Guidance on the Assessment and Interrogation of Subsurface Analytical Contaminant Fate and Transport Models

National Groundwater & Contaminated Land Centre report NC/99/38/1

Guidance on the Assessment and Interrogation of Subsurface Analytical Contaminant Fate and Transport Models

January 2001

Authors

A McMahon, M Carey, J Heathcote & A Erskine

Entec UK Ltd

National Groundwater & Contaminated Land Centre
Environment Agency
Olton Court
10 Warwick Road
Solihull
B92 7HX

National Groundwater & Contaminated Land Centre report NC/99/38/1

Publishing Organisation

Environment Agency
Rio House
Waterside Drive
Aztec West
Almondsbury
Bristol BS32 4UD

Tel: 01454 624400 Fax: 01454 624409

ISBN 1 857 05486 5

Dissemination status
Internal: Released to Regions
External: Released to Public Domain

Statement of Use
This document provides guidance to Environment Agency staff on the assessment and interrogation of analytical fate and transport models of subsurface processes that have been submitted to the Agency by problem-holders and their consultants. This document forms one of a set of three reports produced under this project.

Research Contractor

This document was produced under Project NC/99/38 by:

Entec UK Ltd
160-162 Abbey Foregate
Shrewsbury
Shropshire
SY2 6BZ

The Environment Agency's Project Manager was Dr John Davys, National Groundwater & Contaminated Land Centre.

The Project Board consisted of Sarah Evers, Paul Hulme, Dr Janet Macmillan, Tony Marsland, Dr Martin Shepley, Jonathan Smith, Jenny Thomas.

CONTENTS

Tables

List of Figures

List of Appendices

Executive summary

The increased use of contaminant transport models to determine risks to the subsurface environment has led to an increase in demand for Agency personnel to assess these models and make use of their outputs in decision making. This document provides guidance on the assessment and interrogation of subsurface analytical contaminant transport models submitted to the Agency by external organisations.

Checklists and tables of 'what to look for' are provided to enable easy and systematic assessment of all stages of the modelling process. The first check on any modelling study is to ensure that all the necessary information has been provided with the report and that the key stages have been carried out. It should be clear what the objectives are and that a modelling approach is appropriate. A comprehensive and clear conceptual model should have been developed. The sources of all data and the justification for all decisions and assumptions should be presented in the modelling report. The mathematical model selected should be appropriate to simulate the conceptual model, to meet the objectives of the study and have regard to the quality and quantity of data available. The model design will depend on the type of model used, but the input parameters required for all models will be similar and should always be derived, wherever practicable, from site-specific data used in the conceptual model. The results from a model should address the original objectives and take account of the uncertainty in the input parameters. The required sophistication of analysis and the acceptable level of uncertainty in model results will depend on the sensitivity of the receptor(s) and the magnitude of potential impacts.

In general, external organisations carrying out modelling work should be encouraged to consult with the Agency on an on-going basis and reach agreement at key stages of the project. Clarification and/or further information should be sought where important data have not been provided or where justifications are inadequate.

Key words Groundwater, risk assessment, fate and transport, modelling

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 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.

1. Introduction

1.1 Background

A key aspect of the Environment Agency's regulatory role is the assessment of risk to the environment and determination of the need for protection or remediation. 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 in the subsurface and also encourages external bodies to adopt the 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 also 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 analytical model codes/equations which simulate the transport of contaminants in the subsurface, which includes the unsaturated and saturated zones, and model codes used for determining impacts on groundwater and surface water receptors, but does not address surface water model codes.

The Agency is required to assess the contaminant transport models submitted to it by external organisations and to make decisions based on the results of modelling studies. Agency staff must establish that the approach used is appropriate and that the model code/equations, input parameters and results are valid for the site in question. The environmental professionals performing contaminant transport modelling have a diverse range of qualifications and experience and this can result in the inappropriate application of models. Problems can occur at any stage in the study, from data collection through to interpretation of model results. Inconsistent and inappropriate approaches to modelling can cause potential problems for the Agency. Acceptance by the Agency of proposals based on an inadequate modelling study could result in harm to the environment.

1.2 Purpose of this document

The purpose of this document is to assist Environment Agency Officers in the assessment and interrogation of contaminant fate and transport models, to ensure that:

- a modelling approach is appropriate;
- an appropriate model code/equation(s) has been used;
- the model is supported by appropriate data;
- the model adequately represents field conditions; and
- model results are realistic, adequately documented and can be justified.

The format of this document is intended to enable Agency personnel to carry out thorough and efficient assessments of analytical models submitted to them and to identify problem areas at an early stage in any modelling study.

1.3 Target audience

This document is written for Agency staff and assumes that Agency personnel carrying out the assessment of contaminant fate and transport models are hydrogeologists or environmental professionals with a good understanding of the principles of hydrogeology. Its aim is to develop a thorough and consistent Agency approach to assessing subsurface contaminant transport modelling studies.

1.4 Relationship to other guidance

This guidance note is one of a number of technical guidance documents produced by the Environment Agency's National Groundwater and Contaminated Land Centre which are aimed at improving understanding and capability, both inside and outside the Agency, in the risk based approach to environmental protection. 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:

- 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 (Environment Agency 2000a).
- Technical Guidance on Assigning Values to Uncertain Parameters in Subsurface Contaminant Fate & Transport Modelling (Environment Agency 2000b).

These documents are intended to be used in conjunction with 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.

This document is also intended for use with other Agency risk assessment tools such as LandSim and ConSim (refer to 'Risk Assessment Model Fact Sheets', Environment Agency, in preparation).

1.5 How to use this document

This document should be used in conjunction with the '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' (Environment Agency 2000a) which contains more detailed and comprehensive discussion of the key topics. For ease of use this report includes checklists and tables of key points to consider when assessing modelling projects.

Chapter 2 gives an overview of the key topics that should be covered in any modelling study and which should be presented in a modelling report. The appropriate use of models is also discussed.

Chapter 3 looks at how to assess a conceptual model and includes checklists of the things that should have been considered by the modeller in the development of the conceptual model.

Model code/equation selection is discussed in Chapter 4 and reference is made to those most commonly used. The assessment of model design and input parameters is discussed in Chapter 5 and includes reference to what should be considered for each of the main types of models.

Chapter 6 looks at the assessment and interpretation of the results of modelling and how these may be incorporated in decision making.

A list of technical terms used in this document is presented in the glossary.

2. Overall approach to reviewing contaminant transport models

2.1 Introduction

The assessment of contaminant fate and transport models may be either qualitative or quantitative and will always require an element of subjective decision making or ‘expert’ judgement. The environmental professionals developing both the conceptual and mathematical models should have an appropriate level of technical expertise and Agency personnel should also be aware of the limits of their own experience and seek advice from Area colleagues, or Regional specialists who will refer to National colleagues as appropriate, when assessing complex models.

Before any detailed assessment of a modelling study is undertaken, it is sensible to look at the proposals being made and the report’s conclusions . If these appear acceptable based on knowledge of the hydrogeology and previous experience, it may not be appropriate to spend a long period of time assessing the model produced in great detail. A short initial assessment of the model, as given in Figure 2.1, to check that key steps have been followed may be adequate. However, if you accept the proposals/conclusion without reviewing the model/code, this should be stated explicitly in your response. Otherwise the situation can arise where an incorrect code is applied to a low risk site, the conclusions accepted at face value, but the consultant states that the code is ‘Agency approved’ by that Region, when in fact it was never checked.

2.2 Summary of 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 2.2. An initial assessment should be undertaken to check that key stages have been carried out. Figure 2.1 shows an overview of this assessment procedure and the action that may be required at each step. Table 2.1 gives a tick list to check that the appropriate information has been provided in support of the modelling study. Early and ongoing discussion with the individuals and organisation doing the modelling will help to ensure that the necessary work is done at each stage.

The procedure for detailed assessment of the various steps is discussed in Chapters 3, 4, 5 and 6.

Figure 2.1 Overview of assessment of a modelling study

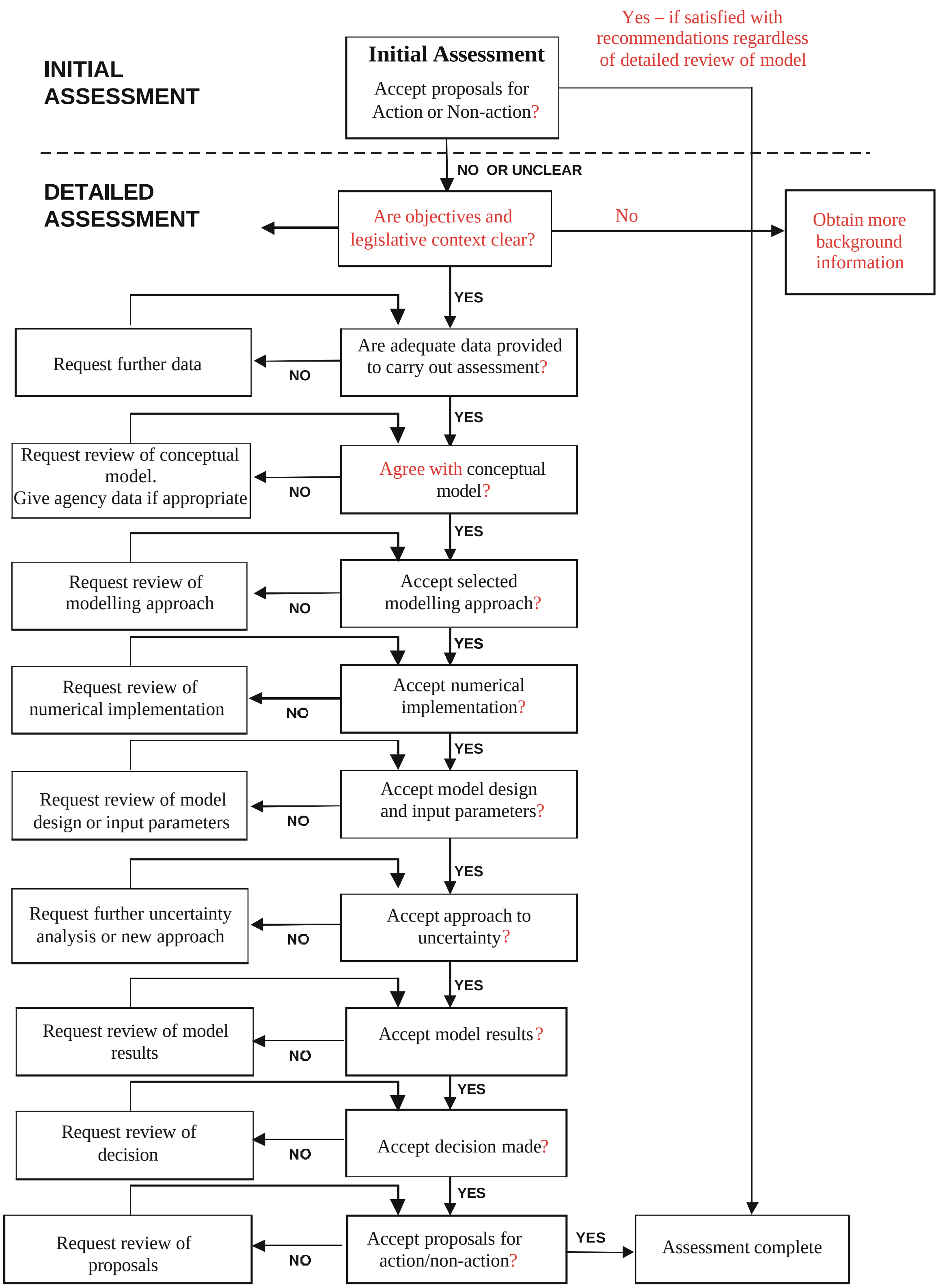


Table 2.1 Tick list of information to be provided with subsurface contaminant fate and transport model

Topic	Specific Information	Y/N	Comments
Reports	Desk study report / site reconnaissance		
	Site investigation report/s		
	Modelling report		
	Remediation report		
Supporting information for model	Model input files (preferably on disk) Range of values and sensitivity runs		
	Copy of model (if spreadsheet, or client in-house model) together with overview of model capability (equations, assumptions etc.)		
	Model output files		
Key stages in modelling	Clear objectives		
	Desk study information (review / collation of information)		
	Site investigation factual report		
	Conceptual model. Identification of sources, pathways and receptors		
	Modelling approach selection explained		
	Transfer of conceptual model to mathematical model explained including simplifications		
	Verification		
	Model design and validation		
	Model results		
	Conclusions/decision making		
Supporting information (including raw data)	Borehole locations and logs (including water levels and strikes)		
	Geological, soil, groundwater vulnerability, Source Protection Zone maps		
	Geological cross sections		
	Groundwater level hydrographs		
	Groundwater level contour maps		
	Results of field testing (tabulated)		
	Results of chemical analyses (tabulated) plus bias and precision of results		
	Contour or distribution plots of contaminant concentrations, time series graphs		
	Sources of information (full references of literature data)		
	Methods of measurements		
	Quality of data (number of samples, accuracy of measurements)		
	Discussion of data inadequacies		
	Statistical analysis of data		

This list is for guidance only and will vary according to the stage of modelling and type of model.

2.3 Appropriate use of models

It is essential that any modelling study has well defined objectives from the start and that the 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?

In a risk assessment context, a mathematical modelling approach is appropriate only if a robust conceptual model[1] has been developed that can adequately be described by mathematical relationships. Modelling may then help to provide a quantitative evaluation of the risks. In some situations, particularly when the sensitivity of the environment is low, it may be unnecessary to develop anything more than a simple calculation (e.g. of travel time and/or dilution). Where more complex systems or processes need to be represented, more sophisticated models are required. Models may also be appropriate for remediation design or optimisation where they may provide a means for 'collating' data and predicting performance.

2. Has an appropriate modelling approach been used?

The modelling approach used must take account of the objectives of the modelling, the availability of data and the complexity of the system and transport processes. The conceptual model[1] should identify those elements of the system that need to be represented; justification should be given for anything not represented in the model. Chapter 4 discusses model code/equation selection in more detail.

For the majority of projects, the development of a conceptual model and modelling approach will be iterative. Typically the modelling approach will start with relatively simple calculations or model codes/equations moving through to more complicated analytical or numerical codes/equations 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. This approach is in accordance with the 'Methodology for the derivation of remedial targets' (Environment Agency 1999a) which sets out a tiered approach, where increasingly sophisticated models and further data are required as the assessment moves progressively through each tier.

2.4 Reporting

The report is the main record of any modelling study and should include sections on the following:

- **Introduction** - site location (NGR), site plan, regional setting, 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 investigation –** Summary of results, sampling, testing methods and results should be presented as a separate report with raw data presented in appendices and key data summarised in tables or spreadsheets;

---

[1] 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.

- **Conceptual model** - flow and transport mechanisms, source-pathway-receptor linkage(s). The conceptual model should be presented graphically wherever possible and all figures should be clearly annotated and labelled. All background information should be presented in appendices;
- **Model/code/equation selection** - basis for selection of modelling approach, mathematical description, limitations/assumptions/simplifications, code verification;
- **Transferring conceptual model to mathematical model** - description and justification of model input parameters, assumptions and simplifications, including cross references to sources, where appropriate. Any data pre-processing should be explained and all calculations presented in appendices;
- **Model design and development** - building the model, validation process and sensitivity analysis. Include modelling log or QA;
- **Model results** - results of model verification and validation, results of uncertainty analysis and sensitivity analysis. Inputs and outputs should be presented where appropriate. A copy of the model data files (e.g. model runs) should be provided to the Agency on disk. If the model code has not yet been agreed with the Agency then this should also be provided (see Section 4.1);
- **Conclusions** - assessment of model results and subsequent decision making.

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

The information submitted should be sufficient to allow the work to be audited and, if necessary, reproduced. Models and any conclusions drawn may need to be rejected or further documentation requested if supporting information is inadequate. Table 2.1 provides a checklist of information which should typically be provided for a modelling study.

2.5 Consultation

It is helpful if the Agency is involved in modelling studies from an early stage in order to ensure that the proposed investigations and modelling work are appropriate, adequate and take account of any relevant information held by the Agency. External organisations should be encouraged to consult with Agency staff when the desk study information has been collated. This consultation process should continue throughout the project. The initial liaison should establish:

- the objectives of the study;
- agreement on the interim conceptual model;
- agreement on the priorities for site investigation;
- identification of local Agency issues and concerns;
- identification of any relevant Agency data;
- requirement for additional discussion during the project.

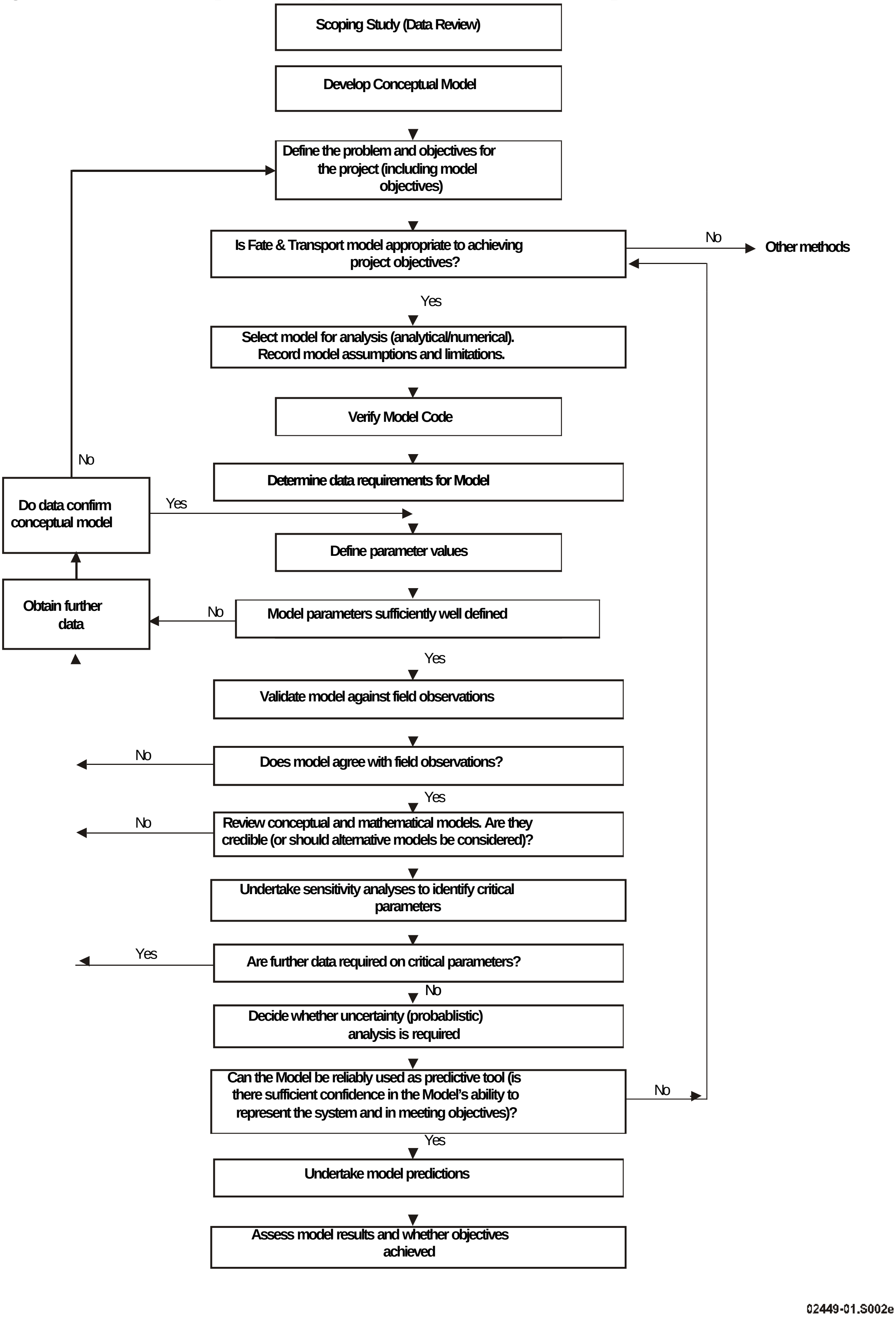
Subsequent liaison will include:

- agreement on refinements to conceptual model;
- agreement on choice of modelling approach;
- agreement on parameter values for model input;
- discussion of model results.

The consultation process serves three main purposes:

1. It ensures that all issues of concern to the Agency are addressed;
2. 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.
3. It ensures the modeller is aware of Agency held data and other local issues of concern/interest to the Agency.

Figure 2.2 Basic steps in the application of a fate and transport model



3. Assessing the conceptual model

3.1 Inputs to the conceptual model

A conceptual model is a simplified representation of how the real system is believed to behave based on analysis of field data. The most critical part of any modelling study is the construction of a robust conceptual model. The conceptual model demonstrates the modeller's understanding of the site (including its history and surroundings), the likely nature of contamination, the hydrogeological system, and the transport processes in and around the site. It is important to establish that site data have been obtained and that an appropriate, adequate and defensible conceptual model has been developed.

The conceptual model should have been developed to the standards recommended in the 'good practice' guide (Environment Agency 2000a) and must consider all aspects of the fate and transport mechanisms which affect the source(s), pathway(s) and receptor(s). These will include:

- definition of the study area/conceptual model domain;
- geology, including stratigraphy and lithology;
- hydrogeology/ aquifer characteristics/aquifer hydraulics/geochemistry;
- inflows/outflows to the system;
- contaminant source term (geometry, distribution, concentrations over time, phase etc);
- processes which control contaminant movement and behaviour;
- receptor(s);
- overall system behaviour.

A detailed list of what should be considered in any conceptual model is given in Table 3.1. Many of these factors will not be relevant for all sites but their exclusion from the conceptual model should be justified. It is important to identify, at this stage, the main uncertainties in the conceptual model, since this will be an important driver in designing subsequent site investigation.

3.2 Data sources

Many of the key inputs into the conceptual model will come from site investigation data. It is important to check that the data collected have been obtained using the current industry 'good practice' and relevant standards and appropriate methods of sampling and analysis. Other information, including from literature sources, may also be of value, but it is important that these are referenced and checked to be of relevance to the site in question.

The data should have been checked for inconsistencies and anomalies:-questions should be asked if these occur and have not been explained. Raw data should be presented. QA checks of information presented in summary tables against the raw data are recommended to ensure errors have not been introduced in copying or transferring information. Calculations should be presented where conceptual model data or model input data have been calculated from field measured parameters. QA checks on calculations are also recommended to ensure that calculation errors have not been introduced.

Table 3.1 Typical details to be incorporated into the conceptual model (this list is for guidance only and will be dependent on site specific conditions)

Topic	Specific information	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 and processes 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, stratigraphy		
	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		
	Other sources of recharge e.g. soakaways		
Characterisation of groundwater flow system	Groundwater occurrence		
	Groundwater vulnerability (resource classification and soil leaching characteristics)		
	Groundwater quality data (background and on-site)		
	Location of SPZs		
	Direction of groundwater flow		

Table 3.1 (continued) Typical details to be incorporated into the conceptual model (this list is for guidance only and will be dependent on site specific conditions)

Topic	Specific information	Y/N	Comments
Characterisation of groundwater flow system	Horizontal and vertical hydraulic gradients		
	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 including mixing zone 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), frequency(ies) and methods(s) of release and duration)		
	Contaminants present/identified		

Table 3.1 (continued) Typical details to be incorporated into the conceptual model (this list is for guidance only and will be dependent on site specific conditions)

Topic	Specific information	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) and whether it is widespread/localised		
	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		
	Volatilisation		
	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		
	Land-use (e.g. vapours to residents)		
	Location of buildings/services (e.g. attack on concrete)		
	Relevant environmental standards (e.g. DWS, EQS) for each contaminant at each receptor		

Table 3.1 (continued) Typical details to be incorporated into the conceptual model (this list is for guidance only and will be dependent on site specific conditions)

Topic	Specific information	Y/N	Comments
Characteristics of soil/rock in relation to contaminant transport	Permeability		
	Thickness		
	Fraction of organic carbon		
	Cation exchange capacity		
	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 (contaminant and natural attenuation indicator species)		
	Aerobic/anaerobic		
	pH, temperature, salinity, redox, dissolved oxygen, indicators such as 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 3.2 Assessment of data

Item	Description	What to look for
Source of parameter value	The report should detail the source of measurement (field, laboratory, literature or expert opinion), the method of measurement and method of analysis.	Is it clear where the data has come from?
Definition of parameter values	Parameter values should be described either by a probability density function, or as minimum, most likely and maximum values. It should be noted that setting maximum and minimum values based on the actual range of observations is likely to underestimate the actual population range.	How have parameter values been selected and justified? How do values relate to raw data? How have extreme data values been identified and dealt with (e.g. included or excluded in the analysis)? Have 'default' data been used and are they relevant?
Consistency of parameter values	Do parameter values make sense when viewed in combination	Unrealistic combinations of parameters e.g. high hydraulic conductivity values and high hydraulic gradient, high leakage and low vertical hydraulic conductivity. Has the assessor thought about the basic science?
Site specific or literature value	Site-specific data should be used when possible. Use of literature values or values based on expert opinion need to be justified including references, their applicability to site conditions, and whether the values have been used conservatively or as worst case.	Literature values are appropriate to site conditions, e.g. partition coefficients for metals can be sensitive to pH conditions, degradation rates may relate to aerobic conditions whereas site conditions are anaerobic**. Literature degradation rates should be supported by redox data and evidence of degradation (e.g. daughter products, electron acceptors etc.) from the field.**
Quality of data	Number of measurements, precision and bias Method of analysis (should be according to recognised standard, when appropriate). Sample handling (has appropriate protocol been followed/referenced). Level of detection for chemical analysis (is this appropriate for the particular contaminant and the decision that needs to be made?)	Assessments based on limited data should be treated with caution, and supported by uncertainty analysis, e.g. for some lithologies the value of hydraulic conductivity can vary by more than an order of magnitude. Method of analysis or level of detection may not be appropriate for parameter. Scale of measurement, e.g. scaling up of laboratory measurement of hydraulic conductivity to field situation is likely to underestimate regional value of hydraulic conductivity. The limit of detection of laboratory analysis should be less than the environmental standard against which comparison is to be made.
Range of data values	For heterogeneous systems, wide ranges of parameter values may be determined from site investigations.	Has the risk assessment taken account of observed range of parameters through sensitivity analyses or uncertainty analysis? If a deterministic approach is taken is it reasonably conservative?
Presentation of data	All information (e.g. raw data) used in assessment should be presented in graphical or tabular form, including statistical analysis.	Is the selected parameter value consistent with base information, if not justification for the selected parameter value should be given.
Uncertainties in data	Field measurements can measure only a small volume of the system, and uncertainty exists over whether the measurement will provide a realistic measure of the system. Uncertainty in parameter measurement, or in calculation of the parameter value based on field measurements	Over reliance on model results when limited or poor quality data are available, unless supported by adequate sensitivity or uncertainty analysis. Is the selected PDF appropriate for the reported data? Unless lots of data are available for statistical analysis, it is probably appropriate to use PDFs such as uniform, normal or triangular (log or linear).

Literature and other sources of data and parameter values should always be referenced and the use of non-site specific data should be justified. The data used must be appropriate to the site conditions being modelled. Table 3.2 gives an indication of what to look for in assessing data.

3.3 General points

It is also important to have an overview of the conceptual model that has been developed and consider whether it makes sense. Any inconsistencies should be questioned. You should be satisfied that the system is sufficiently well understood and that it has not been over-simplified or over-complicated.

The risk assessment should not focus exclusively on risks to controlled waters. Typically assessments will need to consider risks to a number of other potential receptors (e.g. chronic and/or acute risks to human health via inhalation, ingestion or dermal contact, risks to buildings etc).

With regard to contaminant transport modelling the old adage “rubbish in, rubbish out” applies. No matter how smart or complex the model and report, if the conceptual model or input data are wrong or inadequate, the results will be erroneous. Any conclusions made on the basis of such results will probably be invalid.

4. Reviewing the proposed mathematical modelling approach

This Chapter gives guidance on determining whether a suggested code/equation is appropriate to a given problem and whether an appropriate mathematical model has been used in the study. A mathematical model should be used only where the objectives of the study are clear and defensible, and an adequate conceptual model has been developed. The purpose and justification of using a modelling approach should be clearly stated as part of the project. A mathematical model should not be used as an alternative to collecting additional site investigation data. Indeed, any model constructed without adequate data is unlikely to be robust in simulating processes at the site. Conversely, where sound decisions can be made on the basis of the conceptual model or conventional data analysis, development of a mathematical model may be unnecessary.

4.1 Selection of a mathematical model

The choice of model code or equations will be dependent on a number of different factors, and may change as the project develops. For example, the remedial target methodology (Environment Agency 1999a) outlines a tiered approach with the sophistication of the mathematical model increasing at each tier. The decision to move from one tier to the next is based on a combination of environmental risk, and the cost-benefit relationship of collecting more data or undertaking remediation to more conservative standards. There is a requirement for additional data to be obtained at each tier.

Most models can be categorised in one of 6 levels of complexity shown in Figure 4.1. If a model has been used, the first step must be to understand what sort of model it is and into which category it fits in Figure 4.1. In choosing the mathematical model, the modeller should have considered whether it is too simple or over-complicated in relation to the objectives of the study.

The complexity of the mathematical model should have regard to:

- The accuracy required. If simple and conservative models predict that the likely impact at a receptor is several orders of magnitude smaller than the acceptable concentration (target concentration), then there may be no need to produce a more complex model.
- The complexity of the conceptual model. Sometimes simple mathematical models do not do justice to a complex situation (although, with some logical thought, a worst-case can usually be defined). However, a simple 'worst-case' approach may be unrealistically bad. The Agency should identify over-conservative approaches as well as under-conservative approaches, as this may result in unnecessary works, thereby incurring unnecessary costs and use of natural resources (e.g. fuel during unnecessary remediation works).
- Data availability. If there are too few data to justify a complex model <u>and</u> the data are needed, then the solution is not to construct a model, but to acquire more data.

Typically the complexity of the modelling approach should increase progressively. For example a plug-flow calculation would be made first, then a 1-D dispersion equation calculation. Monte-Carlo analysis might then be carried out, perhaps followed by more thorough data collection to understand the attenuation mechanisms. If the plausible range of impacts predicted still overlaps the maximum acceptable concentration, then the next stage may be a numerical model or to proceed with remedial action. Using this approach, the basis for increasing the sophistication of the mathematical model can be justified.

Once it is established that the mathematical model is at an appropriate level of complexity, the following questions should be addressed:

Is the mathematical model an appropriate one?
The model code/equations must simulate the processes identified in the conceptual model and the assumptions made by the mathematical model must correspond to those made in the conceptual model. If further assumptions have to be made at this stage they must be documented. Assumptions should represent simplifications that do not fundamentally alter the mechanisms of the conceptual model, or the assumptions should be demonstrated to be conservative. For example, if for the conceptual model it is concluded that fissure flow is the primary mechanism, then the mathematical model must make some allowance for this (such as assuming flow is through a homogenous porous medium with a low transport porosity).

Is the model code verified?
Verification is the process of checking that the code in the computer program does what it is intended to do. Commercial programs are usually verified internally by rigorous code-checking and externally by checking the results are correct for problems with known answers. A program is generally accepted after these studies and a few years of use (and debugging) have ironed out any problems. For complex model codes, total verification is not really possible – it can only be shown that the program has not failed yet!

Many model codes have been verified in studies open to peer review and are generally accepted as doing what they claim to do. These include LandSim, ConSim, MODFLOW (although the various preprocessors are not always reliable), FLOWPATH, MT3D, SUTRA.

If a model code is not known to be verified or verification cannot be demonstrated to the satisfaction of the Environment Agency, then verification should be sought. In this case a verification report should be provided by the consultant and this could include the results of comparing the model with other solutions including appropriate analytical models. **For an in-house code or spreadsheet produced by the consultant, adequate evidence of verification must be made available to the Agency.**

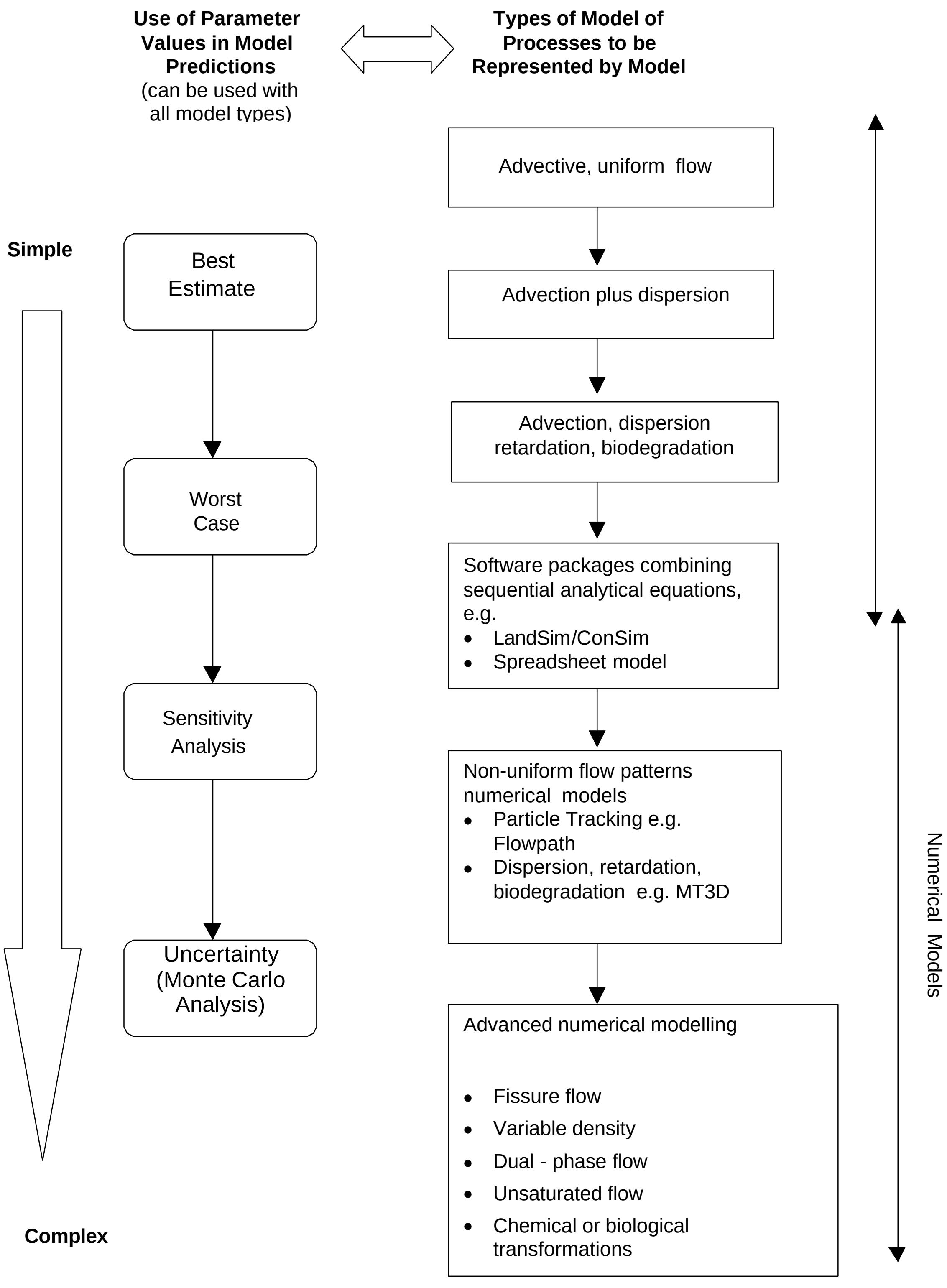
4.2 Guide to commonly used model codes

A full description of all the available contaminant fate and transport model codes is beyond the scope of this guidance but an overview of the two main types of mathematical models is given below and some of the more frequently encountered model codes are described in 'Risk assessment model fact sheets' (Environment Agency, in preparation).

4.2.1 Analytical models

Commonly used analytical models include LandSim (Environment Agency, 1996), ConSim (Environment Agency, 1999b). The LandSim and ConSim software were written by Golder Associates under contract to the Environment Agency and are designed to calculate the potential impact of a landfill (LandSim) or land contamination (ConSim) on groundwater. Further details of these programs are included in 'Risk assessment model fact sheets' (Environment Agency, in preparation).

Figure 4.1 Modelling approaches



4.2.2 Numerical models

Although this document is not intended to cover numerical models, some of more commonly used codes are identified in this section for information only. Many numerical models use the well known groundwater flow modelling code MODFLOW with any one of the popular pre-processors (Groundwater VISTAS (which is the Agency adopted system), VisualModflow, PMWin) to superimpose a contaminant distribution. MODPATH and PATH3D perform particle tracking while MOC and MT3D include dispersion. These model codes are capable of 2D or 3D and time variant or steady state simulations. FLOWPATH is a 2D particle tracking code which has recently included transient modelling of flow. These model codes all use finite difference simulation but other programs such as MicroFem and AQUA use finite element approaches (for a discussion of finite difference and finite element approaches see, for example, Anderson and Woessner, 1990).

Programs that couple the flow equation with the contaminant transport equation (in order to take account of variable density) include SUTRA, SWIFT and NAMMU. Other programs such as ARMOS include multi-phase flow.

5. Reviewing model design and its input data

In the previous chapters, we have established that the conceptual model needs to be robust and the modelling approach acceptable. The next step is to assess whether the model (i.e. code and data) is correct. In essence the criterion must be that it adequately represents the conceptual model. In this chapter we will discuss the transition from conceptual model to quantitative model, and the importance of checking that this process is adequately reported and justified, including discussions of any simplifications that have been made in applying the model.

Summaries are given in Tables 5.1 to 5.3 of the various aspects of models that should be considered in their assessment.

Table 5.1 describes the influence of different parameters (for example bulk density) and processes (for example sorption) on contaminant transport and how these are often represented in a model.

Table 5.2 identifies some of the main components in the model design and what to look for in considering the model construction.

Table 5.3 provides a checklist of the information that should be provided to justify the choice of mathematical model and the model construction (including how it represents the conceptual model).

The judgement as to whether the modelling approach is appropriate, whether a valid mathematical model has been used for the problem, and whether the model adequately represents the conceptual model will be dependent on the different factors identified in Tables 5.1 to 5.3. This decision will be also dependent on the experience of the reviewer and whether the approach used is considered to be reasonable. If in doubt, the consultant should always be requested to provide clarification of any points, or other staff within the Agency should be consulted.

In the following sections, guidance is provided on specific approaches that should be adopted when reviewing different types of models.

5.1 Analytical calculations or spreadsheets

The modelling assessment may have been undertaken based on analytical equations or spreadsheets, often developed in-house by the consultant. These may range from relatively simple mathematical models that consider rates of contaminant migration, to more complicated mathematical models that combine a number of sequential calculations. In assessing such models it is important to have an overall understanding of what the model does, and how it has been built. **The consultant should have provided a clear description of the mathematical model and a copy of the relevant programs or spreadsheets** (see Section 4.1).

Suggested approaches for the evaluation of such mathematical models include:

1. Check whether the equations used are referenced or are common knowledge to a qualified hydrogeologist. Some of the more common analytical expressions are included in

Appendix A. In this way, you can be sure what the assumptions and simplifications are by reference to the literature.

2. Compare the model results with an existing analytical model, such as the 1D Ogata-Banks equation (Appendix A) or the Environment Agency remedial target spreadsheet (available on the Web) to check that the results are of a similar magnitude (be aware that key functions in Excel (Version 7) give incorrect results).
3. Verify the result by checking through the calculations. This is often a case of following it through on a line-by-line basis. Mistakes are most often made with units, so these should be checked carefully.
4. If the calculation is available electronically, examine the sensitivity of the model to changing parameters values. This exercise will benefit in terms of:
   - Understanding the sensitivity of the model to the parameter values and whether this has adequately been taken into account by the consultant;
   - Checking that the model behaves in an expected way (e.g. increasing the degradation rate should decrease calculated contaminant concentrations). This may identify errors in the model coding;
   - Consider whether the modelling approach and choice of model parameters values is over or under conservative.

Some other points of guidance are:

- Is the source term correct? Most solutions either use a constant rate source term, a declining source term or assume a slug of contamination. The model mass balance should be checked to determine whether the modelled mass is comparable to the actual contaminant release. The selection of a constant source term generally implies a conservative assessment.
- The number of dimensions. Usually using 1D or 2D is conservative for an essentially homogenous aquifer in the sense that dispersion in the other one or two dimensions is neglected. Using 3D or 2D with a point source may be under-conservative if the source is large.
- Make sure the calculation presented is roughly consistent with the plug flow calculation. The arrival time of half the source concentration (continuous source) or the maximum concentration should be close to the plug flow arrival time allowing for retardation. The equation is:

  $TT = xnR/Ki$

  where

  TT = travel time (d)

  x = distance (m)

  K = hydraulic conductivity (m/d)

  i = hydraulic gradient

  n = transport porosity

R = retardation factor

$= 1 + K_d \rho/n$

- K_d = partition coefficient (ml/g)
- ρ = bulk dry density (gm/cm3)

- The plug flow time of travel can also be used to check how many half-lives have elapsed in checking the use of a formula incorporating degradation.
- If the receptor/compliance point is not directly down-gradient, it is very important that the transverse dispersion is not underestimated. Assuming that the receptor is directly down-gradient would be conservative. If flow direction changes seasonally, this is a reason to increase transverse dispersion.
- Check that the calculated groundwater flow (*Q*) is roughly equivalent to recharge over the groundwater catchment (*QQ*) e.g.

  $Q = Kbwi.$

  where

  Q = groundwater flow (m^3/d)

  K = hydraulic conductivity (m/d)

  i = hydraulic gradient

  b = aquifer thickness or mixing depth (m)

  w = width of site (m)

  $QQ = AR$

  where

  QQ = total recharge (m^3/d)

  A = area of groundwater catchment to site (m^2)

  R = recharge rate (m/d)

- Make sure that any equations used in the calculation (in-house spreadsheets) are correct.

5.2 Common analytic codes

The LandSim and ConSim model codes (refer to ‘Risk assessment model fact sheets’, Environment Agency, in preparation) are two of the most common codes used by consultants undertaking groundwater risk assessments. Since these codes have been approved by the Environment Agency, the task of assessment comes down to ensuring that the models are applicable to the site and conceptual model, and checking the input data.

Table 5.1 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.
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. For the unsaturated zone travel times are typically calculated as function of unsaturated zone thickness, infiltration or leakage 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).
(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.

Table 5.1 (continued) Influence of model parameters on contaminant transport

Parameter	Influence on contaminant transport	Comments
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. Take care not to assume a large mixing zone and then have vertical dispersion (or you will double count that dilution).
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.

Table 5.1 (continued) Influence of model parameters on contaminant transport

Parameter	Influence on contaminant transport	Comments
Organic partition coefficient (K_{OC})	Used in calculation of retardation of contaminant or in soil water partitioning.	Partition coefficient typically calculated as: $K_D = f_{OC} \times K_{OC}$ (for non-ionised organic contaminants)
	Rate of contaminant migration	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, 2000f) which will increase the surface area, when compared to in-situ samples.
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. metal, Cl 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, 2000e) by observable mass loss and geochemical indicators, and should not normally rely solely on literature data.

Table 5.1 (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, 2000e)

Table 5.2 Assessment of model design

Component	Description	What to look for
Assessment of parameter values	Parameter values used in the assessment should represent a realistic use of conservative and worst case values. Parameter values may be specified as a single value or by a probability density distribution.	Are parameter values optimistic or conservative compared with observed or literature values, e.g. are they realistic, or do they try to present an unrealistically good or bad case? Most analytical models require parameter values to be specified as a single value, whereas actual values may vary spatially and with time. In addition there will be uncertainty as to parameter measurement and whether it describes the system behaviour (Environment Agency, 2000b) Has an uncertainty or sensitivity analysis been undertaken to assess the effect of natural variability or uncertainty in parameter measurements, particularly for parameters with a large natural variation (e.g. hydraulic conductivity)? Has sampling bias and scale-dependency been taken into account? Do model parameter values result in realistic model solutions when compared to field observations? How have values based on point (e.g. borehole) field measurements been distributed across the model domain? Is this distribution credible? Are values conservative, best guess or optimistic and do they result in plausible model results?
Contaminant source (see also initial conditions and boundary conditions)	The contaminant source may be represented using a number of different approaches such as: • constant concentration boundary (e.g. dissolution of organic contaminants from a NAPL source); • initial contaminant concentration in groundwater; • contaminant concentration in recharge to the model.	Important to check whether the initial modelled contaminant mass and subsequent additions to this (e.g. from constant head boundaries) is consistent with original contaminant release. Constant concentration boundaries are likely to represent a conservative condition.

Table 5.2 (continued) Assessment of model design

Component	Description	What to look for
Depletion in the source term	The contaminant mass is likely to decrease with time due to solution, volatilisation, degradation.	How has the decline in the source term been represented (typically this is as a first order reaction)? For example, the LandSim model represents the decline in the leachate source term as a first order decay rate calculated using the waste thickness, waste porosity and infiltration. Where possible, field observations should be used to provide support for a decline in the source term, e.g. decline in contaminant concentrations with time. The modelled contaminant mass balance should be checked to determine if it is consistent with the actual contaminant source. A comparison of results from a constant source and declining source term can be informative.
Model Domain or Area	The model area should include the contaminant source and identified receptors. As far as possible the model boundaries should relate to actual boundaries such as edge of outcrop, faults, groundwater catchment divides.	How do model boundaries relate to actual boundaries (e.g. edge of outcrop)? How accurately does the model portray the geometry of the system (e.g. aquifer thickness)?
Boundary conditions	A range of possible boundary conditions can be incorporated into analytical solutions, and which can have an important influence on the model solution The most common is a constant concentration boundary condition or injection of a specified contaminant mass.	Is boundary condition consistent with conceptual model e.g. history of contaminant release and is modelled contaminant mass comparable to estimated contaminant mass (e.g. spill volume)? How sensitive is the model to changing the boundary condition and location?
Steady state or time variant conditions	Analytical models are either steady state or time variant.	Steady state models are likely to represent a conservative case (i.e. contaminant concentrations after infinite time has elapsed). A number of assumptions will be necessary in setting up a steady state model, particularly how model parameters should be averaged and these assumptions should be checked. A steady state model provides no indication of time scale and this should be checked, for example the plume may take thousands of years to reach the receptor and this may be important when determining an appropriate response to a predicted impact.

Table 5.2 (continued) Assessment of model design

Component	Description	What to look for
Number of dimensions	Analytical models can be set up to represent 1, 2 or 3 dimensional transport, usually by adding a dispersive term in more than one direction.	Dispersion can have a significant influence on contaminant concentrations, and the validity of allowing dispersion in more than one dimension should be checked. This could be assessed through a sensitivity analysis.
Multi-component models e.g. unsaturated zone/saturated zone	Most contaminant problems comprise a number of components, e.g. vertical leakage through the unsaturated zone and lateral migration through the aquifer. In order to model such systems a number of separate models may need to be linked or the system simplified.	Models can be developed to represent such systems based on sequential calculations. For example the LandSim code considers migration through the unsaturated zone, vertical leakage through a confining layer and horizontal flow through the underlying aquifer. The modelling report should provide a clear description of how the system has been represented, including justification and a discussion of the implications of any simplifications.
Initial conditions (including definition of plume geometry)	Analytical expressions can be combined or superimposed to allow variation in starting conditions (plume geometry) to be taken into account.	Where the results of a number of calculations have been combined, evidence of verification of these calculations should be provided.
Representation of contaminant transport processes (see also Table 5.1)	A model will require the processes affecting contaminant fate and transport to be represented by relatively simple equations.	How has the process been represented? For example, degradation is often represented as a first order reaction (see Table 5.1). Do field observations confirm that the assumed process is reasonable? e.g. field observations may indicate that degradation is inhibited at high contaminant concentrations and therefore that a single degradation rate is not a realistic model assumption.
Water balance	Values of hydraulic conductivity, hydraulic gradient, aquifer dimensions will be used in the calculating contaminant concentrations in groundwater. These parameters should also be used to calculate groundwater flow rates or leakage rates to check if these flows are reasonable.	Information on calculated leakage rates, groundwater flows should be provided. Calculated groundwater flow should be checked against estimated flow based on recharge over the catchment area to the site. This may allow an unrealistic for value for hydraulic conductivity to be identified. Calculated leakage rates should be checked against infiltration over the site area.

Table 5.2 (continued) Assessment of model design

Component	Description	What to look for
Contaminant mass balance	Contaminant models typically are used to calculate contaminant concentrations in groundwater. In addition, the contaminant mass should also be calculated.	Is modelled contaminant mass consistent with actual contaminant release, or with an estimate of the contaminant mass with the plume.

Table 5.3 Tick list for model code selection, design and input parameters

Topic	Specific Item	Y/N	Comment
Model code selection	Name and version number of model code (including appropriate references)		
	Basis for selection of model code/method		
	Description of model code/method together with relevant references		
	Details of model code verification (not required for LandSim/ConSim), although the use of check calculations is recommended.		In-house model codes or spreadsheets should be supported with calculation checks
Model design/ results	Model input parameter values		
	Justification/basis for parameter values		
	Description of how contaminant fate and transport processes have been represented (e.g. biodegradation, sorption) and justification for approach		
	Description and justification of model assumptions and simplifications		
	Description and basis for model domain		
	Justification for steady state or time variant model		
	Model results/output including presentation of data (graphs, tables)		
	Does the report provide clear links between model input and model results?		
	Details of model validation including presentation (graphs, tables)		
	Results of sensitivity analyses including presentation (graphs, tables)		
	Are differences between modelled and observed values discussed and explained satisfactorily?		
	Description of model prediction runs		
	Description of relationship of computer model to conceptual model (including schematic figures). Is this acceptable?		
	Do all model parameters seem physically reasonable and consistent.		
	Are model calculation checks provided, e.g. model contaminant mass versus contaminant release, groundwater recharge versus groundwater flow.		

Some useful checks that should be undertaken as part of the assessment of these models include:

General

- Parameter values have been based on site specific data, or if literature or default values have been used then these have been justified (and should be conservative);
- The choice of probability density function and the parameters that describe this function are appropriate and can be justified based on site specific data. Specific guidance on the use of probability density functions (PDFs) in relation to input parameters for stochastic models is given in Environment Agency (2000b);
- Model results are consistent with any field data, e.g. if the model predicts no breakthrough for an existing site then this should be confirmed by groundwater monitoring;
- Check that groundwater flow rates (calculated using the model values for hydraulic conductivity, hydraulic gradient etc) are broadly consistent with recharge over the groundwater catchment.

LandSim

- If a declining source term has been assumed, the rate of decline should be checked to see if this is reasonable and consistent with any leachate quality data for the site. Good practice would be to check the results with a non-declining source term to determine the significance of a declining source to the model results;
- Graphs of concentration against time have been presented, and not just the results for the times specified as default in LandSim.

Consim

- ConSim assumes a constant source term, but does provide a contaminant mass balance. This should be checked against any estimate of the actual contaminant mass. This may provide an indication of how conservative the model prediction is.

In undertaking this assessment it is recommended that the reviewer should have an understanding of how these codes work, including the basic equations and assumptions that are incorporated in them.

Consultants may also propose additional calculations to these codes and provided these can be justified they represent a valid approach. An example of this is that the LandSim (V1.08) code does not allow for degradation of contaminants (although this will be included in LandSim 2). A common approach by consultants is to use LandSim (V1.08) to estimate the travel time for the contaminant to migrate through the unsaturated zone. This travel time can then be used in a separate calculation, taking account of degradation, to determine the contaminant concentration at the water table (simplified example given below):

$C = \quad C_0.\exp(-l\,t)$

where

C = concentration at base of unsaturated zone (mg/l)

C_0 = contaminant concentration at top of unsaturated zone (mg/l)

t = travel time for contaminant to migrate to the water table as derived from the LandSim model (d)

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

In evaluating such an approach some of the issues to consider are:

- Is the approach consistent with the conceptual model and can it be justified;
- Has the modelling approach been adequately explained;
- Have appropriate parameter values been used and can these be justified, e.g. rate of degradation.

5.3 Other models

This document is not intended to provide guidance on how to assess more complicated models (e.g. numerical contaminant fate and transport models). In such cases the normal procedure would be to refer these to a modelling specialist.

In general more complex models should be checked using a simpler method (e.g. plug flow calculation) to check that the results are credible. If an error has been made, it will often manifest itself as an answer significantly different (by orders of magnitude) from a similar but simpler calculation. If this happens, the reason why it happens needs to be explained by the modeller. Evasive answers implying that complicated models “are always right” should not be accepted - complexity gives more room for mistakes.

6. Assessment and interpretation of model results

6.1 Introduction

The specific outputs and results produced from a modelling study will depend on the original objectives of the modelling and the type of model used. For example, the information required for the design of a remediation strategy may be the optimum number, location and pumping rate of the boreholes required to remediate the site to a specified concentration, whereas the information required for a land contamination risk assessment may be the concentration and mass of contaminants likely to reach a receptor, and the predicted travel time from the source to the receptor.

In the case of the risk assessment, the regulator needs to decide whether to accept the model and its conclusions. This decision in turn depends on the acceptable concentrations at the receptor and how the model predictions compare with it, and the uncertainty associated with the model result. Establishing the tolerable level of contamination at a receptor (the target concentration) and the level (or threshold) at which action is required (the remedial target) will depend on the nature and sensitivity of the receptor. Guidance on deriving remedial targets is given in a number of Environment Agency documents (1999a, 2000c).

Guidance on some of the key points to consider when evaluating the results from a model is given in Tables 6.1 and 6.2. Table 6.1 summarises the factors that should be considered in demonstrating the robustness of the model. Robustness, particularly the ability to match existing data, improves the confidence that can be attached to model predictions. Table 6.2 provides a summary of some of the factors that should be incorporated in the risk assessment approach, e.g. the distance to a compliance point and the choice of an appropriate target concentration at this compliance point.

6.2 Presentation of results

Model output should be clearly and succinctly presented and in graphical format where this is appropriate. Validation data (e.g. comparison of modelled and observed contaminant concentrations) should be given for key model runs or checked where models are supplied on disk. Clarification should be sought if important model results are not presented, and decisions made on the basis of model results should be justified with the appropriate model output.

For spreadsheet models and those using common codes such as LandSim or ConSim, the input files or spreadsheets should be provided in digital format, so that the simulations may be re-run and checked (e.g. to check consistency between the model and the reported results).

Table 6.1 Assessment of the model results

Factor	Description	What to look for
Model validation	Computer models should be checked against field observations to demonstrate that the model provides a realistic simulation of the system behaviour. It should be noted that the model solution may not be unique. Where models cannot be checked against field observations, e.g. predictive runs, the model should be run for a number of scenarios to represent the likely range of possible conditions.	Are model results acceptable when compared with observed values both spatially and with time? Have differences between model and observed values been adequately explained?
Model verification	Errors can occur in data entry, in setting up a model, in calculations performed by the model and in processing the model results.	Have independent calculations been provided to provide support for the model calculations?
Parameter values	Parameter values may be modified in refining the model simulation of observed conditions. The values should still relate to field measurements or literature values.	Are parameter values plausible when compared to field or literature values. Limited or poor data to support choice of parameter value. Inadequate account taken of observed system variability?
Sensitivity analysis	A sensitivity analysis is useful in identifying input parameters which have the greatest influence on the model results. The results of the analysis should be used to determine the need for further site investigation, to identify which parameters need to be considered in predictive runs and to define the range in parameters values for predictive model runs.	Have sensitive parameters been considered in subsequent site investigation or model predictive runs? Does sensitivity analysis cover full range of plausible values? Are conservative, or optimistic values used for those input variables identified as being most important by sensitivity analysis?
Uncertainty analysis	The modelling approach should take account of uncertainty in parameter measurements and/or the natural variability of a parameter value through sensitivity analysis or probabilistic analysis.	

Table 6.2 Using fate & transport models as part of a groundwater risk assessment

Factor	Description	What to look for
Are model results sensible	The model results should be compared with observed or expected system behaviour	Initial or modelled contaminant concentrations exceed effective or theoretical solubility. Predicted contaminant concentrations and distribution agree with observed values. Modelled contaminant mass agrees with the actual contaminant release.
Use and selection of mathematical model	Computer code should be selected based on objectives, complexity of conceptual model and data availability.	Sufficient data are available to justify a modelling approach. The system is sufficiently well understood. The proposed computer code is appropriate to the problem and the basis for its selection justified.
Conceptual model	The mathematical model should be consistent with the conceptual model and any simplifications in the system behaviour justified.	Have key processes controlling groundwater or contaminant movement (preferential pathways) been ignored or over simplified.
Target concentration	Target concentration (P20 methodology)* should be selected as either background quality or a water quality standard appropriate to the current or potential use of groundwater.	Would the use of a water quality standard determining a remedial target result in an unacceptable deterioration of existing water quality, e.g. selection of the drinking water standard of 400 mg/l for chloride when the background concentration is 40 mg/l.
Compliance point	Compliance point (used in derivation of remedial targets, P20 methodology)* should be selected to provide adequate protection of the water resource.	Would the selection of a down gradient compliance point result in unacceptable migration of the contaminant plume. Can this point be monitored to validate the model, e.g. can groundwater quality be monitored off site.
Receptors	All receptors should be identified and assessed. An appropriate receptor should be selected. This may include groundwater below the site.	Ensure that the receptor is relevant, sensible and applicable in context of legislation (e.g. for Regulation 15, Groundwater Regulations, 1998, receptor is receiving groundwater; for other situations (e.g. historic contamination), a more remote compliance point may be applicable).
Legislation	Regard should be given to legislative requirements. For example the Groundwater Regulations 1998 prohibit the discharge of List 1 substances to groundwater.	Summary demonstrating that the modeller understands the context and constraints of the legislation. Particularly important to distinguish between requirements to prevent pollution from current (or new) activities (i.e. Groundwater Directive, Landfill Directive, IPPC Directive) and requirements for dealing with historic contamination (i.e. Part IIA, EPA 1990; planning regime).

* Environment Agency, 1999a.

6.3 Approach to uncertainty

The approach used to take account of uncertainty should be clearly documented in the modelling report. The main approaches to uncertainty are as follows:

Best Estimate (BE) Prediction.

The calculation (or model) is performed using the most likely value for each parameter. This should always be carried out in order to gain an understanding of what the model is doing. The value arising from this calculation gives a starting point for uncertainty analysis. This version of the calculation is the one that should be checked thoroughly because this model is, essentially, the foundation of the prediction – if it is flawed then anything that follows from it is of no value.

However, on its own, this version of the model gives no understanding of the magnitude of uncertainty.

Worst Case (WC) Prediction

This is the same model as used for Best Estimate but with the parameters reset at their most conservative possible values. This is a very useful calculation and will usually be over-conservative. The difference between the Best Estimate prediction and the Worst Case prediction indicates the magnitude of the uncertainty involved.

The basis for deriving the best estimate and worst case values should be documented. It is important to note that worst case estimates values should be used with caution. On one hand they may result in implausible model predictions, particularly where worst case values have been combined. On the other hand, a worst case value may have been selected based on observed measurements, but if insufficient field data have been obtained these may not accurately reflect the variability of the system, i.e. they may not be worst case. It is also important to recognise that due to non-linear relationships, the combination of most conservative parameter values may not necessarily yield the worst case result. It is therefore important to understand what is being represented when worst case values are combined and whether this is a credible combination.

The relative size of the Worst Case (WC) estimate compared to the target concentration (TC) can be used to guide the requirement for uncertainty analysis. This is illustrated in Table 6.3 and in Figure 6.1.

Table 6.3 Example actions recommended after best estimate and worst case results known

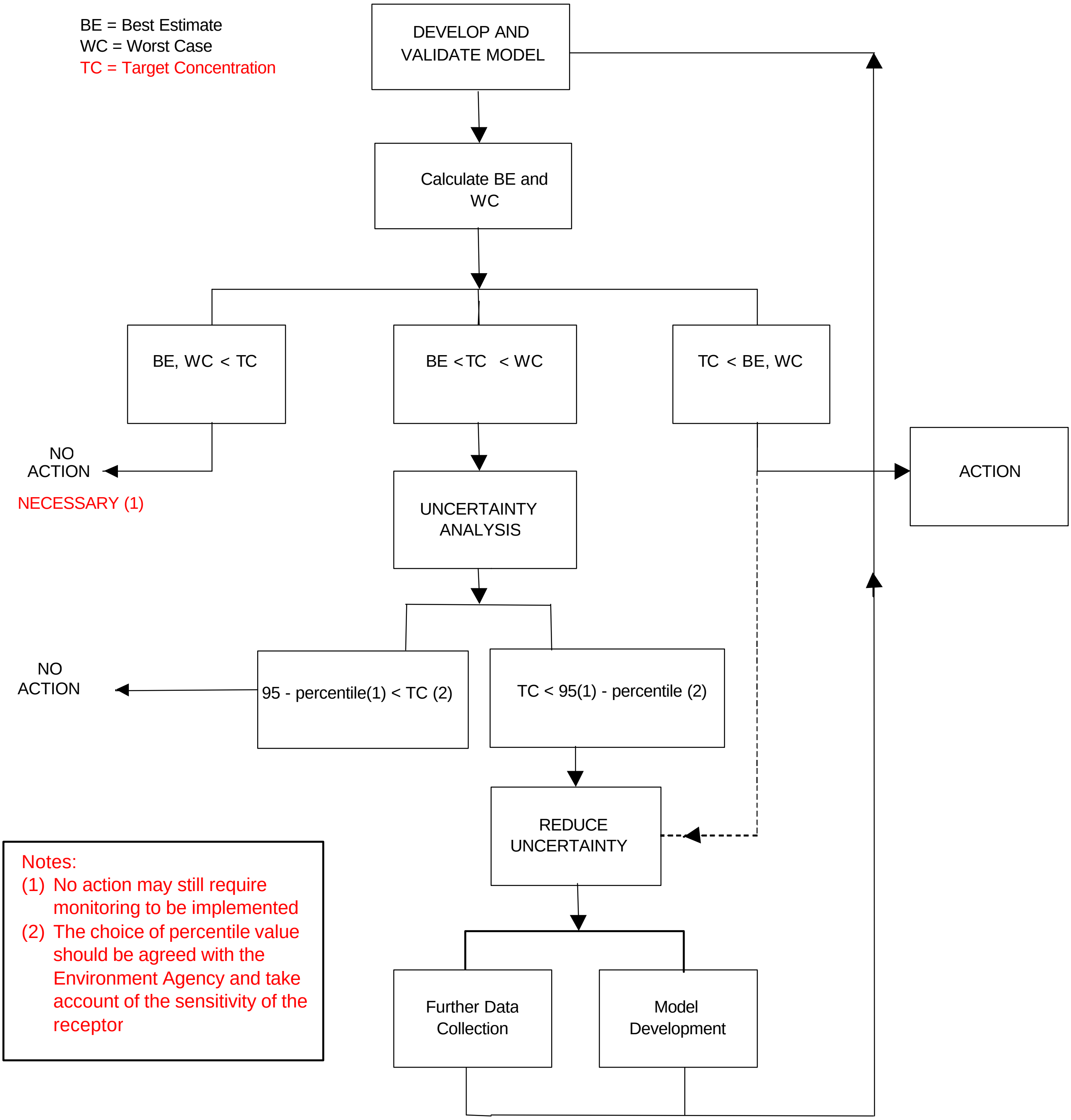
Magnitude of the target Concentration (TC) relative to best estimate (BE) and worst case (WC) results for impact at receptor	Action on site
BE, WC < TC All predictions are less than the 'target concentration' at the receptor	NO ACTION. If reasonable confidence in model and enough margin of safety[1] to allow for uncertainty in model simplifications.
BE<TC<WC 'Target concentration' lies between best estimate and worst case	UNCERTAINTY ANALYSIS. Such a site may be acceptable since the worst case may be very conservative. Carry out Monte-Carlo Analysis and see where the 95-percentile lies (or other value agreed with the Agency). If the 95-percentile is below the target concentration then NO ACTION[2], if above then further assessment may be warranted (including further site investigation to more accurately characterise the site including parameter values) or alternatively remediation implemented.
TC < BE, WC Both the best estimate and the worst case are greater than the 'target concentration'	ACTION/REDUCE UNCERTAINTY. There is no point in uncertainty analysis at this point. Either initiate action now, or gather further data to determine whether there is a case for revising the assessment, e.g. a number of conservative assumptions may have been used in developing the conceptual model (such as assuming there is no degradation of organic contaminants). Further data which may demonstrate that degradation is occurring, would provide the basis for updating the assessment.

1. The margin of safety will need to be determined based on the sensitivity of the receptor, plus comparison of the range between BE and WC, and how this relates to TC, i.e. if the spread is large and the WC result is close the TC, then there is unlikely to be a sufficient margin of safety.

2. The sensitivity of the target should also be taken into account.

Conservative is used in the sense that the model is likely to overestimate any impact.

Figure 6.1 Decision tree



Probabilistic (Monte-Carlo) analysis

A probabilistic modelling approach (e.g. Monte Carlo) may have been adopted, where the input parameters are described by a probability density function. The output from such a model will also be described by a probability density function which will describe the likelihood of a given result being exceeded (Environment Agency, 2000b).

Typically the significance of the results from a probabilistic model will be assessed in terms of whether a given concentration (e.g. drinking water standard) has been exceeded at the receptor at a given confidence level (e.g. 95%ile confidence). The higher the value used the higher the confidence in the model results. The 95-percentile (i.e. there is a 1 in 20 chance of this concentration being exceeded in an infinite number of simulations) is typically used in the assessment of risk to controlled water.

The choice of an appropriate percentile should represent a balance between protecting the identified receptor and the uncertainty attached to the analysis (including definition of parameter values). For most problems a 95 percentile will be acceptable, but should be agreed as part of the consultation exercise with the Environment Agency. The final decision of whether action is required should take into account the practicability and cost of such action.

The basis for determining the criteria for assessing the results of a probabilistic analysis must be fully documented and justified.

Sensitivity analysis

Sensitivity analysis is a recommended approach to understand how the model works and in determining which parameters have the greatest influence on the model result. A sensitivity analysis comprises modifying parameter values and examining the effect of this change on the model results. This analysis is useful in identifying which parameters need to be targeted in any further site investigation.

The modeller should provide details of any sensitivity analysis, identifying which parameters have the greatest influence on the model results and whether these have been adequately defined by the site investigation.

A sensitivity analysis may also have been undertaken in the context of determining how high or low a parameter value needs to be for a remedial target to be exceeded. These values can then be compared to observed data to determine how likely or unlikely the result may be. In general uncertainty analysis provides a more robust method.

Validation

If the model correctly predicts observed contamination at the receptor or at any intervening point, this significantly improves the confidence that can be attached to the model. Only the range of parameter values consistent with the available validation data should then be considered in any further model predictions and this can often decrease the need for additional uncertainty analysis.

In reviewing the results of a model validation exercise the following points should be considered:

- Whether sufficient field data are available to validate the model;

- Does the model fit the observed both spatially and with time. A model may be able to match field data at one particular time, but may fail to represent changes in contaminant concentrations with time;

- The acceptability of the model fit to the observed data and whether any inconsistencies have been adequately explained. In some cases differences between the model and observed data can point to a flaw in the modelling approach;

- The model solution may not be unique (different combinations of model parameter can give the same result).

6.4 Reality check

The assessor must 'stand back' from the problem and check that the conclusions being produced are sensible and reasonable. This is sometimes difficult to do, when involved in the analysis and the 'nuts and bolts' of a model specification. The reality check should be based on two principles: independent input by a fresh mind, uninfluenced by the relationships and previous decision-making at the site, and the value of experience.

Three main methods are recommended to achieve this aim:

- Formalised review procedures, involving senior members of technical staff with much experience and if possible an overview of the Agency's approach.

- Communication with staff who have been involved in similar decisions at the Area/Region/National scale (and international if necessary). For particularly sensitive sites, or contentious decisions, Area staff may wish to consult with relevant colleagues at Regional level, who may then refer to National Centres.

- Contracting an independent review by an expert third party.

If a model has been accepted at all other stages in the modelling process (i.e. conceptual model, model code selection and verification, model design and input data) there is no reason why the output from the model should not be acceptable, assuming it answers the objectives of the study.

However, models can propagate mistakes, sometimes caused by simple mis-typing and other times because code is being used by insufficiently skilled practitioners who do not understand the details. These mistakes can be difficult to spot and may only be picked up because the result does not 'feel' right. There is no substitute for experience.

Mathematical models provide a useful tool in the assessment of contaminant problems, provide they are used correctly. Environment Agency staff play an important role (through consultation and review of the model) to ensuring that good practice is adopted. This does not necessarily mean that the most sophisticated model is used, but rather that models have been used in a logical and systematic way that can be related to the conceptual model, the available data, and the nature of the problem. The development of the conceptual and mathematical model should be seen as an iterative process. The assessment of models requires a range of technical skills and Agency staff should consult with relevant colleagues at Regional level, who may then refer to National Centres.

7. References

American Society for Testing and Materials, 1998 Standard Provisional Guide for Risk Based Corrective Action. ASTM Designation: PS104-98.

Anderson, M.P. and Woessner , W.W. 1992. *Applied Groundwater Modelling*. San Diego: Academic Press.

Bear, J. 1979. Hydraulics of Groundwater. McGraw- Hill Book Company, 679pp.

Bear, J and Verruijt, A. 1987. Modelling Groundwater Flow and Pollution. D.Reidel, Dordrecht, 414pp.

BGS/Environment Agency, 1997. The Physical Properties of Major Aquifers in England and Wales. BGS Technical Report WD/97/34. Environment Agency R&D Publication 8.

Crank, J. 1956. The Mathematics of Diffusion. New York Oxford University Press.

DETR/Environment Agency, 2000c. Contaminated Land Research Report CLR11. Model Procedures for the Management of Contaminated Land. DETR and Environment Agency (In preparation).

Domenico, P.A and Schwartz, F.W. 1990. *Physical and Chemical Hydrogeology*. J. Wiley & Sons.

Environment Agency, 1996. LandSim Manual - *Landfill Performance Simulation by Monte-Carlo Method*. Ref CWM 094/96.

Environment Agency, 1999a. Methodology for the Derivation of Remedial Targets for Soil and Groundwater to Protect Water Resources. R&D Publication 20. Prepared by Aspinwall & Company.

Environment Agency, 1999b. ConSim: Contamination Impacts on Groundwater: Simulation by Monte-Carlo Method. Prepared by Golder Associates (UK) Ltd.

Environment Agency, 2000a. Guide to Good Practice for the Development of Conceptual Models and the Selection of Mathematical Models of Contaminant Transport Processes in the Subsurface. NC/99/38/2. Solihull.

Environment Agency, 2000b. Technical Guidance on Assigning Values to Uncertain Parameters in Environmental Risk Assessments NC/99/38/3. Solihull.

Environment Agency, 2000d. Internal Guidance on the Interpretation and Application of Regulation 15 of the Waste Management Licence Regulations 1994 with Respect to Landfill.

Environment Agency, 2000e. Guidance on the Assessment and Monitoring of Natural Attenuation of Contaminants in Groundwater. R&D Publication 95. Prepared by Aspinwall & Company/LGC.

Environment Agency, 2000f. CEC and Kd Determination in Landfill Performance, R & D Technical Report P340, Prepared by British Geological Survey.

Environment Agency, in preparation. Risk Assessment Model Fact Sheets.

Fetter, C. W. 1992. Contaminant Hydrogeology. Macmillan.

Fried, J. J. 1975. Groundwater Pollution: Amsterdam, Elsevier.

Sauty, J. 1980. An Analysis of Hydrodispersive Transfer in Aquifers. Water Resources Research 16, 145-158.

Appendix A
Some common analytical equations for contaminant transport

This appendix gives details of some commonly used analytical expressions. It is intended for guidance only and it should be noted that the assumptions behind each one of these equations are not described in detail. If in doubt, consult a recognised text book such as Bear (1987), Fetter (1992) and Domenico and Schwartz (1990).

Symbols

TT	Travel time of contaminant (d)
x	Distance to receptor (m)
t	Time since entry of pollutant to aquifer (d)
b	Aquifer thickness (m)
n	Transport porosity
K	Hydraulic conductivity (m/d)
i	Hydraulic gradient
C_0	Source concentration (mg/l).
v	True (or average linear) groundwater velocity (m/d)
a_L	Longitudinal dispersivity (m)
a_T	Transverse dispersivity (m)
a_Z	Vertical dispersivity (m)
R	Retardation factor
λ	Decay Constant (/d)
K_D	Distribution coefficient (l/kg), sometimes called the partition coefficient
ρ	Density (kg/l)
Q	Abstraction rate at well (m^3/d)
M	Mass of solute injected (g)
Y	Width of source perpendicular to direction of flow (m)
y	Distance (lateral) to receptor perpendicular to flow direction (m)
z	Distance (depth) to receptor perpendicular to flow direction (m)
erf	Error function
erfc	Complementary error function erfc(x) = 1 - erf (x)

1. Travel Time Equation under uniform hydraulic gradient

$$\mathrm{TT} = \frac{xn}{Ki}$$

NOTE: In a fissured aquifer this equation is still valid if it is noted that the transport porosity should be set as the fissure porosity (e.g. for Chalk, the fissure porosity may be around 0.01).

2. Travel Time Equation to pumping well with no hydraulic gradient and no retardation

$$TT = \pi x^2 bn/Q$$

3. Groundwater velocity (or conservative tracer) under uniform hydraulic gradient

$$v = \frac{Ki}{n}$$

4. Retardation (R)

$$R = 1 + \frac{r}{n} K_D$$

5. Ogata-Banks, Sauty approximation with no degradation

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

The Sauty approximation is the average of the constant concentration source and the constant injection source – probably a better model than the "full solution" for many cases where the true situation is more like constant injection.

6. Ogata-Banks, Sauty approximation with degradation

$$C = \frac{C_0}{2} \exp\left(\frac{x(1 - b)}{2a_L} \right) \operatorname{erfc}\left(\frac{x - vtb / R}{\sqrt{4a_L vt/R}} \right)$$

with $b = \sqrt{(1 + 4\lambda R\alpha_L/v)}$

7. Ogata-Banks, complete version, constant concentration source, no degradation

$$C = \frac{C_0}{2} \left\{ \operatorname{erfc}\left(\frac{x - vt/R}{\sqrt{4a_L vt / R}} \right) + \exp\left(\frac{x}{2a_L} \right) \operatorname{erfc}\left(\frac{x + vt / R}{\sqrt{4a_L vt / R}} \right) \right\}$$

8. 2D Continuous Solution (retardation but no degradation

An exact solution for the continuous injection of a contaminant is given in Bear, 1979 (Equations 7-156 to 7-158). Domenico's approximate solution is more commonly quoted and is given below (Domenico, 1990)

$$C = \frac{C_0}{4} \operatorname{erfc}\left(\frac{x - vt / R}{\sqrt{4a_L vt / R}} \right) \left\{ \operatorname{erf}\left(\frac{y + Y / 2}{\sqrt{4a_T x}} \right) - \operatorname{erf}\left(\frac{y - Y / 2}{\sqrt{4a_T x}} \right) \right\}$$

An alternative is Emsellem's solution (see Fried 1975, Fetter, 1992).

9. 2D Continuous Solution (Domenico, 1990, extended Domenico equation for retardation and degradation)

$$C = \frac{C_0}{4}\left\{\exp\left(\frac{x(1-b)}{2a}\right)\mathrm{erfc}\left(\frac{x - vtb / R}{\sqrt{4a vt / R}}\right) + \exp\left(\frac{x(1+b)}{2a}\right)\mathrm{erfc}\left(\frac{x + vtb / R}{\sqrt{4a vt / R}}\right)\right\}\left\{\mathrm{erf}\left(\frac{y + Y/2}{\sqrt{4a_T x}}\right) - \mathrm{erf}\left(\frac{y - Y/2}{\sqrt{4a_T x}}\right)\right\}$$

10. 1D Slug Injection Approximation (Crank, 1956)

$$C = \frac{M}{\sqrt{4pa_L vt/R}}\exp\left(-\frac{(x - vt/R)^2}{4a_L vt/R}\right)$$

The dimensions of M are (kg/m^2) so that the dimensions of C are (kg/m^3) or (g/l).

A more complex version of this solution is given in Sauty (1980)

11. 2D Slug Injection (De Jong Approximation)

$$C = \frac{MR}{4pvt\sqrt{a_L a_T}}\exp\left(-\frac{(x - vt/R)^2}{4a_L vt/R} - \frac{y^2}{4a_T vt/R}\right)$$

The dimensions of M are (kg/m) so that the dimensions of C are (kg/m^3) or (g/l).

12. 3D Slug Injection (Baetsle Approximation)

$$C = \frac{M}{8(ptv/R)^{3/2}\sqrt{a_L a_T a_Z}}\exp\left(-\frac{(x - vt/R)^2}{4a_L vt/R} - \frac{y^2}{4a_T vt/R} - \frac{z^2}{4a_Z vt/R}\right)$$

The dimensions of M are (kg) so that the dimensions of C are (kg/m^3) or (g/l).

The above equations are intended to indicate the range of analytical solutions that are available and is not intended to be exhaustive.

In using analytical equations from references, these should be checked for errors (references can contain misprints). The best approach is to check the equations against worked examples or solutions from a comparable equation.