unsaturated zone and the saturated zones, and all the key flow and transport processes therein need to be considered. Pathways along which flow normally occurs should be examined, but potential by-pass mechanisms must also be taken into account.

This will require information on soils, geology, hydrology and hydrogeology to be collated and assessed (Table A1, Appendix A).

3.4.1 The groundwater (geosphere) system

Conceptual models produced by the Environment Agency as part of regional flow models or Source Protection Zone delineation may be available and will hold a synthesis of information available at the time that it was produced. They often include Agency obtained data, a description of the important flow mechanisms operating at the site and some water balances. Discussion with the hydrogeologists responsible for undertaking the work may provide additional background.

Geology
Geological information can initially be gathered from maps or logs of existing boreholes in the area of interest but more detailed information will generally require further site investigation. It is essential to determine the lithologies in the area of study, the geometry of the different lithologies and the stratigraphy. The lithology determines the flow and transport properties of the strata and it may vary laterally and vertically over a short distance and within a single stratigraphic unit. Different stratigraphic units may also have similar lithologies and properties and therefore act as a single aquifer unit. The stratigraphy of the area can generally be determined from maps and will help to establish the lateral extents and outcrop boundaries on a broad scale and indicate the geological boundaries and structures which may be affecting the aquifer system.

The water table
The water table marks the boundary between the saturated and unsaturated zones and may intersect both stratigraphic and lithological boundaries. The influence of these boundaries on groundwater flow and contaminant transport should be considered. The movement of the

water table can also affect the vertical distribution of contaminants. Light non-aqueous phase liquids (LNAPLs), which float on the water table, may be ‘smeared’ across a sequence of strata as the water table rises and falls causing free-phase liquids to be trapped beneath the water table. Historical water table fluctuations may have affected the current distribution of the contamination in the vertical profile. The range of water table fluctuation, both seasonal and long term, should be established.

The presence and significance of perched groundwater should also be established (i.e. is lateral flow via perched groundwater an important pathway).

Unsaturated zone flow and transport

Movement of water through the soil and the unsaturated zone is complex and a function of infiltration, soil moisture/saturation, hydraulic conductivity (usually a function of the degree of soil saturation), soil suction and the properties of the polluted fluid. Detailed discussion of unsaturated zone processes is beyond the scope of this document, but Fetter (1992) and Case (1994) provide a good summary of flow and transport in the unsaturated (vadose) zone.

Mathematical expressions have been developed to describe water movement in the unsaturated zone, but these are often complicated, and still require a number of simplifications to be made about system behaviour. In practice, the rate of flow and travel times through the unsaturated zone are often represented by relatively simple equations as described in Box 3.1.

Box 3.1 Examples of simple methods for calculating flow and travel through the unsaturated zone.

Rate of flow (q) = Ki *(1)*

where

q = specific discharge ($m^3/d/m^2$)

K = vertical hydraulic conductivity (m/d)

i = vertical hydraulic gradient

In solving this equation, it is commonly assumed that the hydraulic gradient is 1, and that the hydraulic conductivity is equivalent to or lower than the value for a saturated soil. These conditions are likely to occur if the rate of flow is significantly less than the annual effective precipitation and therefore this calculated rate of flow should be compared with an infiltration rate estimated from meteorological data. This equation is only really appropriate to fine grained materials with a high soil suction.

Note: For example the leakage through a clay layer of hydraulic conductivity $K = 10^{-9}$ *m/s and vertical hydraulic gradient of 1 is q = 31 mm/year. The effective precipitation in most parts of England and Wales is greater than 100mm/year.*

The travel time for a contaminant to migrate through the unsaturated zone can be estimated as follows:

Travel time (t) = dn/q *(2)*

d = thickness of unsaturated zone (m)

n = transport porosity

q = rate of flow or infiltration rate (m/d)

These simple formulae embody a large number of simplifications about flow through the unsaturated zone including:

- Saturated flow occurs;
- Uniform conditions exist (i.e. no by-pass component).

Note. Porosity calculated using measurements of moisture content is often used in Equation 2. These values will usually be less than the saturated porosity and, therefore, care needs to be taken if the infiltration rate is taken from Equation 1, which assumes saturated conditions.

These calculations are useful in providing an initial estimate of rates of flow and travel times, but should be used with caution unless additional supporting information can be obtained from field measurements.

The representation of unsaturated flow by such a relatively simple mathematical model may, however be inappropriate, for example preferential pathways may exist through the unsaturated zone (e.g. cracks, tree roots, man made-structures). This illustrates the need to ensure that the conceptual model takes account of field observations, and the representation of these in the mathematical model needs to be justified, together with a consideration of whether they are over or under-conservative.

Groundwater system and saturated zone flow

The conceptual model should seek to describe the groundwater flow system in terms of:

- Horizontal and vertical hydraulic gradients;
- Seasonal variations in groundwater levels and flow directions;
- Possible heterogeneity of the flow system, multiple porosity and fractures;
- Inflows (i.e. recharge, river leakage) and outflows (i.e. abstraction, spring discharge) including changes in these flows with time.

This information provides the basis for understanding how contaminants (dissolved in groundwater) are likely to move through the groundwater system.

Sufficient understanding of the aquifer system must be gained to determine which inflows and outflows are likely to influence the transport of contaminants between the site and the receptor(s). Complex problems may require the development of a detailed understanding of the groundwater flow system before any contaminant transport modelling can be undertaken.

The local and regional groundwater flow pattern should be considered as part of the conceptual model, i.e. definition of the flow system should not just be restricted to the immediate vicinity of the site. How much understanding of the regional flow pattern is necessary will depend on the likely magnitude of the plume. If the plume is likely to be kilometres in length, then the regional flow pattern is very important, whereas if the plume is a few tens of metres, then the local direction of flow and any flow mechanisms in the area of the plume may be adequate detail.

Realistic hydraulic gradients and flow directions for a site can be established only with the use of data from both the up and down gradient directions. Regional flow directions are rarely straight lines and it may be that a contaminant plume initially heading in one direction will bend in another direction, as the regional flow pattern changes. Vertical flow gradients may be important, for example near pumping wells, recharge or discharge zones, in some aquifer systems (e.g. multi-layered aquifers) and these must be considered as part of the conceptual model development, including whether they result in a diving plume.

If there is an existing conceptual model or groundwater flow model for the area this could be obtained and, if appropriate, used for an initial study of the regional groundwater flow regime. However, the quality of the data and the model should be established before using this output blindly.

The conceptual model should consider how groundwater flow occurs (via fracture flow, intergranular flow), both on the small scale and regional scale. Field measurements of hydraulic conductivity can often show a variation of more than one order of magnitude. The conceptual model should seek to understand and explain this variation and to identify over what scale (centimetres, metres, kilometres) changes in the system characteristics and behaviour need to be understood. For example, Darcy’s Law can be used to provide an adequate representation of groundwater flow on the regional scale (provided a suitable value for hydraulic conductivity is used). However small scale variations in hydraulic conductivity (due to the presence of fractures, or more permeable lithologies) can have a significant influence on contaminant transport.

3.4.2 Artificial pathways

Man-made structures may form artificial or preferential pathways (e.g. drains, mine workings, adits) or barriers (e.g. walls and foundations) to natural flow. Artificial pathways can provide key routes for the lateral and vertical migration of contaminants particularly where low permeability layers are penetrated by these structures, for example where a service corridor has been excavated through a clay layer and subsequently back-filled with granular material.

Below ground structures may form multiple pathways. The potential for changes in these pathways over time should be considered as old structures are excavated and new ones installed. Pathway changes over time may also result from seasonal changes in infiltration, abstraction, river flows or flows in culverts.

These pathways can be difficult to identify during a site investigation and it is essential that as much information on underground services and structures should be obtained during the desk study from maps or plans of the site and from a site walk over survey. The significance of artificial pathways should be addressed in the conceptual model.

3.5 Fate and transport processes

The conceptual model should describe the processes that control the movement of contaminants in the soil, unsaturated and saturated zones. These processes including:

- Advection;
- Dilution;
- Dispersion;
- Diffusion;
- Sorption;
- Degradation (biotic and abiotic);
- Volatilisation;
- Multiphase flow.

Tables B1, B2 and Appendix B provide a brief description of these processes and how they are typically represented in a mathematical model. A summary of some of the main factors that need to be considered in the conceptual model are outlined below:

Advection

Advection describes the movement of water under a hydraulic or pressure gradient. When dissolved solids are carried along with flowing groundwater, this is advective transport. Understanding advective transport should be the starting point in the development of a conceptual model of contaminant migration. This is why any previous work on modelling the flow system at a regional scale should be investigated.

The rate of advective transport is typically described by the mathematical expression given in Box 3.2.

Box 3.2 Equation describing advection in homogenous, porous media

The rate of advection is usually described by the following equation:

$$v = Ki/n$$

where

v = average velocity of water movement (m/d)

K = hydraulic conductivity (m/d)

i = hydraulic gradient

n = transport porosity

This equation is useful and can be used during development of the conceptual model to indicate:

- The likely extent of the contaminant plume and its consistency with field observations;
- The time before impact might be expected at the receptor and consequently how much time is available to undertake any assessment.

However, this equation can potentially be misleading as it implies that groundwater velocities can be represented relatively simply. In practice, the contaminant migration is more complicated as:

- The hydraulic conductivity can be highly variable. For example the geology may comprise inter-bedded deposits of differing permeability, such that the rate of contaminant migration will vary within each horizon;
- The hydraulic gradient can vary both spatially (with both horizontal and vertical component of flow) and with time (seasonal variation in groundwater levels);
- The transport porosity will depend on whether flow is via fissures or through interconnected pores, with the need to understand what proportion of a rock's porosity is involved in transport. This can be further complicated as contaminants can diffuse between mobile and non-mobile water (Barker & Foster, 1981 and Barker, 1993);
- For some groundwater systems, groundwater movement may be non-laminar (turbulent flow) in which case the above equation would not be appropriate;
- Contaminant breakthrough at a receptor will occur sooner than that predicted from advection alone, due to the influence of dispersion (see below).

The transport porosity of an unconsolidated homogeneous material is likely to be as high as its total porosity. However, most aquifers contain dead-end fissures, unconnected pore-space and lower permeability than average material, and therefore the transport porosity of such materials is generally lower than their total porosity.

In highly fissured aquifers the transport porosity may be as high as the fissure porosity. In dual porosity aquifers (i.e. fractured porous materials), the relevant porosity may be somewhere between the fissure and matrix porosity and may change with average flow velocity. For example in chalk, for very slow velocities (i.e. regional flow of less than 1 m/d), diffusion will ensure the contaminant will spread out through the matrix and a value approaching the total porosity is appropriate. At faster velocities, diffusion into the matrix becomes less significant and the transport porosity reduces towards the fissure porosity.

In addition, the measurement of these parameters can be problematic. For example, whilst it is relatively easy to measure the total porosity of a consolidated rock (e.g. from laboratory measurements), it is generally not straightforward to measure the transport porosity or even the total porosity of a loose gravel. Total porosity for granular materials can be calculated based on grain density and dry bulk density, and for coarser materials the transport porosity will be similar to the total porosity. Measurements of natural moisture content can be used to calculate the water filled porosity in the unsaturated zone (Marshall *et al.* 1996). Tracer experiments can provide a reliable method for estimating the transport porosity, but these can be difficult and costly to undertake.

Dispersion and diffusion

As water and contaminants migrate through the subsurface, they will tend to spread out, parallel to and normal to the flow path. This spreading out is called dispersion and is caused by a number of factors including:

- Diffusion - movement of contaminant from a region of high concentration to a region of low concentration;
- Pore size - some pores are larger than others and allow fluid to move faster;
- Path length - some particles travel along longer flow paths to go the same linear distance;
- Friction in pores - fluid moves faster through the centre of pores than along the edges.

Dispersion is important in terms of the first arrival time of contamination at a receptor and the sharpness of the breakthrough curve. Larger longitudinal dispersion leads to earlier breakthrough, but lower peak concentrations and a longer time for all the contamination to pass through.

Dispersion will also result in a decrease in contaminant concentration through mixing or dilution both along the flow path (longitudinal dispersion) and normal to the flow path (transverse dispersion). Permeability heterogeneity (including fissures and lenses) causes further mixing on a larger scale (macrodispersion), such that the dispersion generally increases with the scale of measurement.

Diffusion causes solutes to move in the direction of the concentration gradient but under most conditions of groundwater flow diffusion is insignificant and it is not possible to distinguish the effects from those of mechanical dispersion. The two are therefore generally combined as hydrodynamic dispersion. However, under certain conditions (e.g. low permeability, low velocities), diffusion may be important. The relative contribution of diffusion and dispersion processes should be established as part of the conceptual model development.

It is important to understand, however, that although we commonly represent dispersion in numerical models by Fickian diffusion equations, this is only done because we are unable to represent the actual processes (refer to Zheng & Bennett, 1995). Hence, when models produce, for example, dispersion upstream of the direction of flow it is not real, but a consequence of the diffusion equation to represent dispersion.

Dispersion is usually described using a relatively simple mathematical expression as given in Box 3.3.

Box 3.3 Equation describing dispersion

Dispersion of contaminants is usually described by the following equation

$\mathbf{D}_h = \mathbf{D}^* + a\boldsymbol{v}$

where

$\mathbf{D}_h$ = the coefficient of hydrodynamic dispersion (m^2/s)

$\mathbf{D}^*$ = the effective diffusion coefficient (m^2/s)

a = the dispersivity of the medium (m), and

$\boldsymbol{v}$ = the velocity (m/s).

and

$\mathbf{D}^* = \mathbf{D} \times T$

$\mathbf{D}$ = the diffusion coefficient (m^2/s)

T **=** dimensionless coefficient related to tortuosity.

For a specified flow direction, dispersion is described mathematically by the longitudinal dispersivity α_L, and two transverse dispersivities $\alpha_{T;}$ (dispersivity is expressed in units of length). A number of empirical expressions exist which describe relation of values of dispersivity to the path length (Xu and Eckstein, 1995).

The measurement of dispersion is difficult and expensive in the field and consequently empirical expressions are used. For example the longitudinal and transverse dispersivity are commonly set to 10% of the flow path length and 1% of the flow path length respectively. This is based on literature studies that indicate that dispersion is scale dependent (Xu and Eckstein, 1995, Domenico and Schwartz, 1990).

The use of simple descriptions of dispersion, leading to simple mathematical expressions can be misleading. This may mean that insufficient thought is given to understanding how contaminant migration is occurring and in particular the importance of particular pathways may be missed. For example, contaminant transport may be occurring via high and low permeability layers, each being important in defining contaminant breakthrough at a receptor. The presence of low permeability layers will limit vertical dispersion. A possible approach could be to describe this behaviour mathematically using a large dispersive term, but this ignores how the actual system is behaving and could lead to incorrect conclusions being drawn. The key is to decide whether the use of simplifying assumptions is reasonable.

Volatilisation

The concentrations of volatile contaminants may be reduced due to volatilisation (forming a gas phase) and the importance of this process should be determined as part of the conceptual model development. Loss of contaminant mass via volatile breakdown products must also be considered.

Box 3.4 Volatilisation (Henry's Law)

The partitioning of volatile contaminants between the dissolved phase and the vapour phase can be described using the following equation:

$$C_v = H\,C$$

where;

C_v = contaminant concentration in vapour phase (mg/l)

C = contaminant concentration in aqueous phase (mg/l)

H = Henry's Law constant (dimensionless)

Effect of fluid properties

Some contaminants may be present in sufficient concentration to modify the physical properties of the water phase, particularly its density and viscosity. Density differences may cause density-controlled flow. For example, the solution of highly soluble contaminants (e.g. halite or rock salt) can result in a dense fluid plume that will tend to sink through less contaminated groundwater. Where solute concentration modifies the properties (e.g. density and viscosity) of the water phase, the flow and transport equations become linked and solution of the equations is particularly difficult as it must be done conjunctively.

The significance of density and viscosity effects should be considered within the conceptual model, and whether, for example, the concentration of inorganic dissolved salts is likely to result in density controlled flow. Such effects may be important for dissolved concentrations of more than a few thousand mg/l.

Multiphase flow

Sites where the contaminants include non-aqueous phase liquids (NAPLs) present particular problems as the controls on migration are numerous and complex. LNAPLs are less dense than water and remain close to the capillary fringe or spread across the water table. Seasonal water table fluctuations may result in NAPL being trapped both beneath and above the water table, especially in fractured aquifers. DNAPLs are denser than water and move downwards through the strata in response to gravity, they migrate down the dip of the geological strata and may flow in a different direction from the groundwater. Further information on the behaviour of NAPLs can be found in Pankow & Cherry (1996) and Fetter (1992).

Box 3.5 Raoults Law

The dissolved concentrations for a mixture of organic compounds can be estimated based on Raoult's law as follows:

$$C_d = SX$$

where

C_d = dissolved phase contaminant concentration in groundwater (mg/l)

S = pure phase (liquid) solubility of organic compound (mg/l) (usually obtained from literature sources)

X = molar fraction of organic contaminant in free product (obtained from laboratory analysis of free product)

A common approach in considering NAPLs is to assume the NAPL is immobile, and that the transport of contaminants is a result of their solution by groundwater and subsequent transport in the dissolved phase. The dissolved contaminant concentration is often defined as the contaminant solubility (Box 3.5). This illustrates that simple models can be used to represent relatively complex systems, but will be reliant on providing supporting information to justify any assumptions, such as the NAPL phase is immobile.

3.5.1 Geochemical and biochemical processes

The conceptual model should take account of geo- and biochemical processes that can influence the transport or concentrations of contaminants in the subsurface. The conceptual model should determine whether or not these processes are operating at a particular site and whether they are significant and need to be represented in a mathematical model.

The chemical and biological processes that influence the concentration of contaminants are often complex and poorly understood and are the subjects of large amounts of research and theorising. Some of the main processes by which contaminants can be removed from the groundwater include:

- Sorption;
- Degradation;
- Chemical precipitation;
- Radioactive decay.

Detailed discussion of these processes is provided by Fetter (1992). A brief summary of issues relating to sorption and degradation are given below.

Sorption

Sorption processes include adsorption, absorption, chemisorption and cation exchange. These processes are complex and are dependent on the geochemical environment, the rate of groundwater flow, the surface area in contact with groundwater and the concentration of contaminants present in groundwater. The actual process of sorption is also difficult to determine directly, such that the conceptual model will require a number of assumptions to be made about the processes that are occurring.

There are two fundamentally different ways of conceptualising sorption in common use:

i) The first is to assume that the quantity sorbed is directly proportional to the concentration in the water (linear isotherm, Box 3.6) and that it happens instantaneously. The ratio of sorbed concentration to dissolved concentration of a contaminant is known as the partition coefficient (k_d). This includes all the sorption processes and has the advantage that it leads to the elegant conclusion that the contaminant travels at a velocity directly proportional to the water velocity – only slower by a factor known as the retardation factor. However this formulation assumes that sorption is unrelated to contaminant concentration which may not be true at high contaminant concentrations and also that there is no upper limit on the amount of sorption that can occur.

ii) The other approach is to assume the matrix absorbs the contaminant up to a limit (e.g. cation exchange capacity, or CEC). This is a common approach for ammonium.

Other relationships have been proposed to describe the ratio between sorbed and dissolved concentrations such as the Freundlich isotherm and Langmuir isotherm. Examples of how these processes are described mathematically are given in Box 3.6. The Langmuir formulation combines the approach of a distribution coefficient with a sorption limit. The sorption process is reversible, therefore, once the contaminant plume passes a particular point, desorption can occur back into the groundwater. Most current modelling approaches assume that sorption and desorption are effectively instantaneous and reversible, which is mathematically convenient. Experimental evidence indicates that these assumptions are an over simplification with desorption typically occurring at a slower rate than sorption.

Box 3.6 Equations describing sorption

1. Linear isotherm

$$K_d = \frac{C_S}{C}$$

2. Freundlich isotherm

$$K_d = \frac{C_S}{C^{1/N}}$$

3. Langmuir isotherm

$$K_d = \frac{C_S}{C(b - C_S)}$$

K_d = partition coefficient (l/kg)
C = concentration in the aqueous phase (mg/l)
C_S = concentration in the solid phase (mg/kg)
b = maximum amount of contaminant that can be sorbed (mg/kg)
N = chemical-specific coefficient (values of 1/N typically range from 0.7 to 1.1)

The partition coefficient can be used to determine the rate of movement of a sorbed contaminant as follows

$$V = u/R_f$$

Where the R_f or retardation factor is defined as:

$$R_f = 1 + rK_d/n$$

Where: Rf = retardation factor

r = bulk density (kg/l)

n = effective porosity

K_d = distribution coefficient (l/kg)

Degradation

Degradation can be a significant process in decreasing the contaminant mass. This process is complicated and the actual rate of biodegradation varies according to a range of factors including contaminant type, microbe type, redox, temperature and chemical composition of groundwater.

This process is usually represented mathematically either as a first order reaction (exponential decay), or by a rate limited reaction. Exponential degradation implies that the rate of decrease in concentration of the substance is proportional to the amount of substance (see Box 3.7) and can be characterised by a half-life (i.e. it is assumed to be a first order reaction). This behaviour is commonly observed in biodegradation (since the activity of a microbial population is proportional to the availability of its food), radioactive decay, and in other non-biological processes where the contaminant is present in trace amounts relative to other reactants.

Box 3.7 First order reactions

A first order reaction (exponential decay) can be represented by the following expression:

$$C = C_o \, e^{-lt}$$

where

C = contaminant concentration after time t

C_o = initial contaminant concentration (mg/l)

l = decay rate (d^{-1})

However, exponential decay may represent a simplification of what is occurring. For example:

- the process may be inhibited at high concentrations (e.g. high levels of contaminant cause toxicity to micro-organisms);
- the process of degradation may vary through the plume (low oxygen tends to result in the growth of a new (anaerobic) microbe population with a different consumption rate and may result in anaerobic degradation at the centre of the plume and aerobic at fringe);
- the process may be dependent on a food source that may become exhausted (e.g. low levels of contaminant cause the micro-organisms to die of starvation);
- there may also be a delay while the microbial community acclimatises to the contaminant;
- the reaction rate may depend on the availability of another reactant i.e. oxygen.

Degradation may also result in the production of daughter products that may have different properties and toxicity from the parent.

Evidence for degradation should be identified at the conceptual model stage and incorporated if observed. The conceptual model should aim to determine from available data whether there is evidence for this process (Environment Agency, 2000b), how it is occurring (i.e. aerobic or anaerobic degradation) and what controls there are on the rate of degradation (i.e. inhibition at high concentration, dependence on oxygen supply). The conceptual model should then consider how this is best represented, for example by a exponential decay function, together with the limitations associated by the chosen approach.

3.5.2 Mathematical representation of transport processes

The conceptual model should consider what processes may be influencing contaminant transport in terms of:

- Contaminant properties (solubility, mobility, persistence);
- Evidence for a process, e.g. biodegradation (for example the Environment Agency, 2000b, guidelines for the assessment of natural attenuation points to looking at several lines of evidence that biodegradation is occurring, although stresses that assessment based on one line of evidence may be adequate provided it is overwhelming);
- The process occurring (e.g. cation exchange or sorption);
- Controls on the process (e.g. do high contaminant concentrations inhibit degradation);
- Representing the process mathematically (linear isotherm) including the use of appropriate simple expressions, and reasonable assumptions can be demonstrated through comparison of the model results with field observations. Good practice is to try a number of different approaches to determine which best matches observed conditions, and to be ready to reject the model if inconsistencies are apparent.

Nevertheless the use of simple equations to describe contaminant movement can provide a very useful approach in determining how far a contaminant would be expected to migrate. Comparison of the expected extent of a contaminant plume with the observed distribution provides a quick check on whether the conceptual and mathematical representation are compatible.

3.6 Defining the receptor

A receptor, in this context, is any protected water or location down groundwater gradient from a contaminated site which may be at risk from the contamination. The potential receptors that must be considered in the conceptual model are:

- Groundwater; including the aquifer below the site, and any deeper aquifers. (e.g. in assessing a discharge to groundwater for the purposes of the Groundwater Directive, or assessing whether land is Contaminated Land);
- Groundwater abstraction boreholes; e.g. for assessing whether Contaminated Land is a Special Site under Regulation 3(a) of the Contaminated Land (England) Regs, 2000;
- Natural groundwater discharge (e.g. springs, wetlands, surface watercourses, marine discharges);
- Compliance point defined by the Agency (e.g. a compliance borehole located down hydraulic gradient of the site).

All potential receptors must be considered and, commonly, there will be more than one. However, not all receptors will need to be modelled and an important part of the process of developing the conceptual model is to identify the key receptor(s). For the purposes of risk assessment the sensitivity of the receptor and the existing background water quality can be used to determine the level of contamination that could be tolerated at any given location and hence the remedial target for the contaminant source (Environment Agency, 1999a).

3.7 Uncertainty

The conceptual model must take into account uncertainty (see also Section 5.6). This may be due to:

1. *Field / Laboratory Data:* There is inherent uncertainty in the point measurement of all field / laboratory data and in producing spatial distributions based on them.

2. *Conceptual model:* The most serious cause of error in modelling results arises from deficiencies in the formulation of the conceptual model (Anderson & Woesner, 1992, p293). The conceptual model is a *simplified* description of the real aquifer system. Alternative conceptual models can be formulated which are equally plausible so that both require testing. This is commonly called conceptual uncertainty.

3. *Model Input Data:* There are errors introduced due to the uncertainty in the model input parameters. For example transmissivity values derived from pumping tests at one location are frequently a factor of 3 higher or lower than those from a nearby pumping test which would be in the same model cell. Model parameters are applied to cells or zones across which the properties are averaged thus not representing the real heterogeneity of the system. This is very scale dependent so greater accuracy requires much greater detail.

4. *Mathematical representation:* There will be inherent errors associated with the mathematical representation of the physical processes (e.g. the governing equations and boundary conditions are simplified mathematical descriptions of the conceptual model). In addition the numerical approximations used to solve these equations and the associated spatial and temporal resolution introduce further errors. (See section 8.3)

5. *Predictive Uncertainty:* There will be errors in the model predictions because future conditions are estimated but will in reality be different (see Section 9.6).

Key areas of uncertainty must be discussed in the conceptual model, including their significance in any mathematical model. Conceptual uncertainty will be one of the main reasons why the results of the modelling exercise are wrong.

3.8 Reporting the conceptual model

Preparation of a clear report is essential in communicating the conceptual model to relevant parties, including the Environment Agency (see Section 10).

The preparation of plans, contour maps, cross-sections and block diagrams is essential in the development of a conceptual model as it often highlights data gaps and inconsistencies and provides a method for checking that any assumptions make sense in the light of existing data. The presentation of these figures in reports also enables others to gain a rapid understanding of the system. Table 3.1 provides a summary of figures that should be produced as part of the conceptual model.

Figures 3.4 to 3.8 provide examples of how the conceptual model for a site should be presented. Figure 3.4 shows a simple plan view of a site and the groundwater contours.

Depending on the hydrogeological complexity, more than one piezometric map may be required. The cross-section for the same site may look like Figure 3.5. Figure 3.6 shows a conceptual model cross-section of a more complicated site and the potential links between sources, pathways and receptors. Figure 3.7 shows a more detailed example of sources and pathways that may need to be considered in a conceptual model and how these could be represented in a cross-section. These figures will represent a simplified representation of our understanding of the system. For example, a number of assumptions may have been made constructing Figure 3.4 including:

- The field measurements of water levels are correct and the borehole datum are correct;
- The observation boreholes monitor the same horizon;
- Groundwater flow is perpendicular to groundwater level contours; this may not be the case in anisotropic aquifers.

In reporting the conceptual model it is important that clarification is given to the following:

- What is known and understood about the site. Supporting data and calculations should be provided;
- What is not known or not understood about the site and whether it is thought to be important. What are the uncertainties in the data. This should also include a list of further data requirements and proposed sampling or investigations to obtain essential information;
- What has been assumed about the system. Justifications for decisions and any supporting data or calculations should be provided.
- What has been ignored or simplified in order to come up with answers to our questions. Again, justifications for decisions and any supporting data or calculations should be provided.

Table 3.1 Examples of presentation of data

Information	**Presentation method**	**Purpose**
Site history	Historical maps	To show possible sources of contamination, below ground structures and identify possible pathways (i.e. services)
Geology	Geological maps Cross sections or 3-D sections Structural contour maps (including top and base of formation, thickness of formation)	To show geology of study area and to identify possible contaminant pathways.
Ground water levels	Distribution map (contoured)	To show direction of groundwater movement. This should be compared with contaminant distribution. Contour maps should be presented for different times to identify whether there are any seasonal or long-term changes in flow direction.
	Hydrographs	To illustrate seasonal variation or any long-term change in water level. This

		should be compared with variations in contaminant concentrations and free product thickness with time.
	Vertical sections (variation in head with depth)	To illustrate if vertical hydraulic gradients are present. This should be compared with observed vertical distribution of contaminants (i.e. 3D plume geometry) and geology.
Contaminant Concentrations	Distribution map (contoured). Time series plots. Distance concentration graphs. Cross sections.	Relevant plots should be presented for different times to illustrate changes in contaminant concentrations and plume geometry over time. To illustrate plume geometry and whether this is changing with time. To provide primary evidence of plume stability (shrinking, stable, growing).
Hydrochemical indicators such as pH, redox, dissolved oxygen	Distribution maps (contoured) Time series plots Cross-sections	To illustrate the hydrochemical environment including whether conditions are oxidising or reducing and whether they are changing with time. It is important to define conditions up hydraulic gradient of the plume, i.e. background conditions.

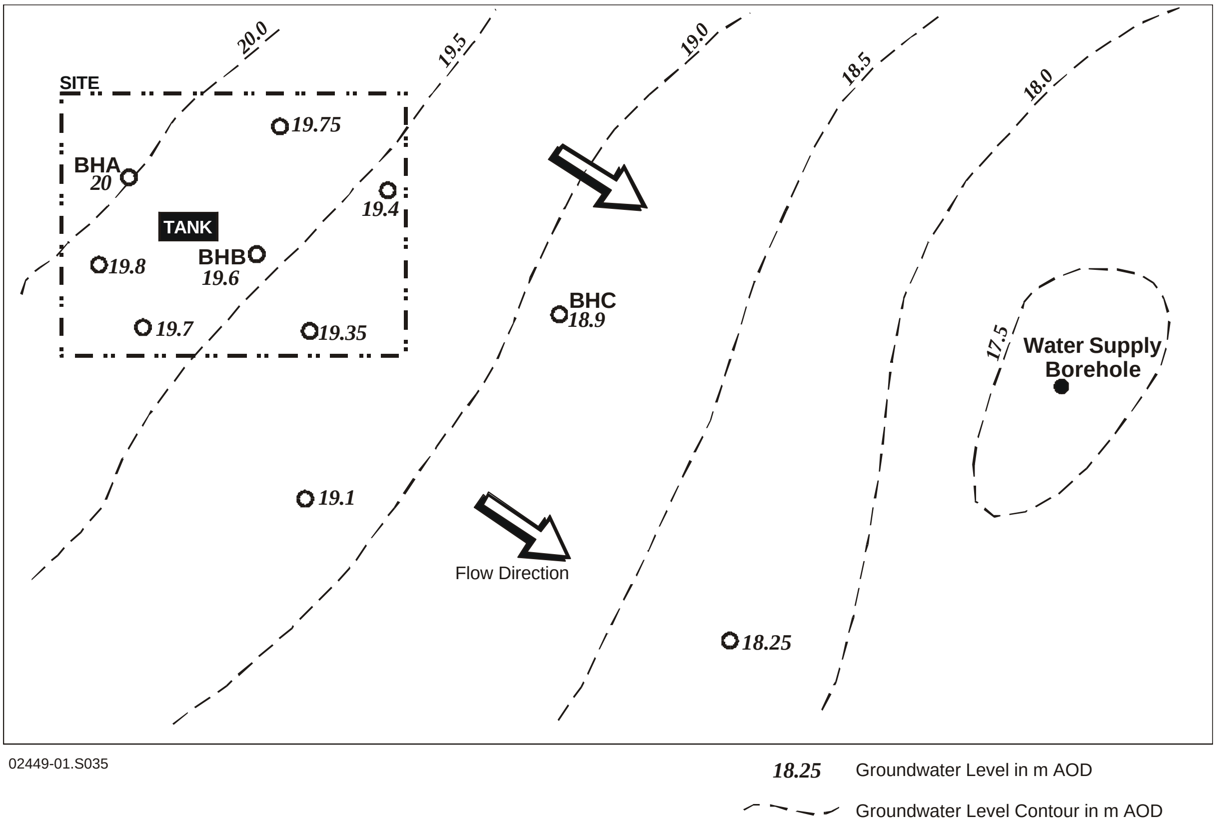


Figure 3.4 Conceptual Model - Plan View and Groundwater Contours

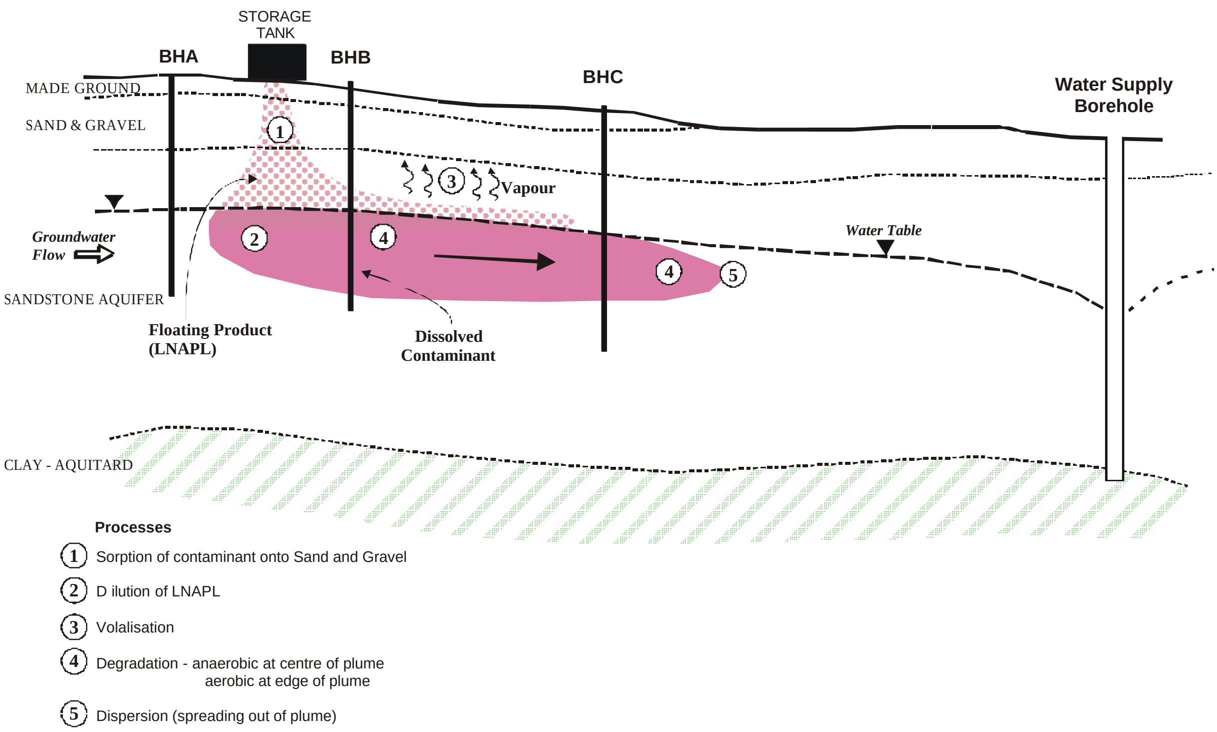


Figure 3.5 Example Conceptual Model - Cross Section Showing Source, Pathway and Receptor

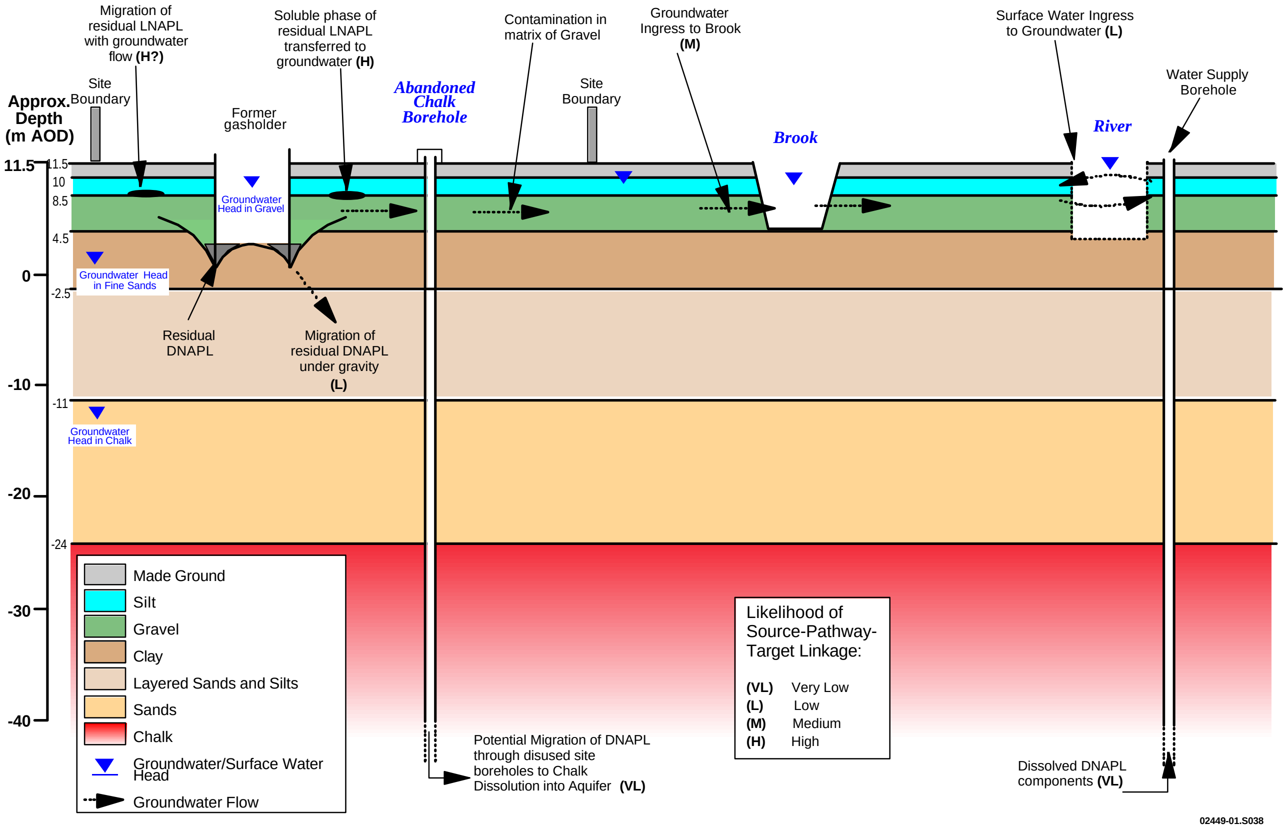


Figure 3.6 Example Conceptual Model of S-P-R (likelihood of linkage will be site-specific)

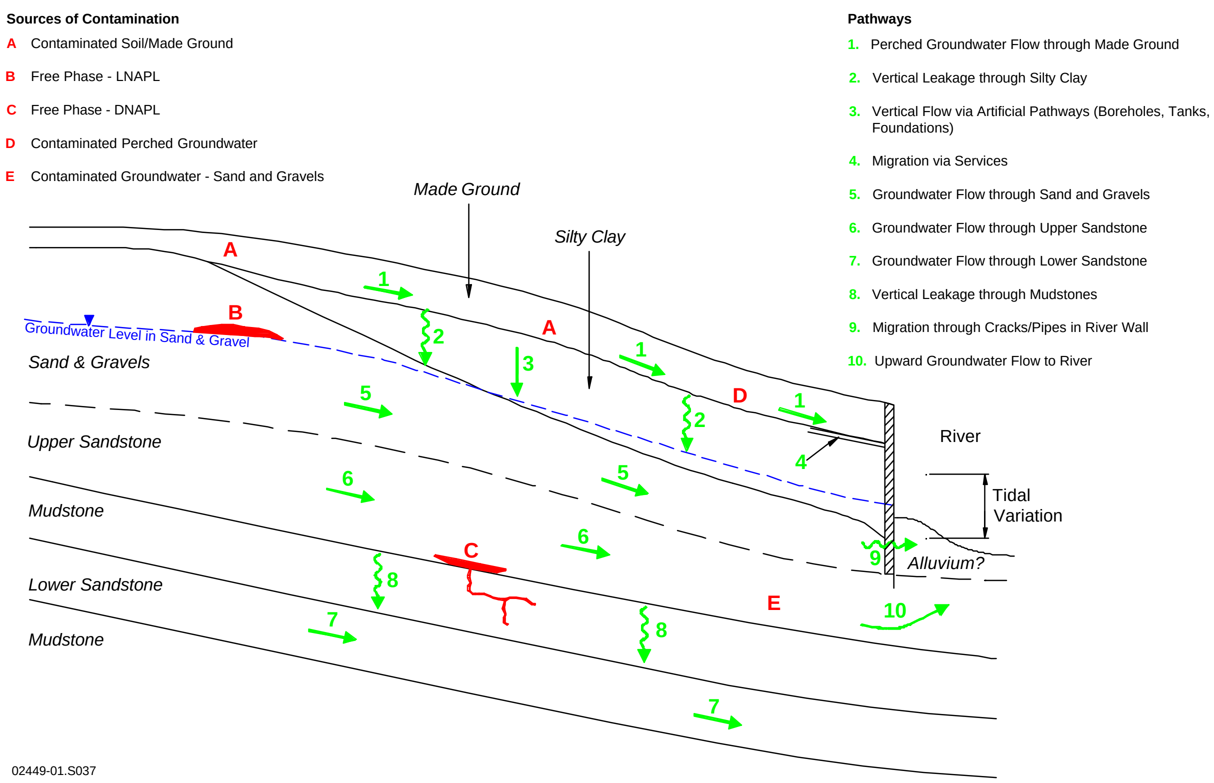


Figure 3.7 Simplified Conceptual Model of Potential Sources and Pathways

4. Data Collection, Collation and Review

4.1 Introduction

The quality and reliability of the results of a contaminant transport modelling study will depend on the data that have been used to develop the conceptual model and to construct, and refine the mathematical model. If the data are inadequate the model results will be unreliable. **The data used should be site-specific and should characterise the site and area being modelled.**

The area of data collection should be defined and (particularly in the case of a numerical model) will be larger than the area of interest. This is to gain an understanding of the surrounding flow patterns that influence advective transport and to set appropriate boundary conditions that will not interfere with the model results.

Inadequate budgeting or limited timescales should not in themselves be used as a reason for not collecting site data. The collection of site-specific data should be carried out in preference to elaborate modelling.

4.2 Data requirements

The data requirements will vary at different stages in the modelling process, but will depend on the objectives of the study, the complexity of the problem, and the sophistication of the analysis, e.g. the type of model. All requirements should be reviewed at the initial stages to assess the feasibility of developing a model. Attempting to construct a complex numerical model, for example, is a pointless exercise if critical input data or validation data cannot be obtained for the site. There are three main stages of modelling at which data are required:

- **Development of conceptual model** – this makes use of available data and requires adequate data to understand the flow system and the transport mechanisms operating at a site. Some parameters may be quantified but others can be estimated at this stage. Developing the conceptual model highlights the data gaps and the data which should be collected during the site investigation and is iterative with further data collection phases. The conceptual model should include an assessment of our understanding of the data, together with any uncertainties (measurement, natural variability).

- **Construction of mathematical model –** the parameters and processes identified in the conceptual model must be quantified. Values or ranges required to be input into the model should be based on site-specific data, if these are not available, substitutes must be obtained from literature or other sources. **Justification of the use of literature values in modelling should always be given.**

- **Assessment of model results against historic data –** these tasks require site-specific data on groundwater levels, flows, and concentrations. The ability of a model to simulate site conditions must be tested by comparing the model results with real data from the site.

Ideally, all data used for contaminant fate and transport modelling should be site-specific relating to the site and area being modelled. However, this is often unrealistic due to the cost that would be involved in obtaining the data, particularly for distributed numerical models. The modeller will need to determine which are the key parameters for which site-specific data are required and those for which literature values would be acceptable. The more site-specific data that are collected, the less uncertainty there is likely to be in the values and ranges used in the model, although in some cases further data collection can increase our awareness of the variability of the system (i.e. a value of hydraulic conductivity is obtained which is an order of magnitude greater than previous measurements leading to the concept that a high permeability pathway may exist). The ease of collection and relative cost of obtaining field measured values for flow and transport parameters are summarised in Table 4.1. The main cost in obtaining site-specific data will usually be associated with the drilling and construction of monitoring boreholes.

Table 4.1 Summary of site-specific data - ease of obtaining values, relative cost and importance

Parameter	Site-specific data essential	Site-specific data useful	Comments on ease and cost of obtaining site-specific data
Aquifer depth/geology(1)	✓		Data relatively easy to obtain but data quality, reliability and cost will depend on site investigation techniques used.
Hydraulic conductivity (2)	✓		Data relatively easy to obtain but data quality, reliability and cost will depend on method used. Pumping tests can provide the best quality data, but may be expensive particularly where contaminated water needs to be managed.
Hydraulic gradient and direction of flow (2)	✓		Data relatively easy to obtain but data quality, reliability and cost will depend on number and construction (depth, diameter) of borehole installations.
Groundwater levels (seasonal range) (2)		✓	As above
Porosity (1)		✓	Intergranular porosity is inexpensive and easy to measure.
Transport porosity (1)		✓	Difficult to measure - requires tracer test.
Bulk density (1)		✓	Inexpensive and easy to measure.
Dispersivity (1)		✓	Difficult and expensive to measure and requiring long term monitoring.
Partition coefficient (K_d) (1)	✓ (for inorganics e.g. metals)	✓	Generally inexpensive and easy to measure. But data quality, reliability and cost will depend on methods used
CEC (1)	✓ (not for organics)		Inexpensive and easy to measure
Moisture content of unsaturated zone (1)	✓		Inexpensive and easy to measure.
Fraction of organic carbon (1)	✓ (for organics)		Inexpensive and easy to measure
Infiltration	✓		Meteorological office data easy and relatively inexpensive to obtain.
Degradation	✓ (not for metals)		Difficult and expensive to measure and requiring long term monitoring. BUT vital to provide confidence
Contaminant concentrations and delineations? (2)	✓		Costs dependant on analytical suite and number of samples
Biochemical environment (2)	✓		Inexpensive and easy to measure (DO, pH, redox, temp)

(1) Requires soil sampling from boreholes/trial pits

(2) Requires construction of monitoring boreholes

The quality and quantity of the available data should be taken into account when selecting the mathematical model. Distributed numerical models should not be considered where data are limited.

Even when simple analytical calculations are used that require a single value for each parameter, those parameter values must be representative of the site and the area being modelled. Single site-specific measurements should be used with considerable caution. Probabilistic models will require parameters to be input as distributions so an appropriate distribution must be fitted to the site investigation data collected and the data collected should be sufficient to define such a distribution. Further information on fitting distributions to field data is included in Environment Agency (2001b).

Data collection should always be seen as an iterative process, often following a tiered approach with a number of phases of site investigation designed to build a more detailed conceptual model or develop an analytical model prior to the development of a numerical model. This illustrates that development of the conceptual model and mathematical model should allow data collection to be targetted at key parameters.

4.3 Data sources

Data sources include;

- Public bodies (e.g. Environment Agency, British Geological Survey, Meteorological Office etc);
- Previous site investigations (investigations from adjacent sites should also be used if appropriate);
- Site investigations undertaken as part of the study;
- Literature (text books, journals etc), databases, web sites.

Models should include site-specific parameter data wherever possible but when these are not available data will need to be obtained from other sources. Data from one part of a site can sometimes be extrapolated to cover areas of the site for which there are no data or information from adjacent or nearby sites or boreholes may be used with caution.

As part of the assessment it may be necessary to use data from literature sources or software manuals. Some useful references for data on contaminant fate and transport modelling parameters in UK aquifers are listed in Table 4.2.

Literature sources should also be consulted as a check, on whether the values obtained from site investigations are credible (i.e. may help to identify errors in laboratory reporting etc).

Table 4.2 Potential literature sources for parameter values

Parameter	Literature References
Chemical and physical properties of contaminants (e.g. solubility, Henry's Law, Koc)	Chemical text references (e.g. Howard *et al* (1991), Montgomery (1996), Howard & Meylan (1997)) Database and model help files (e.g. ConSim)
Hydraulic conductivity	BGS/Environment Agency (1997 and 2000)
Hydraulic gradient	BGS Hydrogeological Maps, Agency piezometric maps
Aquifer depth/geology	BGS Geological Maps and Memoirs, BGS/ Environment Agency (1997 and 2000), BGS borehole database
Groundwater levels (seasonal range)	Environment Agency groundwater monitoring network, EA borehole database
Porosity	BGS/Environment Agency (1997 and 2000)
Bulk density	Soil mechanics and geotechnical textbooks
Dispersivity	Zheng & Bennett (1995), Xu & Eckstein (1995)
Partition coefficient (Kd)	USEPA (1996), Environment Agency (2000c), Model databases (e.g. ConSim)
Degradation rate	Environment Agency (2001g), Wiedemeier (1999), Howard *et al* (1991).
CEC	Environment Agency (2000c and 2001f)
Fraction of organic carbon	BGS (1991), Steventon-Barnes (2000)
Infiltration	Meteorological office data, Environment Agency rainfall data

Parameter values taken from the literature should be used with extreme caution and the context, sampling methods and analytical techniques used to obtain the quoted values should be understood. One exception is that literature values for contaminant physico-chemical properties (e.g. solubility) can usually be accepted. When literature values are to be used they should be from a comparable site or geological, hydrogeological and geochemical environment. They should be applicable to the site being modelled (e.g. do not use an aerobic degradation rate if the site is anaerobic). It is generally more appropriate to use parameters which have a limited range of values and are well defined in the literature. Justification of the use of literature values should always be given. Additional sensitivity analysis should be carried out on those parameters taken from the literature to determine their significance to the model results. **Site-specific data should always be obtained if the parameter has a major impact on the model results**.

4.4 Data quality

Whilst the use of site-specific data is recommended, the quality of those data must also be considered. Inappropriate sampling techniques or testing methods may result in misleading or erroneous data. Detailed guidance on data collection and testing is outside the scope of this report but many aspects of this topic are already covered by existing guidance. All stages of a modelling study should have appropriate QA procedures and include an audit trail for data sources. The sources of all model input parameter values should be given and justified including any assumptions or limitations of the data. The methods of sampling and laboratory analysis for site-specific-data should be carried out in line with current Agency guidance and industry 'good practice'. QA procedures for identifying data errors, particularly when there are large volumes of data, should include plotting or statistical analysis. Outlying values can then be identified and assessed to determine whether or not they should be included (Environment Agency 2001b).

4.5 Data management

Field measured parameters may need pre-processing in order to obtain data suitable for input into a model. Raw data and calculations, including any assumptions made, should always be presented as part of the justification of model input parameters. Where large numbers of data are involved the use of databases, spreadsheets or GIS systems should be considered both for data processing and presentation purposes.

The data should be checked to:

- Ensure units are correct;
- Reported correctly (particularly when transferring from one table to another);
- Credible (i.e. values are physically sensible), comparison with literature values provides a useful check;
- All valid data are used (i.e. extreme values should be used, unless it can be demonstrated that they are anomalous).

Data should be presented graphically wherever possible, particularly where large quantities are involved, and incorporated as part of the conceptual model. Plans, plots, graphs, cross sections and contours are easier and quicker to interpret than columns of numbers, however, tabulated data should always be reported in full as an appendix.

5. Selection of Mathematical Models

5.1 Introduction

There is a wide range of possible modelling tools that can be used in fate and transport modelling. In general, no one tool is appropriate for all situations. It is not the purpose of this chapter to describe mathematical models in detail, but rather to outline the key factors in selecting an appropriate mathematical model in relation to:

- What we are trying to achieve by modelling (i.e. what questions do we answered?);
- What do we need to model (a model may be used to represent only part of the system);
- How are we going to translate the conceptual model to a mathematical model (e.g. what processes need to be represented and how are these going to be represented);
- What information does the mathematical model need and how are we going to obtain this (regional data, site-specific data, literature values).

For most contaminant problems, a phased approach to modelling should be adopted, moving from analytical models through to numerical models, with distributed numerical models requiring the most effort and data. In many cases, it may be necessary to use only simple mathematical models. This process should be closely linked to development of the conceptual model and data acquisition, and continually referred back to the objectives of the study. A phased approach is consistent with the tiered approach set out in the Environment Agency's Remedial Targets Methodology (Environment Agency 1999a).

A mathematical formulation of the conceptual model needs to be developed if any quantitative modelling is required in order to (a) further the conceptual model, and (b) make predictions. This step is common to both numerical and analytical models. If a conceptual model cannot be expressed mathematically, then no quantitative calculations can be made. It is usually necessary to make assumptions (and simplifications) about the physics of the situation to arrive at the mathematical formulation. In the choice of these assumptions, a trade-off has to be made between over-simplifying the problem (which may introduce extra uncertainty) and extra time and difficulty if more complicated assumptions are included.

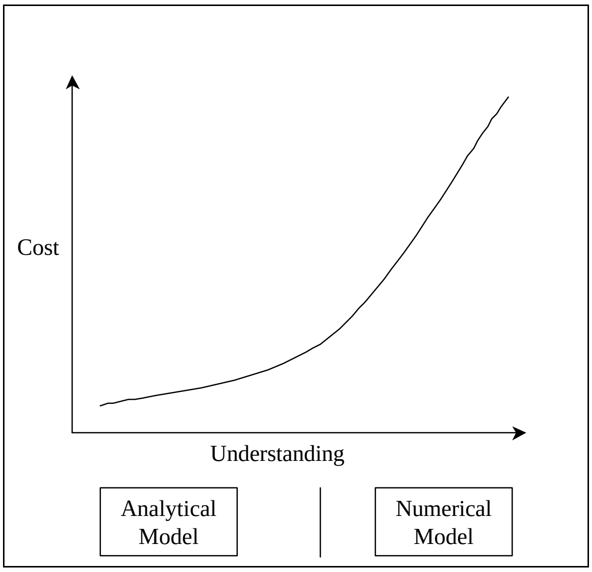
A range of commercial programs exist to model contaminant flow. These can be powerful programs that allow the user to develop models that would not be attainable without considerable mathematical understanding. Tools such as ConSim standardise an entire sequence of analytical calculations and then carry out a Monte-Carlo analysis – a process that could be carried out on a spreadsheet but would involve considerable time to develop and check. It is important that these programs are not treated as black box models, the user must understand what processes are being considered, how they are being represented, and how the input parameters influence the result. It is important to recognise that just because the model is easy to use and has an impressive front end, it is not necessarily the right model to use and the answers may not be reliable for a specific site. The most important aspect is the conceptual model and how this is being represented by the mathematical model.

Guidance on model selection is given in Belgin (1991), Zheng and Bennett (1995), Spitz and Moreno (1996), NRA (1995b), Geraghty & Miller (1992), IGWMC (1991) and van der Heijde (1993).

5.2 Selecting a modelling approach

The choice of model to use will be dependent on:

- **Study objectives** (this should include whether modelling is appropriate);
- **Level of accuracy** required (which may in turn depend on how close the situation is to its action thresholds, and the sensitivity of the receptor);
- **Stage of assessment** (e.g. assessment tier under the Environment Agency methodology for the Derivation of Remedial Targets, Environment Agency, 1999a);
- **Time scale** of the project in relation to the potential risk to an identified receptor. Simple analytical models can be set up and run in days, whereas distributed numerical models can take months or years to construct and test;
- **Cost** - are there sufficient resources to meet the cost of constructing a model?, is the use of a model justified through cost savings (e.g. optimisation of groundwater remediation scheme)? The cost associated with gaining additional knowledge or confidence in the system behaviour will increase substantially when a robust numerical code is used. A decision should be made over whether these costs are necessary given the complexity of the problem



- **Expertise** - are the appropriate technical resources (hydrogeologists, chemists, mathematicians etc.) available to support the model and interpret its output?
- **Data availability and quality** - are data sufficient to justify the proposed application of the model?
- **Complexity** - of the system to be represented and which simplifications can be made without prejudicing the required level of accuracy; does the model allow key processes to be represented?;

- **Regulator -** have the appropriate authorities been consulted and is the proposed modelling approach likely to be accepted?

It should be noted that although data availability is included in the list above, it should not be the driving force behind the decision of how to model a problem. In some situations there may be large amounts of data available for a regional model, but simple calculations using a uniform flow gradient in a limited area around the site may adequately demonstrate that the site is not close to the action threshold. A more complex model would be an inappropriate use of time and resources.

In choosing a mathematical model it is essential to consider how the conceptual model will be represented. It is important to recognise that the mathematical model will represent only a simplification of the conceptual model, which in turn will represent a simplification of the real system. The modeller will need to decide which are the key processes that need to be represented and whether this can be achieved using the mathematical model (i.e. is it acceptable to represent sorption as a linear process). The modeller will also need to take account of these simplifications in interpreting the results from the model and not to treat the results as absolute.

The modeller will need to determine the type of model (analytical, numerical) and what conditions will be represented (i.e. steady state or time variant). Some of the issues that need to be decided are:

- **Analytical or numerical model** This will be largely determined by the complexity of the system to be represented. Analytical models can prove particularly useful in obtaining an initial understanding of system behaviour which may not be so apparent from using more complex models. This emphasises the need to take a phased approach to modelling, starting with relatively simple models.

- **Steady state or time variant model** The simplest type of model is steady state where in-fluxes and out-fluxes to the model are constant with time. These types of models are used to represent relatively simple flow systems and/or contaminant transport (i.e. the contaminant plume has stabilised; there is no significant change in contaminant concentrations with time). Time variant models allow changes in the system behaviour with time to be examined and will be appropriate where monitoring has shown a changing flow pattern and/or contaminant concentrations are changing with time. Analytical models allow changes in contaminant concentration with time to be modelled. Numerical models have the advantage that changes in flow and contaminant fluxes can be simulated.

- **Deterministic or probabilistic model** This will partly depend on how uncertainty in parameter measurements or the natural variability of parameters will be taken into account in the analysis. Where field data are available to validate the model, then a deterministic approach can often be justified as these data allow the possible range in parameters values to be constrained. Where monitoring data are limited then a probabilistic approach should be considered. Uncertainty analysis of numerical models can be computationally expensive.

- Mathematical models allow **one, two, or three dimensional** contaminant transport to be represented. Analytical models consider only flow in one direction but can take account of dispersion both parallel and normal to the flow direction. Numerical models allow both horizontal and vertical flow to be taken into account.

Further factors that should be considered in choosing a model are:

- **Definition of the source term** Most analytic solutions assume that the source term is either constant, a step-curve or decays exponentially with time. If the source history is more complicated, then more complex analytical solutions should be adopted (such as superimposition of analytical solutions, Section 6.4) or a numerical model used. Numerical models have the advantage that fluxes (flow or contaminant) into and out of a model can be more readily varied with time.

- **Complexity of flow pattern** Analytical models allow only simple flow systems to be represented (e.g. uniform flow). If the flow system is more complex (e.g. multi-layered aquifer system where the groundwater flow direction varies spatially and/or with time groundwater/river interaction), then a numerical model is probably necessary (e.g. MODFLOW in combination with MT3D or particle tracking).

- **Flow or transport mechanism** Contaminant migration can occur via intergranular flow, fissure flow, and through the interaction of fissure and pore water. Analytical and numerical solutions exist for these flow mechanisms although numerical models can allow more complicated systems to be represented. The use of analytical solutions should not be ignored as they are particularly useful in gaining an initial understanding of the system behaviour.

- **Homogeneity** Analytical solutions assume that the aquifer is homogenous and cannot, therefore, directly take account of lateral variations in aquifer properties. Numerical models can take account of lateral variations, but only on the scale of the model grid. Nevertheless modellers can use analytical methods to represent heterogeneous aquifers through intelligent use of the model, either by looking at only part of the system, examining the influence of different parameter values on the model results, or through the use of probabilistic analysis. The key is to understand how and why the model is being used, and in interpreting the model results appropriately.

- **Transport process** to be represented, including advection, dispersion, degradation (e.g. decay, kinetic processes), sorption (including type of isotherm). Analytical solutions exist for dispersion, linear sorption and exponential decay. Non-linear sorption and non-exponential decay need specialist (numerical) programs (or occasionally semi-analytical solutions).

Where limited data are available, which is frequently the case at an early stage in an investigation, then an analytical approach is recommended. Sometimes such a calculation based on credible worst-case estimates can provide justification/or not for further analysis and data collection.

A phased approach should be adopted to the use of mathematical models, similar to the Tiered approached recommended in the Environment Agency R&D Publication 20 (EA, 1999) as follows:

Tier 1 involves the use of simple theoretical calculations of soil/water partitioning;

Tier 2 involves the use of simple calculations to determine dilution by groundwater flow;

Tier 3 involves the use of analytical equations to take account of attenuation, dispersion and sorption; and

Tier 4 involves the use of more sophisticated numerical models to represent contaminant transport.

In deciding whether to move from one model to the next the modeller needs to consider:

- Benefits obtained in analysing the problem using a more sophisticated approach (i.e. a higher remedial target can be justified which may avoid the need for unnecessary and expensive remediation measures);
- Whether the uncertainty in parameter values is so large such that this would overshadow any benefit from moving to a more sophisticated model (as illustrated by Box 5.1).

The improvements in moving to more sophisticated models is not easy to quantify, and such understanding is often something held only by experienced modellers. As long as the conceptual model is not seriously flawed, the improvements may be relatively small compared with the potential inaccuracies in parameters such as hydraulic conductivity, which sometimes may be more than an order of magnitude.

The example below is intended to illustrate the dangers of failing to appreciate which uncertainties are the most important – and directing efforts towards improving a model where they would be better spent on collecting data and staying with a simpler model.

Box 5.1 Example

Suppose we are modelling contaminant movement in an aquifer. We have no pumping test data and only a few measurements of sorption coefficients. The travel time from source to target is estimated to be between 10 days and 10 000 days (based on a simple advection model with retardation, where the uncertainty is dominated by uncertainty in the value of hydraulic conductivity).

OPTION A: We have a more advanced model which simulates retardation (by ion exchange) with the Freundlich isotherm, rather than the usual linear isotherm, supported by extensive measurements of sorption. Using this model at a cost of £10 000, we show that the uncertainty in travel time is over-estimated and that the range of travel should have been 15 days to 6700 days.

OPTION B: We spend the £10 000 on additional boreholes and pumping tests. The results of the pumping tests allow the range in values of hydraulic conductivity to be defined with greater confidence and the calculation of travel time using the simple advection model gives a travel time of between 120 days and 840 days.

Option B provides a more useful reduction in uncertainty for the same investment of money.

It is often the case that one of the complex mechanisms can be modelled analytically, but if two or more are required to be represented together, then a numerical simulation is required.

5.3 General procedure

In choosing the model the following general guidelines should be followed:

- Identify sources, pathways and receptors that need to be represented (e.g. vertical pathway through unsaturated zone);
- Identify the area or domain that needs to be represented;

- Identify processes that need to be represented by the model (e.g. biodegradation, sorption);
- Decide how these processes will be represented mathematically.

The modeller should then evaluate the model in terms of:

- Data requirements and whether sufficient data are available to construct the model (this may indicate that too complex a model is being used in relation to our definition of the problem);
- Can the model allow the source term to be represented adequately, particularly if the source term is known to change with time?;
- Can the model incorporate relevant pathways and receptors?;
- Does the model allow key processes to be represented adequately (e.g. sorption, biodegradation)?;

Good practice is to list each component of the conceptual model that needs to be represented and note how these are dealt with by the model.

For most problems the model will not meet all of these criteria, in which case the following questions need to be considered:

- Is a modelling approach still valid;
- Can the model still be used intelligently by considering just part of the system or through the use of conservative assumptions regarding how the model is used.

The choice of model will be subjective and a function of experience. In practice the modeller will have a number of possible modelling approaches or specific models in mind and will choose the one which best fits the situation.

The modeller will also need to check that:

- The model code has been verified (Section 5.5), if not then this needs to be undertaken and agreed with the regulator, and that the
- Model is acceptable to interested parties.

5.4 Parameter values

The factors that will need to be considered in defining parameter values includes (refer also to Environment Agency 2001b):

- Natural variability of a parameter (e.g. values of hydraulic conductivity will vary both laterally and vertically);
- Uncertainty in the measurement of parameter values (e.g. as a result of sampling method or analytical practice);
- Scale dependency; measurements of a parameter value (e.g. dispersion) may vary according to the scale of the measurement;

- Time; some parameter values will vary with time (e.g. aquifer recharge will vary according to climatic conditions);
- Environmental conditions; some parameter values may vary according to the geological or biochemical environment (e.g. degradation will be dependent on whether the environment is aerobic or anaerobic);
- Limited or no field data; some parameter values will not be known or only a few field measurements will be available, such that an initial estimate may need to be made based on literature values or professional opinion. This assumed value may subsequently need to be revised as part of refining the model to improve the modelled simulation of observed conditions – even if the value remains the same, the significance of it needs to be examined. The determination of the sensitivity of the model results to such parameters should be a critical part of the modelling process and, where it is found to be critical to the model results, then field data should be obtained;
- Discrete measurements of parameter values; parameter values are typically measured at specific points (e.g. boreholes), so measurement needs to be interpolated between boreholes.

The recommended strategy for determining model input parameter values is:

- Review all of the available data. Tables or graphs (histograms) to show the variation in parameter values should be used;
- Define parameter values (see below);
- Document the basis for choosing parameter values. This should include the basis for including or excluding extreme values;
- Consult with regulator and agree ranges of values – the regulator may also have useful information.

This may influence the choice of how parameter values will be defined and whether a deterministic or probabilistic modelling approach should be adopted (Environment Agency, 2001b). The potential options in defining parameter values are to:

- Use best estimate or most likely values (this should be based on some statistical analysis of the available data). If field monitoring data are available, then the model can be refined by adjusting the model parameters to improve the fit (see Chapter 9). If the model provides a close match to field conditions then the confidence that can be attached to the model and model parameter values increases. The disadvantage of using average values is that the natural variability of the system is not taken into account, which may lead to misleading results, particularly if contaminant migration via discrete (more permeable) pathways is a key feature of the system.
- Use worst case parameter values to give conservative model predictions. It is important to think about what the effect of combining different parameters values (are the combinations plausible) has on the model results, including whether the combinations (for example high hydraulic conductivity and high hydraulic gradient) result in unrealistic predictions or misleading results. The use of worst case values also does not necessarily mean that the model results can be interpreted as conservative. For example, worse case values are usually selected as the minimum or maximum value in a data set, however

these data set may underestimate the actual range in values of the population (Environment Agency 2001b).

- Use of a probabilistic analysis, where probability distribution functions can be used to describe the expected variation or uncertainty in a parameter. In this case the model results are described by a probability distribution function that describes the likelihood of a range of outcomes (Chapter 9).

Analytical models require hydraulic and contaminant parameters to be represented by a single value. This requires careful consideration in defining the parameter value. Combining analytical and stochastic approaches provides a means of dealing with ranges in parameter values, but will not represent spatial or temporal variations in parameter values.

Numerical models allow lateral and vertical variations in parameter values to be taken into account, although an average parameter value will need to be defined for each model nodal area, and will generally require interpolation of parameter values between measurement points.

5.5 Model (Code) verification

The mathematical code should be verified, and the modeller should be able to provide confirmation of the following:

- The flow and transport equations are correctly and accurately solved (analytical expressions in textbooks are prone to type-setting errors, some spreadsheet functions can also be incorrect);
- There are no calculation errors;
- The model code is fully operational;
- The computer coding is doing what it is meant to i.e. that the code produces the right result for the equations it is supposed to represent.

The most common and easiest method of verifying a model is to check the model against another analytical or numerical model. This is also good practice in using any new model in understanding and checking what the model does. Analytical models can be checked by observing that the result depends on input parameters in an intuitive way, and that simple problems for which the answer is obvious by inspection are correctly calculated (e.g. does movement cease when the hydraulic gradient is zero?). It is essential to check that the results of any modelling exercise can be reconciled with hydrogeological professional judgement, a process requiring significant hydrogeological experience. The Agency have recently completed a bench marking study for a number of contaminant models (Environment Agency, 2000e).

Part of the consultation with the Environment Agency should be to determine what additional information/ documentation is required to provide verification of the model code. For models such as LandSim and ConSim, this should not be necessary. It is emphasised that the assessment must also consider whether the model is applicable to the problem, that is mathematical models are based on a conceptual model of how contaminants are migrating (i.e. sorption is linear) and this should accord with the conceptual model of the system behaviour.

5.6 Reporting

The choice of mathematical model should be fully documented (see also Chapter 10) including:

i) The objectives of the modelling exercise;

ii) Why a modelling approach is appropriate to achieving the project objectives;

iii) Description of the mathematical model (including relevant references) and why it is considered as an appropriate modelling tool. For models that have been developed by the consultant, then a thorough description of the model (including equations) should be provided together with a copy of the software;

iv) Details of how the model has been verified;

v) Details of how the conceptual model has been translated into a mathematical model, together with a discussion of the significance of any simplifications required;

vi) Details and justification of assumptions and limitations of the model, and how these have been taken into account in interpreting the model results.

The Environment Agency should be consulted to agree what documentation (including model input and output files) should be provided.

6. Analytical Models

6.1 Introduction

Analytical models use exact solutions to the equations that describe the migration of contaminants. In order to produce these exact solutions, the flow/transport equations have to be considerably simplified such that they are typically applicable only to simple flow and contaminant transport systems. Analytical models can be simple formulae, spreadsheets or even sequences of calculations packaged up in a piece of software (for example LandSim and ConSim).

The main advantages of analytical models are:

- Calculation of the result using a calculator or spreadsheet can be very quick. With the aid of a spreadsheet the results of using hundreds of parameter variations can be determined very quickly;
- Since the model can be written down as one, or a few, equations, the dependence of the result on each parameter can be seen clearly;
- Analytical models provide a relatively quick method of examining contaminant transport systems. They can even be used to examine relatively complex systems by making a number of simplifying systems, provided it can be demonstrated that these assumptions do not affect the outcome of the modelling exercise;
- Techniques such as Monte-Carlo Analysis are more easily applied to analytical models than to numerical models, allowing uncertainty in model parameters to be taken into account.

The main disadvantages of analytical models are:

- They require most of the parameters to be constant in space and time (for example horizontal and vertical variations in hydraulic conductivity cannot be taken into account). There are exceptions to this rule but, in general, as soon as a parameter takes different values in different areas, the mathematics becomes too difficult to solve;
- There may not be an analytical solution if the physics is complicated (e.g. if the Freundlich isotherm is thought to control sorption instead of the linear isotherm, then the transport equation becomes too difficult to solve);
- They can generally be applied only to relatively simple flow systems, although by the careful use of simplifying assumptions (e.g. superimposing solutions, Section 6.2.2) more complex systems can be examined. In such cases a supporting argument should be presented to support the approach adopted and why it is reasonable.

Analytical models should be used as the starting point in the assessment and before moving on to more sophisticated numerical models, i.e. they may provide justification that a more sophisticated model would be useful, alternatively they may indicate that our understanding of the system is so poor that modelling is not worthwhile.

6.2 Implementation

The main uses of analytical models are to:

- represent contaminant movement and to predict possible impacts;
- test ideas/hypotheses in the conceptual model, i.e. how far a contaminant plume would be expected to have migrated;
- check numerical models. It is useful to understand the analytical framework of contaminant transport as this will help in understanding more sophisticated numerical models. Numerical models are founded on the same basic equations – simply with variable parameters. Analytical solutions can often be used to check that numerical solutions are producing approximately the right answer. It is very easy to mistype input for complex models and an analytical check (which may require only a calculator and an A4 piece of paper) can generate confidence in the numbers produced.

Analytical models are used at various levels of complexity. At the simplest level, a calculation on a piece of paper is an analytical model using a formula. Examples of analytical models include:

- Simple calculations using calculators;
- Spreadsheet models;
- In-house or commercial programs.

Spreadsheet calculations are also essentially calculations, but the use of spreadsheets has a number of benefits:

- Spreadsheet models are relatively easy to set up and check. However errors can arise through the mis-typing of data and or equations, so it is essential that the spreadsheet should be rigorously audited;
- Good quality graphs can be generated quickly to assist in the presentation and interpretation of results;
- Sensitivity analysis can be carried out easily because spreadsheets allow calculations to be carried out many times;
- Monte-Carlo analysis can be easily incorporated into the spreadsheet though the use of commercially available packages such as @Risk and Crystal Ball.

The categorisation given in the rest of this section divides analytical approaches on the basis of what they actually do, rather than whether they are packaged as calculations, spreadsheets or programs. The three groupings are:

- Simple formulae;
- Superposition of formulae;
- Sequences of formulae.

6.2.1 Simple formulae

The simplest transport model is given in box 6.1 below. This is the basic formula for travel time.

Box 6.1 Example:
The travel time of an unretarded, non-degradable contaminant from a site to a receptor located down hydraulic gradient of the site can be calculated using the following equation:

$$t = xn/Ki$$

where	t	= travel time of contaminant (d)
	x	= distance to receptor (m)
	n	= transport porosity
	K	= hydraulic conductivity (m/d)
	i	= hydraulic gradient

There are a number of basic assumptions associated with this formula:

- Darcy's Law is applicable;
- The aquifer is homogeneous in K and n;
- There is no dispersion (i.e. plug flow);
- The contaminant travels at the same speed as groundwater (no retardation or attenuation).

Nonetheless, this equation is fundamental and should always be the first step in an assessment. A numerical model that uses the above assumptions should produce the same answer (and even if dispersion is included the median travel time should be roughly determined by this formula - or a little slower if transverse dispersion is also included). If it does not, then the numerical model may be flawed and it is necessary to understand why it does not reproduce the analytic solution.

There are a number of more complicated equations (example given in Box 6.2) which can include for:

- The effects of dispersion in one, two or three dimensions;
- Retardation;
- Degradation.

There are a number of strong assumptions associated with these formulae:

- Darcy's Law is applicable;
- The aquifer is homogeneous in K and n;
- Degradation can be described as a first order reaction, i.e. exponential decay;
- Retardation can be described by a linear isotherm;
- The source concentration is constant.

Other analytical solutions exist which allow for injection of contaminant mass and for a declining source term and these can be found in Bear (1979), Domenico (1987), Domenico &

Schwartz (1990) and Fetter (1992). Each solution will have assumptions associated with them, and it is important to understand these and how they could influence the predicted results. Table B2, Appendix B outlines how some of these assumptions can influence the model results.

Box 6.2 Example (Ogata-Banks equation):

The Ogata-Banks equation (Sauty approximation without degradation) is given below:

$$C = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x - vt/R}{\sqrt{4a\, vt/R}}\right)\right]$$

where

C = concentration of contaminant in groundwater at distance x from the source (mg/l)
C_0 = initial concentration of the contaminant (mg/l)
t = time since contamination started (d)
x = distance from source to compliance point or receptor (m)
R = retardation factor
a = longitudinal dispersivity (m)
v = groundwater velocity (m/d)

6.2.2 Combination of equations using the Principle of Superposition.

More complicated problems can be considered by superimposing analytical solutions (as illustrated by the example given in Box 6.3). The principle of superposition does not apply to all equations (for example where the relationships are non-linear), but it does apply to contaminant flow with constant hydraulic gradient. This fact allows us to combine different solutions by adding them together to get more complicated versions.

Box 6.3 Example:

Q. Suppose a contaminant source exists for a period of 10 years and then is removed. Assuming homogeneity and constant groundwater gradient, what is the formula for contaminant strength directly downstream?

A. Use a combination of two versions of the Ogata-Banks equation starting at different times. This formula can be used to assume a source starting at time t = –3650 days. If we assume another, negative source, starting at time t = 0, then the two cancel out after time 0.

$$C = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x - v(t+3650)}{\sqrt{4a\, v(t+3650)}}\right) - \operatorname{erfc}\left(\frac{x - vt}{\sqrt{4a\, vt}}\right)\right]$$

The same principle is used in pumping test analysis to calculate recovery pressures curves and to simulate boundary conditions using "image wells".

6.2.3 Sequences of formulae

These types of analytical model involve calculations involving a series of formulae, each depending on the results of one or more of the previous formulae. These sorts of models can become complicated involving flow charts and if-statements. LandSim and ConSim are examples of these sort of analytical models. In these models, the calculations are divided into "modules" which cover the source term, the containment barrier, the unsaturated zone, the saturated zone and the receptor.

6.2.4 Note on Semi-Analytical Models

The term 'semi-analytical' is often used in describing modelling software. Its usage has become confused (so the term has been generally avoided in this document), but usually refers to one of the two variants below:

- The situation where the formula is not explicit. A non-explicit formula is one that cannot be tapped out on a calculator. It may involve an infinite series or an integral or simply a formula that is not fully solved (i.e. an unknown parameter occurs more than once in the formula). The final solution must use numerical methods to solve the equation (e.g. integration, numerical integration or an inverse Laplace transform). However since the method is still essentially analytical, parameters that vary in space can seldom be modelled.

- Models that allow the complicated superposition of a number of equations (as in 6.2.2) also frequently call themselves semi-analytical. The program, QuickFlow, for simple flow problems, is an example of this type of model.

LandSim and ConSim qualify as semi-analytical under the first definition in the sense that both use a complicated formula that is not explicit in one module (the aquifer transport module) if the declining source term is used. Otherwise they are in fact a sequence of formulae with Monte-Carlo analysis.

6.3 Data requirements and selection of parameter values

For most analytical models a single value of each of the aquifer parameters is required for the entire area of interest. These parameter values should be established as part of the conceptual model. If a spatially variable pattern or trend can be established, then an analytical model may not be appropriate

The detailed data requirements depend on the model used. An example is given below of the data requirements for the use of the Ogata-Banks equation with retardation. The assumptions are also discussed.

Box 6.4 Example:

An area of contaminated ground produced a leachate containing benzene from 1980 until 1990. The aquifer beneath is a thin layer of sand, homogeneous with a roughly constant saturated thickness. Estimate the graph of concentration against distance for benzene 10 years after (i.e. in year 2000) assuming the contaminant is retarded but not degraded. The Ogata-Banks equation (superposed with the negative source after 1990) is given below:

$$C = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x - vt_S / R}{\sqrt{4a\, vt_S / R}}\right) - \operatorname{erfc}\left(\frac{x - vt_F / R}{\sqrt{4a\, vt_F / R}}\right)\right]$$

where;

C = concentration of the contaminant in the groundwater at distance x from the source (mg/l)
C_o = initial concentration of the contaminant in the groundwater at the source (mg/l).

The initial concentration has been estimated using the following equation:

$$C_0 = \frac{L \cdot I \cdot A}{(A \cdot I) + (w \cdot b \cdot K \cdot i)}$$

L = leachate strength (mg/l)
I = infiltration rate (m/d)
A = area of contaminated soil (m^2)
w = width of source(m)
b = mixing zone thickness (m)
t_S = time since contamination started (=7300 d) and
t_F = time since contamination finished (=3650 d).
x = distance (m)
R = retardation factor = $1 + \frac{K_d \cdot r}{n}$
K_d = partition coefficient (ml/g)
r = bulk density (g/cm^3)
a = longitudinal dispersivity (m)
v = groundwater velocity (m/d) = $\frac{K \cdot i}{n}$
K = hydraulic conductivity (m/d)
i = hydraulic gradient
n = effective porosity

This equation can be solved using a calculator and an error function table or programmed into an EXCEL spreadsheet. Parameter values will need to be defined for eleven parameters L, I, A, K, i, b, n, K_d, r, a, t and x.

The analytical solution represents an initial useful approach, as a range of contaminant processes are represented namely advection, dispersion, retardation and a change in the source term. However in using this equation a number of assumptions are required.

Some of the weaker assumptions in this analytical approach are listed below:

- Benzene may have taken a significant time to pass through the unsaturated zone and this may not have been a continuous source over the ten year period;
- The contaminant source can be represented as a line source;
- Instantaneous mixing to total depth of the aquifer has been assumed (probably acceptable if the aquifer is thin, but almost certainly not valid if the aquifer is thick);
- Assumed that the distribution coefficient follows a linear isotherm (unlikely to be true where contaminant concentrations are significant);
- Assumed homogeneity in aquifer parameters. However, this will rarely be the case and the conceptual model will need to consider whether the length-scales over which the heterogeneities occur are of importance to the problem being investigated;
- It has been assumed that benzene does not degrade (this would be a conservative assumption in fully aerobic conditions, however it may be realistic where the oxygen supply or nutrient availability is limited). The assessment may conclude that further analysis taking account of degradation would be warranted. This would need to include site-specific data relevant to degradation, e.g. pH and redox conditions.
- Transverse dispersion has been neglected; although this is a conservative assumption since some of the contamination will have moved sideways.

The above points illustrate some of the uncertainties in undertaking fate and transport modelling including:

- Our conceptual understanding of system behaviour, e.g. is degradation occurring;
- The ability of the mathematical model to represent system behaviour, e.g. retardation has been represented using a linear isotherm, whereas laboratory testing may have indicated a non-linear isotherm;
- Definition of parameter values, e.g. an average value for hydraulic conductivity may have been assumed, but there may be some evidence that high permeability pathways may influence contaminant transport.

The key will be deciding whether these assumptions are important and how they could influence decisions made on the basis of the model results.

6.3.1 Good Practice

Experimentation with analytical equations to examine the influence of changing parameter values on the model results is a vital exercise to gain an understanding of which are the key, i.e. most sensitive, parameters and to identify incorrect conceptual models. This experimentation should normally be undertaken using the credible range of values. A sensitivity analysis represents a more rigorous approach to this assessment (chapter 9). For example, experimentation with the Ogata-Banks equation will illustrate that the most sensitive parameters are usually K, K_d and, in the case of fissured aquifers, the transport porosity, n. This assessment may show that the level of uncertainty in the model parameters results in considerable uncertainty in the predictions i.e. the assessment may show, depending on the choice of value whether breakthrough occurs or not at the receptor. Clearly in this case, the next step should be to collect more data to reduce the parameter uncertainties, rather than try and reduce the model uncertainties by developing a more advanced model.

7. Numerical Models

7.1 Introduction

Numerical models allow more complex systems to be represented than can analytical models, providing approximate solutions to the equations governing contaminant transport. Numerical models still require simplifications to be made about system behaviour.

The development of a numerical model should represent the last stage in a contaminant problem, i.e. only when an understanding of the system behaviour has been developed through the use of analytical models and where it can be demonstrated that the use of a numerical model will be beneficial. The application of a numerical model should also be dependent on a robust conceptual understanding of the problem and the availability of adequate data. Numerical models are relatively time consuming and costly to construct and should not be used as an alternative to data collection. For this reason, the application of a numerical model will be undertaken only in a limited number of cases

In distributed numerical models, space and time are divided into discrete intervals (as illustrated by Figure 7.1 and 7.2) where for each model grid cell, parameter values are defined including hydraulic conductivity, porosity, aquifer thickness, initial contaminant concentration etc.

The main advantage of numerical models is that different parameter values can be assigned to each cell, such that lateral and vertical variations in property values can be taken into account. The geometry of the model can also be designed to reflect the geometry of the system to be represented. In addition, models can be constructed as more than one layer to allow multi-layered aquifers to be represented. For time variant models, model inflows (e.g. recharge and its contaminant concentration) and outflows (e.g. groundwater abstractions) can be specified for each model time step.

Numerical models will generally be applicable where:

- Previous modelling studies using simple analytical models have shown that a more sophisticated approach such as incorporating spatial variability is required;
- The groundwater regime is too complex to be robustly represented by an analytical model;
- Processes affecting contaminant transport cannot be readily represented by simple equations;
- An analytical model is inadequate for the design of mitigation measures, e.g. in determining the optimal location and pumping rate for boreholes in a pump and treat scheme.

Numerical models should be considered where the scale and importance of the problem warrants the use of a more sophisticated approach. For such sites the scale of the problem should demand detailed investigations which should provide sufficient information to allow the construction of a numerical model.

The use of a numerical model will require technical expertise in groundwater and contaminant movement, together with specialist and detailed investigations to define the flow regime and contaminant transport processes.

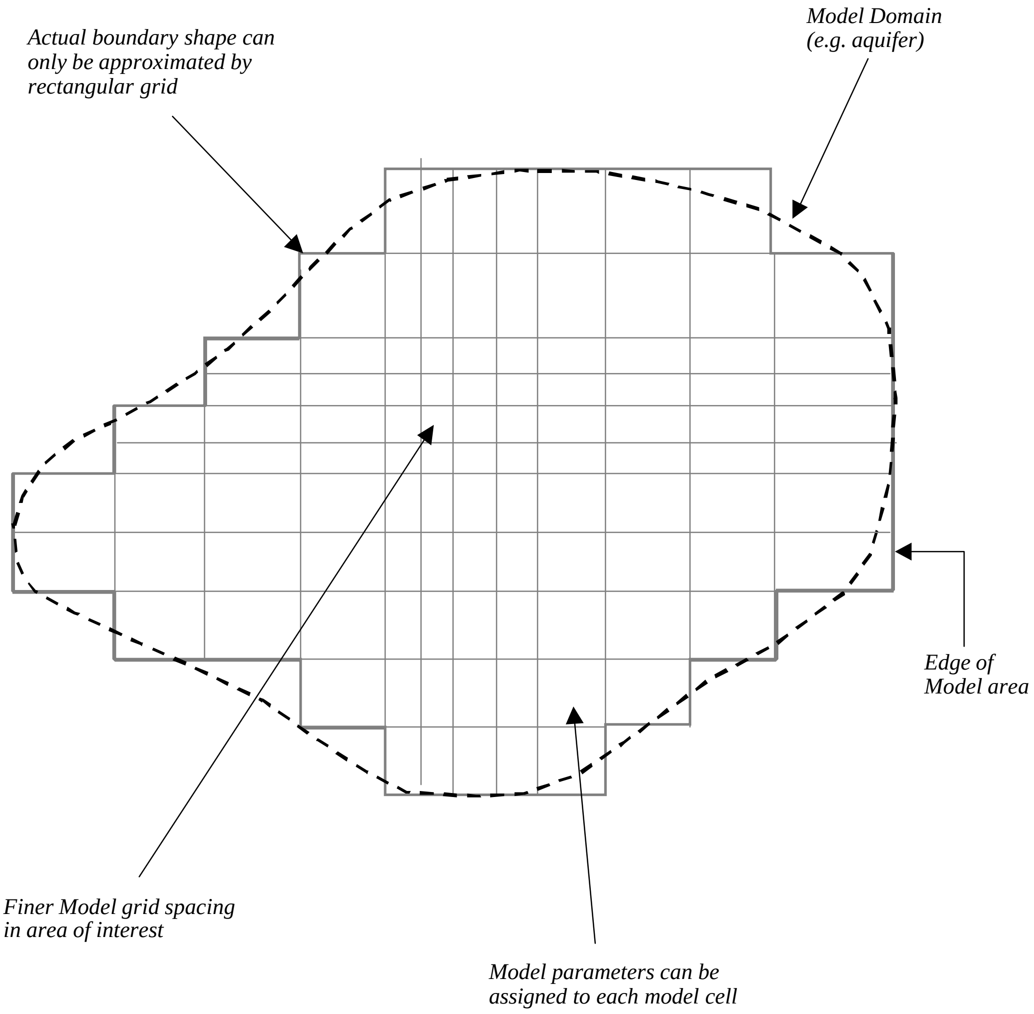


Figure 7.1 Example of a Finite Difference Grid

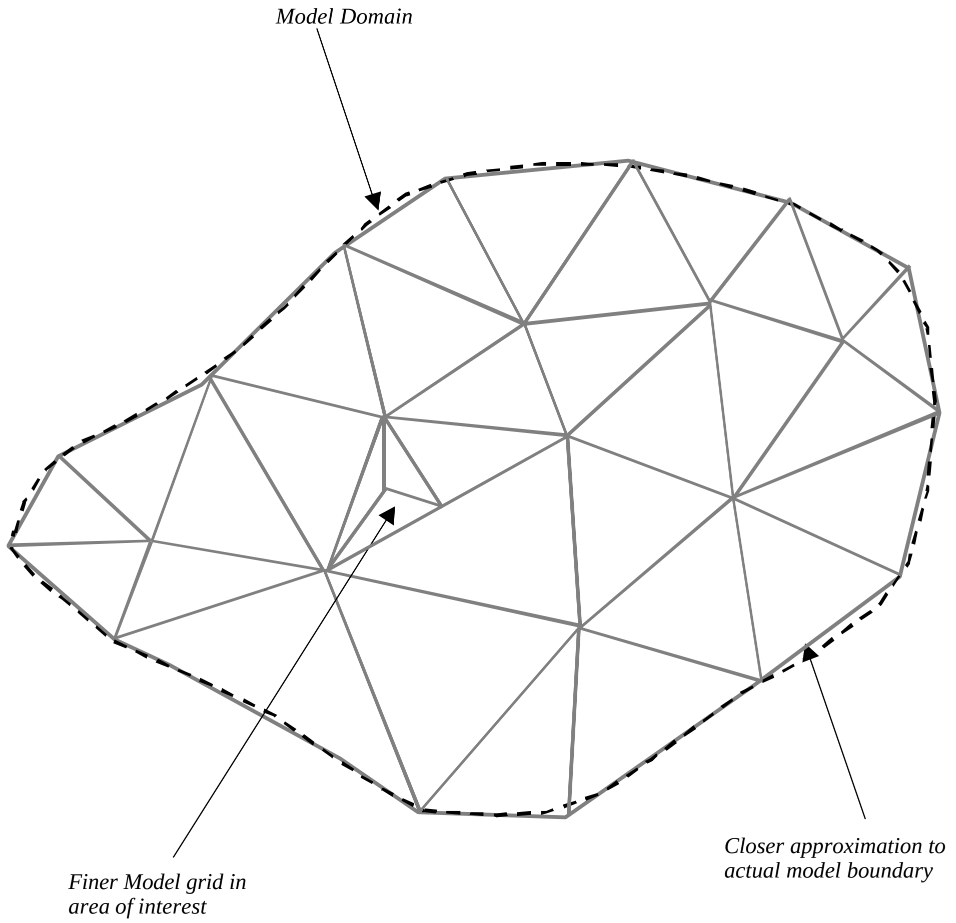


Figure 7.2 Example of a Finite Element Grid

In comparison with an analytical model, the advantages of using a numerical model include:

- They provide more powerful tools to help in representing and understanding contaminant transport because more aspects of the system behaviour can be represented. It should be noted that numerical models still require a number of assumptions or simplifications to be made about the system behaviour;
- A higher degree of confidence can be attached to the model where it has been able to simulate observed groundwater flow and contaminant transport with time (this is assumes sufficient field observations are available).

The main disadvantages are:

- Time and cost involved in setting up and running the model;
- The tendency to believe that the model and the results are correct, because a numerical model has been used even though there may be considerable uncertainty about the system.

Numerical models must be first applied to the groundwater flow system since this determines the advective component of transport. When this is satisfactorily modelled, the model can then be extended to include contaminant transport. Unless the model can provide a realistic simulation of groundwater levels and discharges, it is clearly inappropriate to use the model to simulate contaminant transport. Where it fails to represent the field conditions adequately, it points to the need to review the conceptual model and modelling approach, and to decide if further data collection is needed. It is important that the modeller should consider why the mathematical code is failing to represent field conditions.

A number of model codes (e.g. MT3D, MOC), are designed to be used in conjunction with a groundwater flow model (e.g. MODFLOW). For problems where the effects of density variation are significant, the solution of the flow and solute equations needs to be coupled together (Zheng & Bennett, 1995).

Numerical contaminant fate and transport modelling (i.e. the nuts and bolts) is covered in detail by a number of text books (Section 7.4). It is not the purpose of this document to provide a description of numerical models, but to highlight the key features that need to be considered.

7.2 Types of numerical model and numerical techniques

There is a wide range of numerical codes and solution techniques available to solve the equations describing contaminant transport. Box 7.1, provides a brief description of some of the main types of code. The numerical solution methods for contaminant transport require a solution of the flow field, which can be obtained using finite element, finite difference, or the less used integrated finite difference and boundary integral equation methods (see Box 7.1). The contaminant transport solution can be used for either steady state or time variant flow fields.

A number of solution methods have also been developed to solve the contaminant transport equations; Box 7.2 provides a brief summary.

The choice of whether to use a finite difference or finite element model will generally be a matter of personal preference.

Box 7.1 Types of numerical model

Finite Difference is the most commonly used approach in numerical modelling. For most finite different models the space and time co-ordinates are divided on a rectangular grid, and model parameters (hydraulic conductivity, aquifer thickness) are specified for each model grid cell. Wang & Anderson (1982) and Zheng & Bennett (1995) provide a description of this method. The flow and transport equations are solved by direct approximation. The grid spacing represents the degree of accuracy of the model in representing lateral or vertical changes in the property values that describe the system. Finite difference methods have the advantage in being relatively simple to use, but have the disadvantage of not accurately representing irregular boundaries and it is also difficult to change the grid spacing to provide greater precision in areas of interest.

Finite Element Method. The spatial domain is divided into a mesh of elements, generally of triangular or quadrilateral shape. The variation in a model parameter across the model element is normally approximated by a polynomial function. This technique provides greater flexibility than finite difference methods in representing the model domain, particularly complex geological boundaries. The model mesh can be easily modified to provide greater precision in areas of interest although complex meshes require software tools for their management. Finite element models are less susceptible to numerical dispersion than finite difference models (Zheng & Bennett, 1995), but for the same number of elements/cells the computing cost is higher.

Other methods include the integrated finite difference method and the boundary integral equation method (Zheng & Bennett, 1995).

The method of transport calculation depends on the approach to the co-ordinate system i.e. Lagrangian (the particle is fixed in relation to a moving co-ordinate system) or Eulerian (the particle moves in a fixed co-ordinate system) or a hybrid (i.e. a combination). The choice of solution technique (Method of Characteristics, random walk etc) is important and depends upon whether we have an advection-dominated system or a dispersion dominated (i.e. low permeability) system.

7.3 Grid spacing and time step

Distributed numerical models require the model area or domain to be divided into a polygonal grid. For each model grid cell, parameter values (e.g. hydraulic conductivity, porosity need to be defined). This allows the lateral and vertical variation in parameter values to be taken into account. However, dependent on the grid spacing, an individual model node can represent an area of hundreds to thousands of square metres. Since the variation in a parameter value is likely to be at a smaller scale, then an average value will need to be determined for the grid cell area.

The grid and time discretisation will determine:

- The ability of the model to describe variations in system behaviour (e.g. variation in hydraulic conductivity);
- The data requirements for the model; these increase the finer the model grid and time discretisation;

- Computer memory and model run time requirements; these increase with the fineness of the model grid and time discretisation;
- Numerical dispersion. The coarser the discretisation of space and time, the greater the likelihood of model instability.

The model grid and time step will always be a balance between the above factors. In an ideal study, the effect of grid spacing will be subjected to sensitivity analysis, but because of the considerable effort to do this the test is seldom made, relying instead on an assessment of the likely effects of grid spacing by other means, such as calculation of the maximum grid Peclet number (Appendix C).

A common problem in setting up and running a numerical model is in preventing or minimising numerical dispersion. Figure 7.3 illustrates the effect of numerical dispersion. Numerical dispersion can be minimised by a number of methods:

- Decreasing the model grid spacing and time step to minimise dispersion particularly for models that are solved by Eulerian methods (Appendix C), although this will increase model run times;
- Choice of the solution method; for example, Lagrangian methods are less susceptible to numerical dispersion;
- Choice of initial or starting conditions;
- Choice of convergence criteria for the model.

The change in grid spacing and time step will also need to be designed carefully as changes in the grid spacing can result in model instability. In general, the change in grid spacing from one row or column to another should be less than a factor of 2 (a multiplier of 1.5 is typically recommended in the supporting documentation to codes). Changes in the model time step can also result in model instability. Most codes will provide guidance on the appropriate time step.

A key part in reviewing the results from numerical models is to check the:

1. Mass balance: Errors in the mass balance provide evidence of numerical instability;
2. Time series: Oscillations in predicted contaminant concentrations with time may indicate instability;
3. Contaminant distribution: Anomalies in contaminant distributions may also indicate instability.

Box 7.2 Solution methods

Particle Tracking Models represent contaminant movement (see Lagrangian methods below) by tracking the movement of particles through the groundwater flow field.

Eulerian Method involves approximate solutions to the equations governing contaminant transport by advection and dispersion. These methods can be subject to numerical instability, artificial oscillations and numerical dispersion when compared to exact analytical solutions. These problems can be minimised by using a finer model grid and time step, but this will increase model run times. The **Peclet** and **Courant** numbers provide a means of designing the model grid to minimise numerical dispersion (Appendix C). Solution techniques have also been developed, such as the Crank-Nicholson Method, to minimise numerical instability. The amount of numerical dispersion can be estimated based on the model grid size and time step. A 'fix' that is sometimes used is to set dispersion to zero, but to modify the time step and grid size such that the numerical dispersion generated by the model will be roughly equivalent to the expected physical dispersion. This approach is a 'fix' and the model results should be interpreted with care, i.e. the spreading of the modelled plume is a result of numerical dispersion. The Eulerian method is particularly prone to numerical instability when applied to advection dominated equations, but provides a better solution where dispersion dominates. Examples of code that use this method include SUTRA, CFEST, SWIFT.

Lagrangian Method represents contaminant transport by a large number of moving particles to avoid solving the advection transport equation. The method is free of numerical dispersion, although numerical problems may be associated with irregular grids or contaminant sources or sinks. The method is most suited to problems where advection dominates contaminant transport. The effect of dispersion is dealt with by adding a random displacement **(Random Walk)** to the particle location after each advective movement or time step.

Contaminant concentrations are calculated based on the density of particles within each model cell. Sorption and decay are represented by adjusting the velocity and mass of the particles. The model accuracy is dependent on the number of particles used, although this will also affect model run times. An element of trial and error is required to determine an optimum number of particles, although some models will provide guidance on the number of particles. Examples of models that use this technique include RANDOM WALK, PLASM, INTERTRANS.

Mixed Eulerian - Lagrangian Approach. This method combines the advantages of these two techniques and uses the Lagrangian approach to solve the advection term and the Eulerian approach to solve the dispersion term. The Method of Characteristics (MOC), the Modified Method of Characteristics (MMOC), and the Hybrid Method of Characteristics (HMOC) are examples of this approach.

Method of Characteristics (MOC) uses a particle tracking technique to solve the advection term, but is different in that each particle is assigned a concentration equal to that of the cell in which it is located. At each time step the concentration of each particle is recalculated according to the concentration field. Two approaches are used in the method of characteristics. The first is where a uniform number of particles is used across the model grid (the concentration assigned to each cell will vary from one cell to another). The second is where the model distributes particles between the model cells, such that the highest number are placed in regions of sharp contaminant fronts. The latter method improves computational efficiency. An element of trial and error is required in setting up the model in terms of the number and distribution of particles. The method has the advantage of being relatively free of numerical dispersion. The main disadvantage of the technique is that it is not as computationally efficient as Random Walk methods and errors in the mass balance may occur as the solution technique is not entirely based on the principle of mass conservation. Examples of models include MOC, MOCDENSE, BIOPLUME, MT3D.

Particle tracking and random walk methods can be done on analytical flow fields.

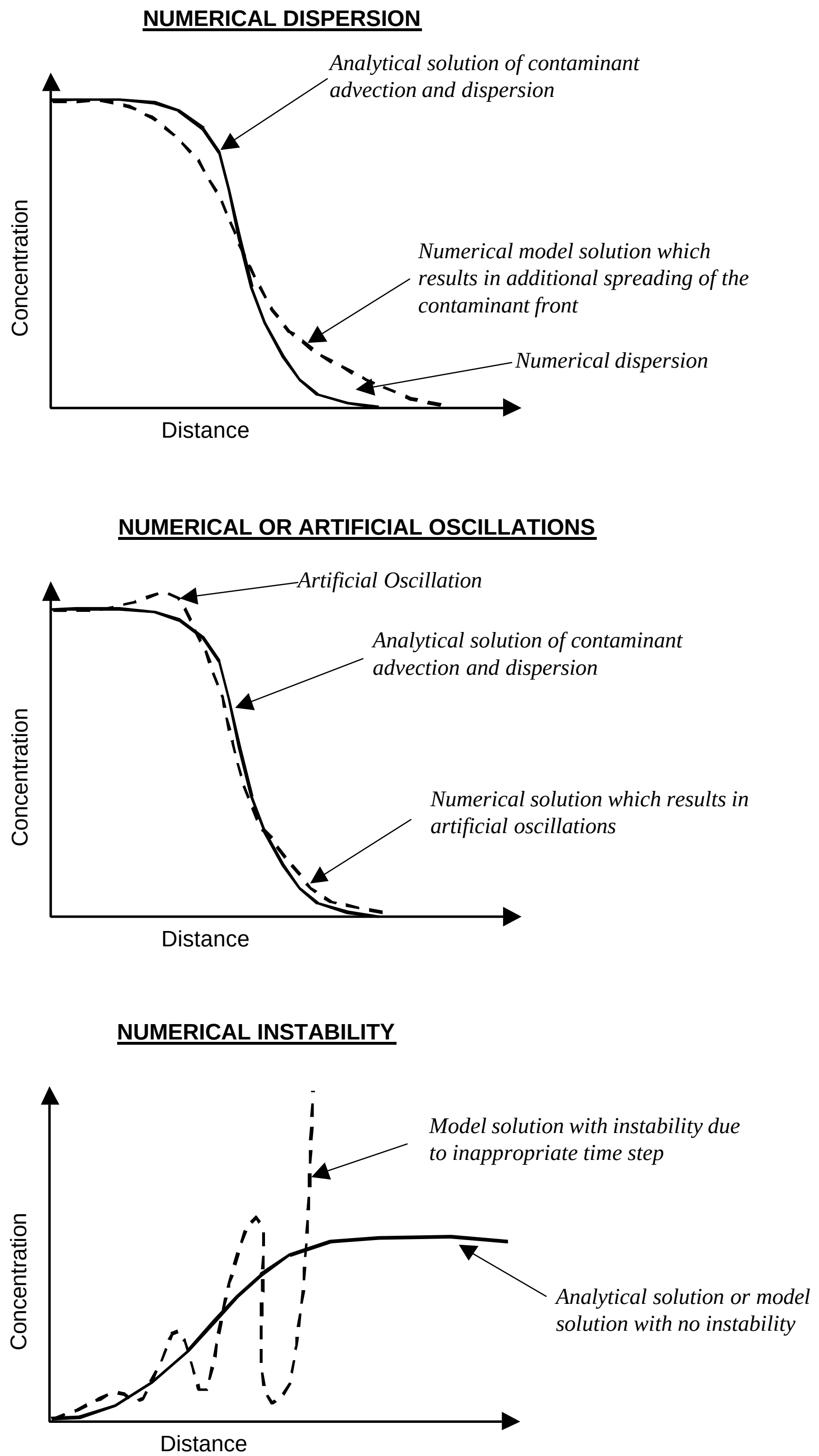


Figure 7.3 Illustrative examples of numerical problems

7.4 Data requirements

The data requirements for distributed numerical models can be considerable depending on the number of model cells, and whether the model is used to simulate steady state or time variant conditions. For each model cell it may be necessary to define:

- Aquifer parameters (hydraulic conductivity, aquifer properties etc);
- Transport properties (transport porosity, dispersion etc);
- Initial contaminant conservative.

The number of cells can vary from 100's to 1000's with the need to define parameter values for each cell. No site will ever have sufficient data to define values for each cell, such that the modeller will need to make judgements as how to distribute field measurements from the model grid.

7.5 Useful references

Numerical models can range from relatively simple one-dimensional to three-dimensional codes and can consider advection, dispersion, retardation, biodegradation, multiphase flow and density.

In selecting a numerical model, the following factors need to be considered:

- What processes need to be represented, e.g. advection, dispersion, linear and non-linear sorption, first order decay, variable density;
- How are these processes simulated, e.g. linear or non-linear sorption, first order decay and reaction limited biodegradation (usually oxygen, but possibly nutrient supply);
- Solution technique (e.g. Eulerian, Lagrangian) and is this appropriate to the flow field;
- Number of model layers;
- Steady state or time variant conditions;
- Pre/post processors.

Details of numerical models are not been provided in this text, however, the reader is referred to the following references: Zheng & Bennett (1995), NRA (1995b), IGWMC (1991), van der Heijde (1993), Anderson & Woessner (1992), Spitz & Moreno (1996) and Bear & Verruijt (1987). In addition recommended web sites include:

United States Geological Survey (www.usgs.gov)

ASTM (www.ameritech.co.uk)

United States Environmental Protection Agency (www.epa.gov)

8. Model Design

8.1 Constructing the model

The basic steps in constructing a mathematical model are summarised in Figure 1.1. It is not the purpose of this document to provide details of how to set up and construct a model as this is more than adequately covered in many text books (e.g. ASTM (1994a) and (1994b), Bear & Verruijt (1987), Spitz & Moreno (1996), Zheng & Bennett (1995), Anderson & Woessner (1992)). A further key reference is the Environment Agency report ‘Strategic review of groundwater modelling guidance notes’ (Environment Agency, 2001c) which provides guidance on the appropriate use of all types of model. In addition, the supporting documentation for most models (e.g. MT3D, ConSim, LandSim) provides the relevant information on how to set up and run the model.

It is essential that a code should not be used as a black box, but that the modeller should understand how the code represents transport processes and what are the main assumptions behind the code. Experimentation with the model to determine how changing different parameters influence the model results is recommended.

8.1.1 Model domain and boundary conditions

The first stage in model construction is to define the area or domain of interest, i.e. the region of the system to be represented by the model. All models require the model domain to be specified, and the following criteria will determine the model domain:

- Source and area of contamination;
- Location of receptors;
- Presence of natural boundaries, such as the edge or limits of the geological formation or aquifer, faults, rivers, groundwater catchment divides.

These factors should have been defined as part of the conceptual model.

There are a number of different types of boundary condition that can be specified in a model in terms of flow and/or contaminant flux (see Box 8.1), including constant head, constant concentration, specified contaminant flux, and no flow, ASTM (1994a) and (1994b), Zheng & Bennett (1995). Examples of boundaries include a river fed by the aquifer, solution of contaminants into groundwater from a NAPL source. Boundaries may be specified at the edge of the model (external boundary) and within the model area (internal boundary).

Numerical models provide the greatest flexibility as irregular boundaries can be readily incorporated. For analytical models, the choice of possible domains is restricted and may be infinite or semi-infinite.

Boundary conditions can have a significant effect on the model results, and consequently the location and type of boundary condition needs to be selected with care. The influence of the boundary condition on the model results should be evaluated including:

- Examining the influence of moving the boundary location;
- Examining the influence of different contaminant release histories on model output;

- Checking modelled inflows or contaminant fluxes from constant concentration or specified flux boundaries.

8.1.2 Steady state or time variant conditions

Models can be run as steady or time-variant simulations. There are various types of simulation that can be considered:

- Steady-state transport problems where groundwater flow and contaminant concentration do not change with time;
- Steady-state groundwater flow where groundwater heads will not change, but the model will calculate changes in contaminant concentrations with time;
- Time-variant models where groundwater flow and contaminant concentrations will be calculated as a function of time.

The initial conditions, e.g. groundwater heads and contaminant concentrations will need to be defined. These may be based on background quality or on the observed contaminant distribution (plume geometry). The assumed starting condition (numerical models) can have a significant influence on the model results, particularly in high porosity aquifers. Examination of the influence of the starting conditions should form part of the model refinement and sensitivity analysis, particularly where there is some uncertainty on definition of the contaminant plume.

Inflows (e.g. recharge rate and concentration, flows from rivers) and outflows (e.g. abstraction, flows to rivers, springs) will also need to be defined. Where the model is used to represent time variant conditions, changes in these flows with time will need to be defined.

8.1.3 Model input parameters and physico-chemical processes

The physico-chemical properties of the aquifer (i.e. hydraulic conductivity, porosity), the pore fluid and the contaminant will need to be defined in setting up the model. These values should be defined as part of the conceptual model. Section 5.6 provides guidance on determining parameter values.

Box 8.1 Types of boundary condition - numerical models

Flow boundary conditions

1. **Constant head.** The head within a cell is specified and remains fixed during the model simulation. The cell acts as either a sink in removing water from the model or as a source in adding water to the model depending on the water levels within the model relative to the fixed head. The main problem in specifying fixed head cells is that an unrealistic volume of water could be added to or lost from the model. Inflow or outflow from the constant head cell to the adjacent model cells is usually controlled via a hydraulic resistance.

2. **Specified flow.** The flow into or out of the model is specified at this boundary.

3. **No flow** No component of groundwater flow across them and they are used to represent impermeable boundaries, groundwater catchment divides, or groundwater flow lines.

Mass transport boundary conditions

1. **Constant concentration** (referred to as the Dirichlet condition). The contaminant concentration of a cell on the boundary or within the model remains fixed during the model simulation. The cell may act as a sink in removing solute mass from the model or as a source in adding solute mass to the model. The dispersive flux is calculated based on the difference in concentration between the boundary cell and the adjacent internal cell and is directly analogous to the flow of water from a constant head cell. There may also be an advective component, if flow occurs at that boundary in the flow model. An illustration of this boundary condition is that the dissolution of contaminants from a NAPL plume could be specified as a constant concentration boundary. The main problem in specifying fixed concentration cells is that an unrealistic mass of contaminant may be added to the model (which may far exceed the actual contaminant source). The mass balance for the model should be reviewed to check on contaminant fluxes into and out of the model.

   The assumption of a continuous contaminant source in an analytical model is analogous to a constant concentration boundary.

2. **Specified concentration gradient** (referred to as the Neumann condition). This boundary considers the dispersive flux only and is dependent on the specified concentration gradient and dispersion coefficient. Typically the dispersive flux at a model boundary is small and this condition is rarely used.

3. **Specified concentration and concentration gradient** (referred to as the Cauchy Condition) The dispersive and advective fluxes are specified. The advective flux is calculated based on a specified concentration and flow rate.

4. **Impermeable boundaries** (no flow boundaries in groundwater flow models) are special cases of the Neumann or Cauchy boundary condition where the advective and dispersive flux is zero.

8.2 Defining acceptance criteria

The acceptability or validity of a model should be based on demonstrating that it can adequately simulate field observations (e.g. measured contaminant concentrations). The model design should include:

- Identifying the field observations against which the model should be checked. This will be based on what field data are available. At a later stage, the model may be used to identify future monitoring points to validate model predictions;
- Determining an acceptable range or how close the model results need to be (e.g. within an order of magnitude, within ∀20% etc.), such that the model can be considered to be an acceptable simulation of the system behaviour. This range should be based on the observed behaviour i.e.:
    - Long-term trends;
    - Seasonal range;
    - Concentrations at monitoring points.

The acceptance criteria will vary depending on the nature of the problem, but should be agreed with the regulator.

8.3 Review of model limitations and simple checks

In developing and using the model, the assumptions made in setting up the model and the limitations of the model should be documented and routinely reviewed to check that conclusions drawn from the model are realistic and applicable to the site.

The following checks should be made (these are dependent on the type of model):

- Examination of the water balance (i.e. difference between the modelled inflow and outflow) may identify:
    - errors in the model calculations;
    - failure to converge;
    - incorrect choice of boundary conditions such that too much water may be entering or leaving the system.
- Examination of the solute mass balance for a model as this may identify:
    - errors in the model calculations;
    - evidence of numerical dispersion;
    - evidence of non-convergence of the model;
    - incorrect choice of boundary conditions such that too much contaminant may be entering the system;
    - the contaminant mass or flux is inconsistent with the observed contaminant mass in the aquifer or the with the original spill volume;

- The model has converged, e.g. the model equations have been solved to the expected degree of accuracy. For numerical models, failure to converge will normally relate to insufficient numerical precision in model calculations and will often be evident in the model water or solute mass balance. In these cases the solver parameters (number of iterations, convergence criterion) should be checked. For probabilistic models (e.g. a Monte Carlo simulation) if too few model realisations are undertaken, then a different result may be obtained each time the model is run.
- Model accuracy, for example is the grid spacing or the time step acceptable in terms of definition of the system and in minimising the potential for numerical errors. Grid spacing is particularly important for particle tracking models.
- Parameter values have been correctly entered into the model.
- The initial model results are physically reasonable and comparable with simple analytical calculations.

Table 8.2 Summary of Basic Model Checks

Parameter	Comment
Model convergence	Numerical precision or instability. Repeatability of model results. Acceptable water and solute mass balance errors.
Parameter values	Plausible when compared with field or literature values, incorrect data entry, extrapolation or averaging of data sets over the model area.
Boundary conditions	Correct or appropriate boundary conditions, influence of boundary on model results, particularly constant head or concentration boundaries.
Initial conditions	Available data may be limited to defining starting conditions. Incorrect initial conditions may affect model results, particularly for aquifers characterised by high effective porosity.
Model code	Equations and calculations are correct.
Model grid spacing*	Definition of system, such as spatial variation in hydraulic conductivity, numerical errors e.g. numerical dispersion.
Time step*	Definition of system, such as transient changes of recharge, numerical errors, e.g. numerical dispersion.

*Numerical models only

9. Model Refinement, Application and Review

9.1 Introduction

In developing the conceptual and mathematical model a number of assumptions and simplifications will have been made about the system and how it is represented mathematically. In addition, the model parameter values will not be known with certainty. It is important, therefore, that the model should be tested against field observations. The confidence that can be attached to a model will be very dependent on the extent to which it has been tested and whether it agrees with field observations. In most cases, the model parameters will need to be adjusted or refined, so that the model produces results that agree with field conditions. This is referred to here as model 'refinement' rather than 'calibration'. This is because in the United Kingdom, considerably more thought and effort is expended in producing a model which best represents the long-term, seasonal and short term flow behaviour of the spatially distributed groundwater and surface water system than merely the best fit implied by the term 'calibration' (Environment Agency, 2001c). Where the model output differs from the observed data the conceptual and the numerical model are revised. Any such change to a model parameter will need to be justified, i.e. is this parameter still credible compared with field measurements. It is important that all modifications made to the model during refinement, including reasons and outcomes, are fully reported. This should include those modifications that are rejected. The model can subsequently be checked by comparing the model results with additional field observations (i.e. ongoing monitoring).

Model verification. Confirmation that the model code is correct in solving flow and transport operations, i.e. that outputs follow correctly from inputs. Typically the model results are compared with the results from analytical solutions and other accepted codes to check agreement.

Model refinement. The adjustment of model input parameters so that the model produces results which agree with field observations to the required degree. All credible historical data should be used. This process should be a critical review of whether the assumptions incorporated into the conceptual and mathematical models are valid, how accurately does the model fit with observed data, and are the model parameters used to obtain a best fit credible. Where the model provides a poor approximation to field observations, then the modeller should be prepared to reject or revise the conceptual and/or mathematical model. The mathematical model should be updated as more data become available to confirm that it continues to simulate observed behaviour.

A sensitivity analysis (Section 9.4) should be undertaken to determine which parameters have the most influence on the model results, so that the modeller can decide whether further information is required.

For some model applications, it is not possible to check the model against field observations, e.g. in evaluating the impact of a proposed activity such as a landfill site that could give rise to pollution of groundwater. In such cases, the model results should be used with care and the use of probabilistic analysis is particularly important to take account of the uncertainty of model parameters.

It is noted that even though a model may provide an acceptable representation of the observed conditions this does not mean that the model is correct. For example, the model may simulate observed contaminant concentrations at a particular time, but fail to simulate the subsequent migration of the plume. It is also important to note when comparing the model result to field data, that there are usually a number of possible combinations of parameter value that can give the same model result, i.e. the solution is not unique. Typically the process of model refinement will be an iterative or ongoing process, where model parameters are continually refined as further data become available. At the same time the conceptual model should be updated.

The modeller should always keep in mind that the mathematical model and the conceptual model on which it is based, is uncertain and built on a number of assumptions, i.e. our knowledge of the system and our ability to represent it is imperfect.

9.2 Methods of refinement

The data requirements for model refinement will depend on the objectives and type of model. Examples of the information that can be used to check a model are given in Table 9.1. The development of a fate and transport numerical model is often a two-stage exercise comprising firstly, modelling of groundwater flow conditions and secondly modelling of contaminant migration.

Flow models can be tested against:

- Absolute water levels;
- Groundwater flow directions;
- Horizontal and vertical hydraulic gradients;
- Variations in groundwater levels and spring flows with time (for most models it is important to simulate maximum and minimum groundwater level conditions);
- Recession in groundwater levels and spring flows;
- Gains or losses in stream flows due to interaction with the aquifer.

Transport models can be checked against:

- Spatial variation in contaminant concentrations, including plume geometry;
- Changes in contaminant concentrations with time;
- Contaminant breakthrough or arrival times.

Throughout this exercise the modeller should continually review the results in the light of the limitations of the definition of the system behaviour and the assumptions used in representing this system mathematically. (i.e. we can obtain a fit by changing a parameter value, but is this realistic in terms of field measurements and our conceptual understanding of the system).

Refinement can be undertaken by manual (trial and error) or automatic techniques (often referred to as inverse modelling). Manual techniques are the most commonly used and are the recommended approach. They should be performed by an experienced modeller. The process involves:

i) Changing a parameter value;

ii) Examining the effect of this change on the model results;

iii) Readjusting the parameter value based on the previous result to improve the model simulation of observed conditions, whilst making sure that it is still realistic (i.e. within the range determined from field testing, literature values etc);

iv) Assessment of whether the model provides an acceptable fit of observed conditions or is further data collection or refinement necessary. A model will never be able to provide a perfect fit of observed conditions. The skill will be in determining whether the fit is appropriate to the proposed use of the model. Consultation with the Agency will be essential in agreeing this end point, but recognition must be given to the need to go back and check the model as more data becomes available;

v) Dependant on the results of this exercise the modeller may need to review the conceptual and mathematical models, and or decide that there is a need for further site-specific data.

Parameters may be changed singularly or in combination. The advantage of this trial-and-error technique is that the modeller gains a good understanding of the sensitivity of the model to parameter values and can readily check that parameter values are plausible. The main disadvantage with this process is that it is time consuming.

Automated techniques use an algorithmic approach to vary parameter values to obtain the best fit to a set of field observations. This practice is generally not recommended as the modeller does not gain an intuitive understanding of how parameter values affect the model result and why aspects of the model don’t work.

9.3 Assessment of model results against field observations

The assessment of the match between model response and observed conditions will be qualitative (visual comparison) and quantitative (statistical techniques). In the early stages of modelling, visual assessment of the model results will be the main method for assessment.

Examples of quantitative or statistical techniques that can be used for groundwater flow models are given in Anderson & Woessner (1992) and Zheng & Bennett (1995).

The criteria that will determine whether a model provides an acceptable match to field data will depend on:

- The purpose of the model, i.e. how accurate does it need to be;
- How the model has been set up to represent the system;
- The observed magnitude of variation in a measurement used to validate the model, e.g. if there is a large range in contaminant concentrations within a plume, then differences between modelled and observed concentrations will need to be assessed in relation to this variability. In setting up the model, consideration should have been given to defining an acceptable variation between modelled and measured values.

Where a model gives a poor fit to field conditions this needs to be investigated. Possible considerations are (Table 9.1):

- The observed data value is an error (incorrect borehole datum for water level measurement, or error in laboratory measurement of a contaminant);
- The model does not allow direct comparison with observed measurements, e.g. comparison of a measured contaminant concentration in a water sample from a borehole

with the calculated concentration for a model cell that may represent an area of several hundred square metres;

- The model does not adequately represent the system e.g. a multi-layered aquifer has been represented as a single layer; i.e. the conceptual model or the translation from conceptual to mathematical is inadequate;
- The model solution is wrong because of input data errors (this is easily done), calculation errors, numerical instability etc.

It is important to recognise that there may be more than one combination of parameter values that simulate observed conditions, i.e. the solution is very unlikely to be unique. It is essential, therefore, that all historical data should be used in checking the model as this will improve the confidence that can be attached to the model results.

Presentation of the results of the model refinement and validation exercise is important and should be presented in tabular and/or graphical format, such as:

- Tabular comparison of observed and modelled values;
- Contour or distribution plots;
- Time series plots; and
- Cross sections.

Table 9.1 Examples of field observations used in model refinement

Measurement	Field observation	Examples of problems associated with the model that may give rise to anomalous results	Examples of errors in field measurements
Groundwater levels	Spot water levels. Groundwater level contours or distribution plots. Horizontal hydraulic gradients. Vertical hydraulic gradients. Groundwater level variation. Groundwater level recession.	Initial conditions. Boundary conditions. Coarse grid spacing. Coarse time step. Model parameters. Simplification of flow system e.g. multi-layered aquifer represented as single layer. Observation borehole not in centre of model grid.	Error in measurement of water level or borehole datum. Borehole construction (more than one aquifer or layer penetrated).
Spring or baseflow	Spot flows. Flow recession. Flow variation. Gains or losses in stream flow.	River/aquifer interaction coefficients.	Error in flow measurement. Separation of baseflow and surface water runoff.
Contaminant concentrations	Spot measurements. Contaminant contours or distribution plots. Vertical sections. Variation in time. Travel or breakthrough times.	Initial conditions. Boundary conditions. Coarse grid spacing. Coarse time step. Simplification of physico-chemical processes. Numerical precision or instability.	Laboratory error. Sampling or handling error. Borehole construction (short circuiting, long borehole screen section may result in mixing of groundwater from different horizons).

9.4 Sensitivity analyses

The purpose of undertaking a sensitivity analysis is to identify which parameters have the greatest influence on the model results and then to decide whether further data need to be collected to define this parameter. This is particularly important for deterministic models, where single parameter values have been used, and for models where limited field observations are available to test the model. The analysis should also consider other components of the model, including model boundaries, source release history, model time step etc.

It should be noted that this analysis provides information on the sensitivity of the model to a change in a parameter value, and does not necessarily reflect the actual sensitivity of the real system.

A sensitivity analysis involves changing one or more parameter values, usually by a certain percentage (e.g. ±20%) and examining the influence of this on the model response (e.g. contaminant concentrations, break through times, plume geometry). However, it should be recognised that the number of possible contributions may be large and that this process may also result in unlikely combinations of parameter values, particularly for dependent parameters. For example, the hydraulic gradient will be partially dependent on the hydraulic conductivity, such that steep hydraulic gradients would not be expected in areas of high hydraulic conductivity. The combination of a high hydraulic conductivity and high hydraulic gradient could result in unrealistic modelled flows, for example in excess of known recharge.

The change in a model parameter value should be related to the measured or observed range in the parameter. For example, the analysis may show that the model calculation is equally sensitive to bulk density and hydraulic conductivity. Field measurements may show that values of bulk density fall within a narrow range, whereas values of hydraulic conductivity vary by more than an order of magnitude. Clearly hydraulic conductivity is the key parameter.

The results of the analyses should be presented in both tabular and graphical format.

The results of the sensitivity analyses should be critically reviewed to determine:

- The parameters which have greatest influence on the model results;
- Do the results of the analyses relate to observed conditions? For example, if changing a parameter value by 20% results in predicted values that fall outside of the observed range this may imply an unrealistic selection of parameter values;
- Are further data required to define the parameter, in order to increase confidence in the model predictions;
- Whether the operational conclusion (e.g. whether or not remediation is necessary) is sensitive within the likely range of parameter uncertainty;
- Are the results of the sensitivity analysis consistent with the conceptual models, i.e. are the same parameters important, or is the sensitivity of the mathematical model a function of the equations used.

The results of the sensitivity analyses should be taken into account in applying the model and in defining scenarios that need to be tested.

9.5 Uncertainty analysis

Uncertainty analysis provides a means of taking account of the effects of uncertainty in input parameter values on the model results. This can be achieved by either:

i) Running a deterministic model using best estimate, worst case and optimistic values for the input parameters to provide information on the range of possible outcomes. Minimum and maximum observed parameter values are often used to define worst case and optimistic values, but this needs to be undertaken with care as the observed values may underestimate the actual range of a parameter (refer to Environment Agency 2001b). Care also needs to be taken in ensuring that this does not result in combinations of parameter values that are implausible and consequently in results that are unrealistic;

ii) Using a probabilistic model where the range or distribution in parameter values is described by a probable density function and the model results are described by a probability distribution. A sensitivity analysis should also form part of this analysis in determining which are the most sensitive model parameters, and which may warrant further data collection.

Environment Agency (2001b) provides a detailed description of uncertainty analysis. Reference should also be made to the results of the sensitivity analyses (Section 9.4) which will provide an initial indication of how changing a parameter value will affect the model result.

9.6 Application of the model

Prior to the use of the model as a predictive tool, the modeller will need to be satisfied as to its acceptability (refer to Section 9.7).

Figure 9.1 summaries some of the key stages in the application of a model, but these will obviously be dependent on the purpose of the modelling exercise.

Defining the appropriate model run scenarios is essential and should be discussed with all interested parties including regulatory bodies. This will include definition of the conditions under which the model will be run; e.g. groundwater abstraction scenarios, recharge conditions, contaminant releases etc.

In using a model as a predictive tool, the main difficulty is determining future conditions, for example:

- Changes in the site characteristics, e.g. placement of hardstanding over the site;
- Changes in groundwater abstraction patterns, e.g. change in the direction of groundwater flow and rise in groundwater levels due to a cessation of pumping;
- Changes in system behaviour, e.g. a hydraulic barrier may have been constructed to control contaminant movement, but for which a deterioration in performance may occur over time;
- Changes in physico-chemical processes e.g. a change from anaerobic to aerobic conditions may significantly affect biodegradation processes.

The results from a fate and transport model are usually compared with a standard, for example, a target concentration to protect a groundwater or surface water receptor. Guidance on the selection of target concentrations is given in Environment Agency (1999a). Where a probabilistic analysis has been undertaken, the criterion for deciding whether the results comply with, or exceed, the standard needs to be determined. Typically the 95%ile is used as the criterion, although this will be dependent on the sensitivity of the receptor. The basis for determining the criteria for determining whether action is required must be fully documented.

There are a number of different approaches to determine input parameters for a predictive model run. These are:

Best Estimate (BE) Prediction using the most likely value for each parameter. These values may be based on analysis of the available data that have been refined in matching modelled results with field data. This approach will provide no indication of the uncertainty in model parameters on the model result.

Worst Case (WS) Prediction where the model input parameters are set at their most conservative values. The difference between a best estimate and a worst case prediction will provide an initial indication of the magnitude of uncertainty in the model results.

The results of this exercise can be compared with the target concentration (TC) as illustrated by Figure 9.2 to determine possible actions, including whether a probabilistic analysis is warranted (refer also to Environment Agency, 2001b).

9.7 Model review

Throughout the development of the model, the modeller should regularly review the acceptability of the approach adopted including:

- The model objectives have been met;
- The model code/equations have been verified;
- The model adequately represents the conceptual model, including the processes which affect contaminant transport (e.g. sorption);
- The model input parameters are sufficiently well defined, and the parameter values are justified;
- The model parameter values are credible (e.g. are they consistent with field or literature values);
- The model accuracy is acceptable, i.e. to what degree has the model converged?
- Sufficient data have been used to validate the model;
- The model adequately simulates observed conditions, and any significant differences between the model and observed values have been explained;
- Uncertainty in the conceptual model has been adequately taken into account;
- Uncertainty in model parameters has been adequately taken into account;

- The sensitivity of the model to input parameters has been assessed through a sensitivity analysis and the results of this exercise has been taken into account in model predictions;
- The model limitations and assumptions have been taken into account in assessing and using the model results;
- The scenarios investigated by the model are relevant;
- The model predictions are based on under- or over-conservative parameter values, such that the results need to be treated with care;
- The model results make sense.

This exercise will determine whether:

- The model can be accepted (e.g. it adequately represents the conceptual model and observed conditions) and therefore, the model results can be used in decision making;
- The model should be rejected or an alternative model selected;
- Further data are required to define the system (e.g. the sensitivity analyses concludes that certain key parameters have a major influence on the model results and only limited site-specific data are available to define these);
- Further data investigation and or model development is not warranted (e.g. the analysis may have shown that there is no impact on the identified receptor, even though a range of parameter values has been investigated, such that further assessment would not be justified);
- The model needs to be updated e.g. an analytical model may have been used to undertake an initial assessment, but that further analysis requires a numerical model. In relation to the Agency's Remedial Targets Methodology (Environment Agency, 1999a) this would be equivalent to moving from a Tier 3 to Tier 4 assessment;
- The conceptual model should be reviewed.

This review will be mainly a subjective exercise and reliant on professional judgement and should involve regulatory bodies and other interested parties.

It is also important that information should continue to be collected (e.g. as part of compliance monitoring for a remediation scheme). These data should be used to:

- Update the conceptual model;
- Update the fate and transport model;
- Test the validity of the model predictions. If the model predictions are found to be incorrect, the conceptual model and mathematical model should be revised and model predictions and findings reassessed.

It is emphasised that the overall process should be one of continual updating and challenging the conceptual and mathematical models. The modeller should not be afraid to reject the modelling approach adopted where this is found to be inadequate.

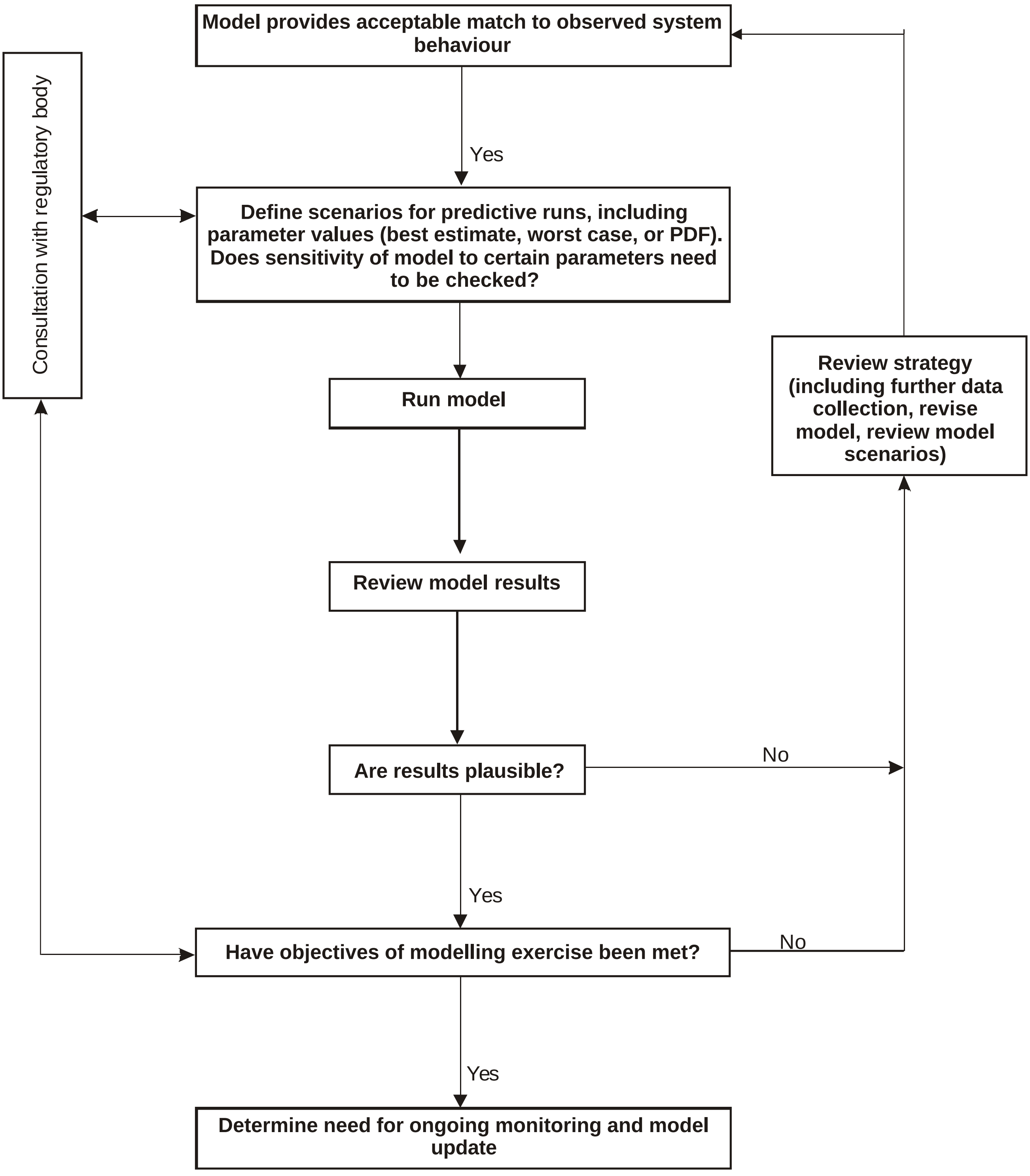
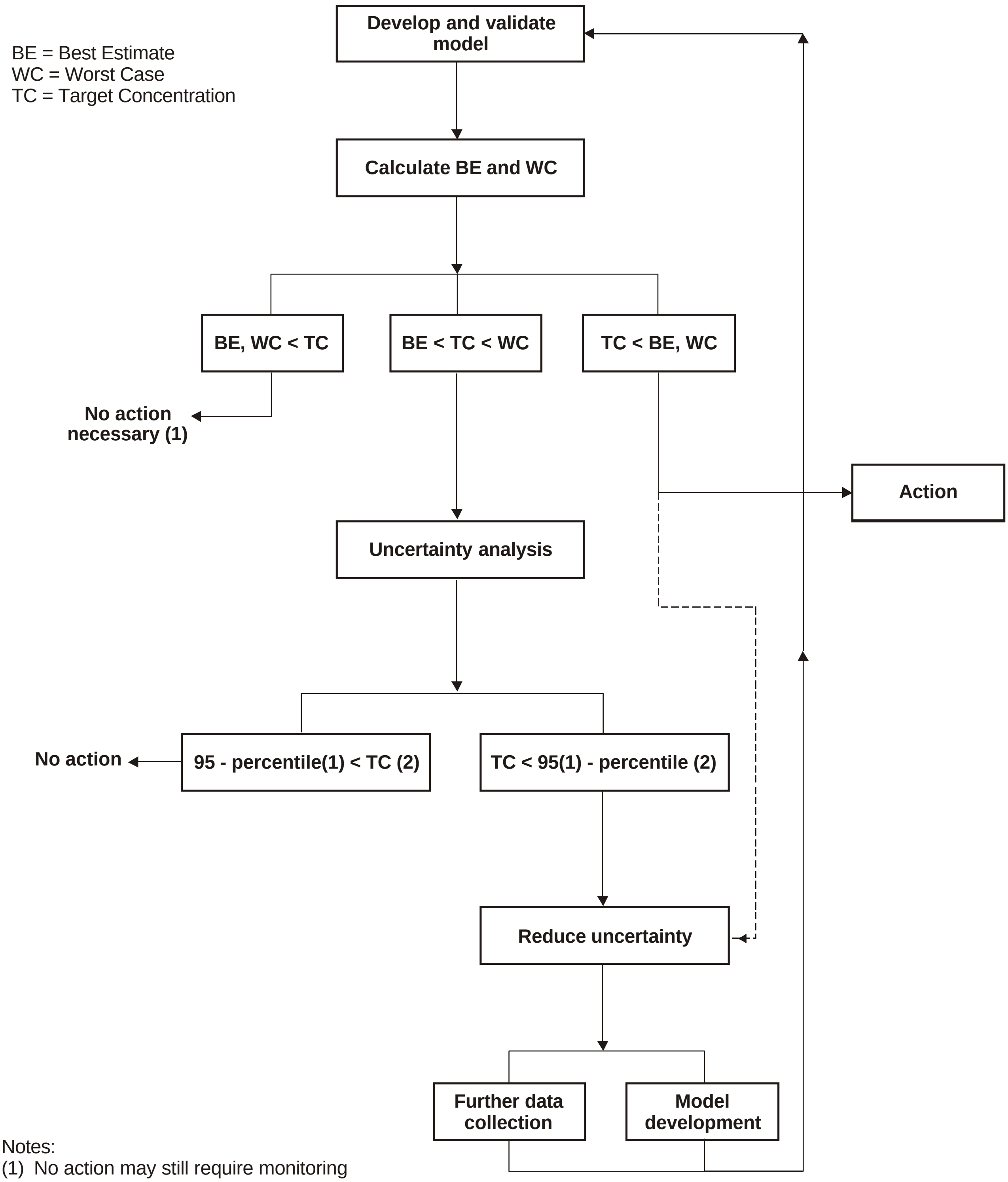


Figure 9.1 Model Application



Notes:
(1) No action may still require monitoring to be implemented

(2) The choice of percentile value should be agreed with the Environment Agency and take account of the sensitivity of the receptor.

Figure 9.2 Decision Tree

10. Project Reporting

10.1 Introduction

The purpose of this chapter is to outline the information that should be included in any report for a modelling study submitted to the Agency. All studies are different but should follow the same broad approach and each stage should be included in the report. Even when no mathematical model has been developed, the conceptual model may be the justification for that approach and must be clearly presented and explained. Agreement with the Agency on the conceptual model and the applicability of modelling should have been obtained at an early stage in the project and these aspects should not be an issue at the report stage. On-going discussion with the Agency as modelling progresses will further minimise the risk of issues arising.

Thorough QA procedures for a modelling study will ensure that records are kept of all stages of the study. These records will include all data obtained and all decisions made. Reports submitted to the Agency should be thorough and comprehensive but summarise the key aspects of the modelling. All supporting information should be available on request.

10.2 Reporting

The report for a modelling study should be logical and include the following sections:

- **Introduction** - site location (NGR), site plan – regional and detailed, local and regional setting, source pathway receptor linkages, purpose of report;
- **Objectives for study** - what are the objectives of the study, why is it being carried out now, what is to be achieved;
- **Desk study information** - background, historical data and maps, previous investigations, site reconnaissance;
- **Site investigation** -details of investigation including rational for number and location of sampling points, sampling and testing methods and results, analytical methods and limits of detection, raw data should be presented in appendices and key data summarised in tables or spreadsheets. Details of quality assurance should be included;
- **Conceptual model (Section 3.9)** - flow and transport mechanisms, source-pathway-target. Conceptual model should be presented graphically wherever possible and all figures should be clearly annotated and labelled. All calculations should be presented in appendices.

The above sections should be presented in a separate report to the Agency such that agreement on the conceptual model can be obtained, prior to commencement of any detailed mathematical modelling.

- **Code selection** - basis for code selection and modelling approach, code description, model limitations/assumptions/simplifications, model verification;
- **Transferring conceptual model to mathematical model** - description and justification of model input parameters, distributions, assumptions and simplifications. Any data pre-processing should be explained and all calculations presented in appendices;

- **Model design and refinement** - building the model, refining the model, sensitivity and uncertainty analyses. Include modelling log or QA;
- **Model results** - Results of model predictions. The model (including input and output files) should be provided electronically;
- **Conclusions** - assessment of model results and justification of recommendations/decision making.

Model reports should be concise but comprehensive and should clearly document the basis for any decisions made at the various stages of the modelling study. Other Agency guidance includes information on reporting requirements Environment Agency (1999a, 2000a, 2000d and 2001c).

The information submitted should allow the work to be audited and, if necessary, reproduced. Models may not be accepted or further documentation may be requested by the Agency if supporting information is inadequate. In many cases this could significantly increase costs and timescales on projects.

10.3 Liaison with Environment Agency

The majority of contaminant fate and transport modelling studies are carried out in response to issues of land or groundwater contamination or in connection with landfill licensing. The reports for these studies will be submitted to the Environment Agency and assessed as part of the relevant regulatory process. It is essential that the Agency is involved in the modelling study at an early stage in order to ensure that the proposed investigations and modelling work is appropriate for the purpose intended and within the legislative context. Consultation with Agency staff should start at the beginning of the project and this initial liaison should establish:

- The objectives of the study (including legislative and policy context);
- Agreement on the interim conceptual model;
- Agreement on the priorities for site investigation;
- Reporting requirements.

Subsequent liaison will include:

- Agreement on refinements to conceptual model;
- Defining objectives for the modelling;
- Agreement on choice of model and modelling approach;
- Agreement on parameter values for model input;
- Discussion of model results;
- Reporting requirements.

The consultation serves two main purposes:

- It ensures that all issues of concern to the Agency are addressed;

- Unnecessary site investigation and modelling work is avoided as agreement is obtained at key stages of the project rather than waiting until the work is completed to identify areas of disagreement.

10.4 Quality Assurance (QA)

QA for modelling studies will consist mainly of clear documentation and organisation of records and computer files. It is important to record and justify data sources, calculations, assumptions and simplifications. Any decisions made during the study or changes made to the model during its development should also be justified and recorded. A modelling log sheet is essential to record the development of the model. The details of the QA procedure will depend on the type of model used but records for a large numerical model may be extensive and a system should be developed at an early stage in the project. The key elements of the model QA should be included in the final report so they can be checked as the model is assessed.

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Appendix A
Conceptual Models

Table A1 in Appendix A Details to be covered by the conceptual model (this list is for guidance only and will be dependent on site-specific conditions)

Topic	Specific Information	Data (Y/N)	Comments
Site description and history	Grid references, site plan (at an appropriate scale), site boundary, area of site		
	Relevant site history including activities that may have given rise to contamination (should also include land adjacent to the site)		
	Current use (including site layout)		
	Proposed future use of site (including development of site)		
	Details of abstraction licences, discharge consents, authorisations etc		
	History of pollution incidents, including prosecutions, Notices etc.		
	Drainage systems, soakaways		
	Topography		
Characterisation of site geology	Local and regional setting		
	Solid and drift geology and soil details		
	Lithological description		
	Geometry (thickness and lateral extent) of the main lithologies		
	Structure (including faulting, fissuring)		
	Geological maps, sections, structural contour maps, isopachytes		
Characterisation of hydrology and climate	Surface water drainage		
	Surface water flows, including low flows		
	Groundwater/surface water interaction		
	Surface water quality		
	Abstractions and discharges		
	Surface water catchments		
	Rainfall, potential and actual evaporation		
	Infiltration through soil and surface water run-off		
Characterisation of groundwater flow system	Groundwater occurrence		
	Groundwater vulnerability		
	Location of SPZs		
	Direction of groundwater flow		
	Hydraulic gradients (horizontal and vertical)		

Table A1 (continued) Details to be Covered by the Conceptual Model (this list is for guidance only and will be dependent on site-specific conditions)

Topic	Specific Information	Data (Y/N)	Comments
Characterisation of groundwater flow system	Variations (seasonal and long-term) in groundwater levels and flow direction		
	Flow mechanism (fissure/intergranular flow)		
	Aquifer properties (porosity, hydraulic conductivity)		
	Lateral and vertical variation in aquifer properties		
	Groundwater interaction with surface water bodies (rivers, lakes, canals etc.)		
	Artificial influences on the groundwater regime, e.g. fracturing of strata due to collapse of underground mine workings		
	Recharge and indirect recharge		
	Discharge to springs and streams		
	Groundwater abstractions		
	Historical, current and future aquifer management which may affect the groundwater regime, e.g. rising groundwater levels in response to a cessation of abstraction		
	Influence of geological structures (faults) on flow		
	Single or multilayered aquifer and significance of aquitards		
	Aquifer thickness and effective thickness		
	Unsaturated zone thickness and flow characteristics		
	Groundwater level maps, groundwater hydrographs, aquifer geometry, cross sections		
Source Term characteristics	History of contamination (volume of spills, number of releases, locations(s), dates, frequency(ies) and methods(s) of release and duration)		
	Contaminants present/identified		
	Likely contaminant form (e.g. DNAPL, LNAPL, dissolved, particulate)		

Table A1 (continued) Details to be Covered by the Conceptual Model (this list is for guidance only and will be dependent on site-specific conditions)

Topic	Specific Information	Data (Y/N)	Comments
Source Term characteristics	Contaminant phase (solid, sorbed phase, free phase, dissolved phase, vapour phase)		
	Contaminant distribution (soil zone, unsaturated zone, saturated zone)		
	Contaminant concentration (soil zone, unsaturated zone, saturated zone)		
	Continuous, plug or declining contaminant source		
	Contaminant properties (solubility, partition coefficient, density, persistence etc)		
Likely pathways	Unsaturated zone pathways		
	Saturated zone pathways		
	Geological, structural and topographic controls		
	Influences of preferential flow via fissures, drainage systems, soakaways, man made structures, foundations, old mines, boreholes etc.		
Contaminant migration characteristics	Porosity/dual porosity/fracture flow		
	One or two phase flow		
	Density controlled flow		
	Degradation kinetics		
	Sorption characteristics		
	Volatisation		
	Dispersion processes		
Receptors	Groundwater below or adjacent to site.		
	Existing and potential users of groundwater, abstractions.		
	Surface water (springs, streams, ponds, wetlands)		
	Distance from site to receptors		
	Sensitivity of receptors		

Table A1 (continued) Details to be Covered by the Conceptual Model (this list is for guidance only and will be dependent on site-specific conditions)

Topic	Specific Information	Data (Y/N)	Comments
Characteristics of soil/rock in relation to contaminant transport	Fraction of organic carbon.		
	Cation ion exchange		
	Mineralogy (e.g. clay content, Fe/Mn oxides etc.).		
	Grain size distribution.		
	Moisture content		
	Significance of preferential pathways		
Observed contaminant behaviour	Plume shrinking, stable, expanding Plume diving (due to density effects recharge or vertical hydraulic gradient)		
	Seasonal and long-term changes in contaminant concentrations		
	Processes affecting contaminant transport (e.g. advection, dispersion, sorption, degradation)		
	Presence of breakdown products, if applicable		
	Influence of reactions/competition between contaminants		
	Influence of biochemical environment on contaminant processes (e.g. pH on metal mobility)		
	Significance of natural attenuation processes, and evidence in support of natural attenuation (Environment Agency 2000e).		
	Influence of future changes on contaminant behaviour (e.g. effect of remediation scheme)		
	Distribution and/or contour plots, sections, time series graphs		
Bio-geochemical environment	Background quality		
	Aerobic/anaerobic		
	pH, temperature, salinity, E_h and/or redox, indicators such as dissolved oxygen, alkalinity, NO_3^-/ NH_4^+, Fe^{2+}/Fe^{3+}, SO_4^{2-}/S^{2-}		
Uncertainty	Uncertainty in definition of the conceptual flow model (e.g. processes affecting contaminant transport), definition of parameter values		

Table A2 Summary of important processes affecting solute fate and transport *(modified from Wiedemeier et al., 1999)*

Process	Description	Dependencies	Effect
Advection	Movement of solute by bulk groundwater movement	Dependent on aquifer properties, mainly hydraulic conductivity and effective porosity, and hydraulic gradient. Independent of contaminant properties	Main mechanism driving contaminant movement in the subsurface
Dispersion	Fluid mixing due to groundwater movement and aquifer heterogeneities	Dependent on aquifer properties and scale of observation. Independent of contaminant properties	Causes longitudinal, transverse, and vertical spreading of the plume. Reduces solute concentration at any point, but not overall solute mass
Diffusion	Spreading and dilution of contaminant due to molecular diffusion	Dependent on contaminant properties and concentration gradients. Described by Fick's Laws	Diffusion of contaminant from areas of relatively high concentration to areas of relatively low concentration. Generally unimportant relative to dispersion at most groundwater flow velocities
Sorption	Reaction between aquifer matrix and solute whereby contaminants become sorbed on organic carbon or clay minerals	Dependent on aquifer matrix properties (organic carbon and clay mineral content, bulk density, specific surface area, and porosity) and contaminant properties (solubility, hydrophobicity,)	Tends to reduce apparent solute transport velocity and remove solutes from the groundwater via sorption to the aquifer matrix. May reduce mobile contaminant mass, but reversible process.
Dilution	Mixing of contamination with groundwater or surface water (driven by dispersion)	Dependent on aquifer matrix properties, depth to groundwater, surface water interactions, and climate	Causes reduction in contaminant concentrations but not total mass.
Volatilisation	Volatilisation of contaminants dissolved in groundwater into the vapour phase (soil gas)	Dependent on the chemicals vapour pressure and Henry's Law constant	Removes contaminants from groundwater and transfers them to soil gas.
Biodegradation	Microbially mediated oxidation-reduction reactions that degrade contaminants	Dependent on groundwater geochemistry, microbial population and contaminant properties. Biodegradation can occur under aerobic and/or anaerobic conditions	May ultimately result in complete degradation of contaminants. Typically the most important process acting to reduce contaminant mass. May produce new contaminants in the ground

Table A2 (continued) Summary of important processes affecting solute fate and transport *(modified from Wiedemeier et al., 1999)*

Process	Description	Dependencies	Effect
Abiotic Degradation	Chemical transformations that degrade contaminants without microbial facilitation, e.g. hydrolysis	Dependent on contaminant properties and groundwater geochemistry	Can result in partial or complete degradation of contaminants. Rates typically much slower than for biodegradation. May produce new contaminants in the ground.
Partitioning from NAPL	Partitioning from NAPL phase into groundwater. NAPL plumes, whether mobile or residual, tend to act as a continuing source of groundwater contamination	Dependent on aquifer matrix and contaminant properties, as well as groundwater mass flux through or past NAPL plume Raoult's Law for mixtures.	Dissolution of contaminants from NAPL represents the primary source of dissolved contamination in groundwater

Appendix B
Influence of Parameter Values

Table B1 Influence of Physical and Chemical Model Parameters on Contaminant Transport Models

Parameter	Influence on contaminant transport	Comments
Source term	Mass of contaminant entering the system. Contaminant concentrations in groundwater.	Source term often represented as continuous source term (conservative assumption). In this case it is possible that the modelled contaminant mass may exceed actual contaminant release. Source term can alternatively be described as a declining source, usually represented as first order reaction (exponential reduction), but in this case important to check that modelled contaminant mass equates to the measured or estimated total contaminant release mass.
Recharge	Dilution Contaminant loading (leaching)	Seasonal variation in effective rainfall and leaching of contaminants. Indirect recharge (leaking drains, rivers, soakaways etc.). Influence of cover (hardstanding, impermeable liners) on infiltration (run-off may flow to leaking drains or soakaway).
Horizontal hydraulic conductivity (K)	Rate of contaminant transport (advection) and arrival time at receptor. Calculated groundwater dilution. If value increased will reduce concentrations due to dilution, but will decrease arrival times at receptor.	Contaminant transport sensitive to this parameter. Field measurements can often vary by more than an order of magnitude (due to the natural heterogeneity of most aquifers). Important parameter to determine by field measurement - literature values unlikely to be sufficiently precise, although Aquifer Properties Manual data may be sufficient if local data are included and relevant to site.
Vertical hydraulic conductivity	Rate of contaminant transport. Leakage rates through low permeability layers.	Usually considered in terms of contaminant migration through the unsaturated zone, mainly in terms of calculation of leakage rates based on vertical hydraulic gradient. If no hydraulic head measurements are available a hydraulic gradient of 1 is often assumed. Unsaturated zone travel times are typically calculated as function of unsaturated zone thickness, infiltration and moisture content. Heterogeneity in vertical hydraulic conductivity may limit vertical dispersion (mixing zone in aquifer).
Hydraulic gradient (*i*)	Rate and direction of groundwater flow. Calculated groundwater dilution. If value increased will reduce concentrations due to dilution, but will decrease arrival times at receptor.	Hydraulic gradient is dependent on hydraulic conductivity. Steep gradients unlikely to occur in zones of high permeability. Important to determine by field measurements (minimum of three boreholes required). Hydraulic gradient and direction of flow can vary with time (seasonality).

Table B1 (continued) Influence of Physical and Chemical Model Parameters on Contaminant Transport Models

Parameter	Influence on contaminant transport	Comments
Transport Porosity (*n*)	Rate of contaminant movement and arrival time at receptor.	Important to determine if fissure or intergranular flow. Fissure-pore water diffusion may be important in some systems. Transport in fissured aquifers is often represented by using a low value for porosity (equivalent to fissure porosity or kinematic porosity) in a homogenous medium.
Dispersivity	Spreading of contaminant. Arrival time at receptor reduced if longitudinal dispersion occurs. Reduction in contaminant concentrations.	Scale dependent. Important to consider when calculating arrival times as results in faster breakthrough than from plug flow calculations. In more complex models relating to biodegradation, dispersion may be important in reducing contaminant concentrations and in introducing electron acceptors (e.g. dissolved oxygen, nitrate).
Longitudinal dispersion		Longitudinal dispersion typically assumed as 0.1 times pathway length (Domenico and Schwartz, 1990).
Transverse and vertical dispersion		Transverse dispersion often assumed as 0.01 to 0.03 times pathway length. Vertical dispersion often assumed as 0.001 times pathway length (because of layering of strata). Different analytical solutions are available depending on whether vertical dispersion can occur (in one or two directions). For a contaminant entering at the water table, the analytical expression should only consider dispersion in one direction (down).
Diffusion	Spreading of contaminant due to concentration gradient	Usually only significant where rates of groundwater flow are low, e.g. strata characterised by values of hydraulic conductivity of less than 1×10^{-9} m/s. Can be important in controlling contaminant movement in dual porosity systems (fissure-porewater diffusion), such as the Chalk.
Mixing depth/aquifer thickness	Dilution by groundwater flow Significance of vertical dispersion (for thin aquifers vertical dispersion should be negligible)	Mixing depth will typically be less than the aquifer thickness. Influenced by groundwater level variation (e.g. smearing of contaminant). Typically estimated based on experience, theoretical calculation, hydrographs (variation), borehole logs (high k zones). Large mixing depths, greater than 20 m, should be treated with caution.

Table B1 (continued) Influence of Model Parameters on Contaminant Transport

Parameter	Influence on contaminant transport	Comments
Bulk density	Used in calculation of contaminant retardation (see below)	Measurement is straight forward and relatively cheap once samples have been obtained. Literature values typically fall in narrow range and can reasonably be used - depends on grain mineralogy and porosity - check for consistency, (1.2 to 1.6 for soils, 1.6 to 2.0 g/cm^3 for rocks) and consequently calculations of retardation rates are relatively insensitive to this parameter.
Sorption/retardation	Rate of contaminant migration. Will indirectly increase time for degradation	Typically represented as a linear reversible reaction. For some situations sorption may be more accurately represented by a non-linear isotherm. Be wary of models relying on sorption at high concentrations (where linear sorption has been shown to be inappropriate). If contaminants are strongly sorbed to aquifer material they may not be bioavailable (and therefore degradable).
Partition coefficient (K_D)	Used in calculation of retardation of contaminant or in soil water partitioning Rate of contaminant migration	Partition coefficients can be sensitive to soil or groundwater pH, pK_a, H, K_{oc}, foc and values can range by more than an order of magnitude. Typically based on literature values, although range of different values may be given in literature sources.
Organic partition coefficient (K_{OC})	Used in calculation of retardation of contaminant or in soil water partitioning. Rate of contaminant migration	Partition coefficient typically calculated as: $K_D = f_{OC} \times K_{OC}$ (for non-ionised organic contaminants) Literature values for organic species can vary.
Fraction of organic carbon (f_{OC})	Calculation of partition coefficient	For low f_{OC} values (less than 0.001), sorption/retardation of pollutants to the substrate may be dependent on mineral surface area and mineralogy. Most UK aquifers have very low f_{OC}
Cation Exchange Capacity (CEC)	Delay for breakthrough of cations (e.g. potassium, ammonium)	Sensitive to pH, Eh, solute concentration and aquifer mineralogy. Aquifers have a finite capacity for cation exchange. Cations will compete for available exchange sites and this is typically handled by specifying a reaction efficiency as a measure of available sites. Cation exchange is a reversible process. Laboratory determination of CEC is normally performed on crushed samples, (Environment Agency, 2000c) which will increase the surface area, when compared to in-situ samples.

Table B1 (continued) Influence of Model Parameters on Contaminant Transport

Parameter	Influence on contaminant transport	Comments
Biodegradation	Reduction of contaminant mass and concentration. Contraction of contaminant plume (where the rate of degradation exceeds the contaminant advective and disperse flux), ultimate plume size.	Calculation of contaminant transport and remedial targets very sensitive to degradation rate. Check contaminant is biodegradable (e.g. metals and chloride are not). Typically represented as first order reaction but degradation: • can be inhibited at high concentrations of contaminant; • is sensitive to environmental conditions (pH, temperature, redox); optimal pH is typically between 6.5 and 8; • is reaction-dependent (i.e. availability of dissolved oxygen or electron acceptors such as nitrate, sulphate, iron (III)); • is dependent on redox (aerobic or anaerobic) conditions (these are likely to vary through the plume): often requires other nutrients especially N and P, or cometabolites (e.g. a carbon source for the reductive dechlorination of chlorinated solvents). Assessors should be expected to demonstrate degradation (Environment Agency, 2000b) by observable mass loss and geochemical indicators, and should not rely solely on literature data.

Table B1 (continued) Influence of Model Parameters on Contaminant Transport

Parameter	Influence on contaminant transport	Comments
		Degradation rates derived from literature values: • may not be appropriate to UK conditions; • may relate to different conditions from that observed at site (e.g. anaerobic conditions may occur at site, whereas the literature value may be for aerobic conditions); • may be unrealistically rapid because degradation rates change by ~2×/10°C, so warm US values (typically 18-25 ^{0}C) may not be valid for cold UK (near-surface groundwater temperature in UK typically 10-12 ^{0}C). • may be derived from laboratory studies which do not reflect field conditions. The breakdown products may be more mobile and toxic than the parent compound. Build up of degradation products can cause inhibition. The determination of field rates of degradation will often be dependent on detailed site investigation and monitoring, supported by modelling and statistical analysis of the data (Environment Agency, 2000b)

Appendix C
Peclet and Courant Numbers

Appendix C

Peclet and Courant Number (Numerical Models)

The Peclet and Courant numbers are used in the design of the model grid spacing and time (Eulerian based models) respectively to minimise numerical dispersion. The Peclet number can be calculated as follows:

$$Pe = \frac{Dx}{a}$$

where

Dx = grid spacing (m)

a = longitudinal dispersivity (m)

Pe = peclet number

The aim of the design of the model grid spacing should be to keep the Peclet number below a critical number (which depends on the solution algorithm, but is typically in the range 1 - 4) to minimise numerical dispersion. i.e. if it disperses more than half a grid spacing then it may become unstable.

The Courant number describes the number of cells or the fraction of a cell that the contaminant is advected across in one time step. The Courant number can be calculated as follows:

$$Cr = v.\frac{Dt}{Dx}$$

where

Cr = Courant number

Dx = grid spacing (m)

v = velocity (m/d)

Dt = time step (d)

To minimise numerical dispersion, then the Courant number should be set no larger than 1. Most models will automatically calculate the model time step, based on this equation. i.e. the particle should not advect more than one grid spacing per timestep. The time step used in contaminant transport can be different from the time variant flow time step.