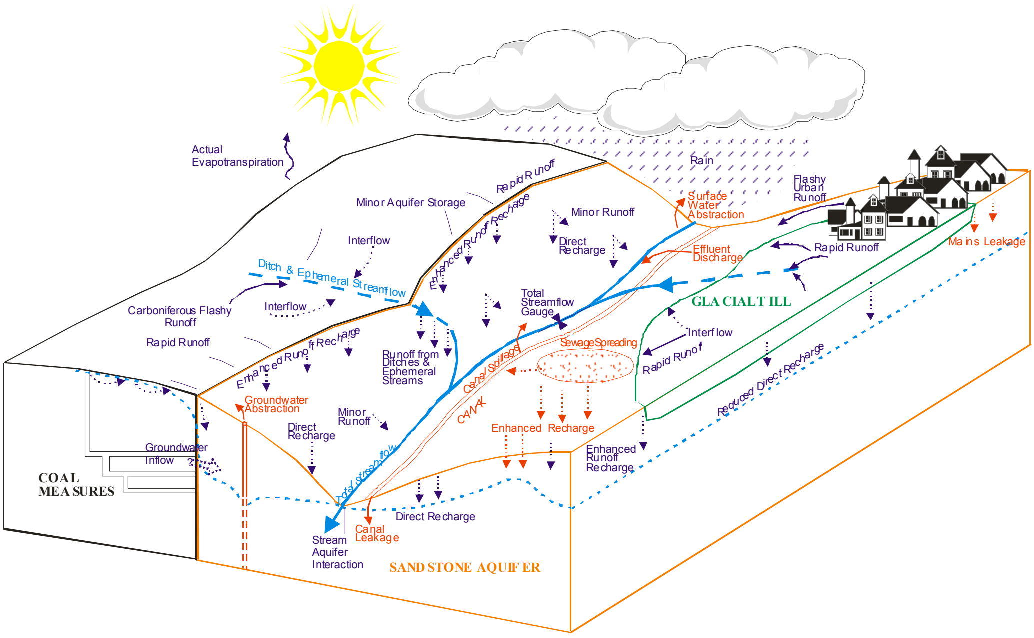
Groundwater Resources Modelling: Guidance Notes and Template Project Brief

Research and Development

Guidance Notes

W213



Strategic Review of Groundwater Modelling

Groundwater Resources Modelling: Guidance Notes and Template Project Brief (Version 1)

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Statement of use
This document aims to complement existing modelling text books and to pass on the Agency's experience of groundwater modelling in England and Wales accumulated over 30 years on to a wider audience both within the Agency and externally.
Evaluation of this version by the Agency and nominated consultees took place during 2003. It is planned to release Version 2 during 2005.

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Comments and Feedback

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Comments have been collected on Version 1and an updated version will be produced during 2005.

AMENDMENT RECORD

The Guidance notes will be updated periodically. Version numbers for each section are recorded on the page footers.
Please ensure all amendments are recorded on this table.

Amendment No.	Amendment Date	Incorporated By	Date

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1.1 Background and Aims of the Guidance Notes & Template Project Brief

1.1.1 Background

These Guidance Notes and Template Project Brief have been produced as part of an Environment Agency R&D project: A Strategic Review of Groundwater Modelling. The Strategic Review of Groundwater Modelling R&D project has two published reports as outputs:

R&D Technical Report W213 - Groundwater Resources Modelling: Guidance Notes and Template Project Brief (this document)

R&D Technical Report W214 - Environment Agency Framework for Groundwater Resources Modelling.

Report W213 (these Guidance Notes) addresses the following objective of the R&D project:

> To consider previous modelling studies and to identify best practice and quality control procedures resulting in the production of Guidance Notes to provide insights on technical and project management topics based on the Agency's experience. This will also include a standard Terms of Reference or Project Brief.

The Environment Agency and its predecessors (the Water Authorities and the National Rivers Authority) have developed over 30 spatially distributed, time-variant groundwater models to simulate and predict the flow behaviour of aquifers at a regional scale since the early 1970's. These models have been used to aid in the assessment of water resources and the prediction of environmental impacts.

Through its abstraction management strategies, the Agency aims to secure the sustainable development of water resources. Where demand for groundwater resources is high, a better quantitative understanding of the groundwater-surface water system is required to achieve optimal use of the resources without compromising the environmental needs. A variety of tools are available to support the assessment of groundwater resources. Numerical groundwater models have the potential to offer the most accurate estimates because they can incorporate the majority of the available data. This is discussed in more detail in the Framework for Groundwater Resources Modelling (Report 214)

1.1.2 Aims

The Guidance Notes are deliberately based on the Agency's experience in regional flow modelling for groundwater resources assessments. The aim is to complement existing text books. The notes do not deal comprehensively with general modelling issues or with source protection or local contaminant transport modelling. Rather, they gather the Agency's experience on topics directly relevant to its operational use of regional groundwater modelling.

The Guidance Notes and Project Brief aim to assist in meeting the need for groundwater modelling to be developed to a high common standard by :

1. Distilling the Agency's experience of the conceptual and numerical modelling components of groundwater resources studies into a working document which can be updated as our experience grows.
2. Setting out the principles which guide the Agency's approach to conceptual and numerical modelling.
3. Raising awareness and understanding of the Agency's approach and providing a focus for discussion within the Agency.
4. Providing a "gateway" to other more comprehensive sources of information.
5. Making the tendering process easier for both Agency staff and our contractors.
6. Being one of the tools to help build the Agency's community of groundwater modellers as they share their experience and contribute to the Guidance Notes.
7. Providing a template project brief for groundwater resource modelling projects with details of the purpose, approach and outputs for each task.

The notes are based on Agency (and contractors') experience which is continually developing as more regional modelling projects are carried out. It is therefore proposed to update the notes regularly to reflect any lessons learned through additional experience. Contributions, suggestions and feedback from relevant parties are therefore encouraged via the feedback form.

The Guidance Notes are a companion to the Template Project Brief (Appendix C), which gives details of the purpose, approach and outputs for all major tasks involved in a regional groundwater modelling project.

1.1.3 Readership

The Guidance Notes are intended primarily for Agency staff involved in modelling projects, both as specialist modellers and as modelling project managers. Inevitably, some of the sections will provide either too detailed an explanation of the broad concepts for the modeller, or too much technical detail for the project manager. To address this, the style and format of the document have been produced so that different readers can readily access what they require. Topics relating to project management are covered in Section 2, whilst technical topics are covered in Sections 3 to 6.

The authors have assumed that the reader is familiar with the background and theory provided by, for example, instruction in groundwater modelling at MSc level. Familiarity with one of the standard texts on groundwater modelling (Anderson and Woessner, 1992; de Marsily, 1986; Zheng and Bennett, 1995) is also expected (and recommended). Other sources of information include Ken Rushton's series of papers on groundwater modelling in the UK and the guidance notes produced by the American Society for the Testing of Materials (ASTM). These are listed in the reference section.

1.1.4 Structure and format of the guide

The Notes comprise six chapters which are further divided into sections. Chapter 1 is this introduction. Chapter 2 deals with project management issues relating to planning and execution of a regional modelling project. Chapters 3 to 6 cover technical issues: Chapter 3 covers collation, processing and interpretation of data, Chapter 4 covers characterisation and modelling of a number of key hydrogeological processes, Chapter 5 covers quantitative testing of the conceptual model, and Chapter 6 covers aspects of numerical modelling.

As noted above, contributions, suggestions and feedback from relevant parties are encouraged, and it is expected that the document will evolve. For this reason, detailed internal referencing to individual sections by title or number has been avoided in order that the structure of the document can change, eg. with the addition of a section, without the need for revision of all internal referencing. Notification that there is other relevant material elsewhere has been given by reference to Chapters (in the hope that the Chapter structure we have adopted has some life in it!). To further assist the user in finding the information she/he requires, second level headings have been included in the Table of Contents.

Those with experience will know that modelling should be a cyclical process, with demonstrable inadequacies of the model (conceptual or numerical) and/or new information causing the modellers to return to an earlier stage in the process. Hard-copy documents do not lend themselves to reflecting this cyclical nature as they tend to be read from front to back, with the danger that modelling is portrayed as a linear process which it is certainly <u>not</u>. Hence, note the content, not the format…..

1.1.5 References

Anderson & Woessner, 1992. *Applied groundwater Modelling: Simulation of Flow and Advective Transport*. Academic Press Inc., New York.

De Marsily, G., 1986. *Quantitative Hydrogeology: Groundwater Hydrology for Engineers*. Academic Press, San Diego, 440p.

Zheng, C. and Bennett, G.D., 1995. *Applied Contaminant Transport Modelling: Theory and Practice*. Van Nostrand Rheinhold. 440p.

1.2 Groundwater modelling

1.2.1 What is modelling?

A model is any device that represents an approximation of a field situation (Anderson and Woessner, 1992).

To state the obvious, modelling is the process of creating a model. A problem or issue is defined, data is analysed and an idealised explanation of the real behaviour, the conceptual model, is formulated in terms of the major physical processes that appear to be operating. These processes are then represented mathematically, and the resulting mathematical model is used to test the initial understanding and then often to make predictions. Therefore, the preliminary conceptual understanding provided by drawing some geological cross-sections and calculating crude water balance estimates constitutes a model, as does the application of analytical solutions such as Theis.

It is this broad definition of modelling that is considered here.

1.2.2 Why undertake modelling?

The Agency has a responsibility for water resources management. It aims to secure the sustainable development of water resources through its abstraction management strategies. Where demands are high, this requires a good understanding of how to achieve optimal development of local groundwater resources for abstractive uses, but without compromising the groundwater resource allocations necessary to meet the environmental water needs of wetlands, springs and rivers, or to manage groundwater quality.

Agency staff are called to make decisions about the future use of these resources, and this raises specific questions such as:

?? will a change in the pattern of abstraction improve river flows or reduce impacts on a wetland?;

?? is a potential river support scheme sustainable?;

?? how might climate change influence available resources?

Groundwater modelling is being used more frequently as a tool to help answer these types of questions because it can lead to a better understanding of how the real system behaves and it can be used to make predictions about the system's future behaviour. This in turn helps the Agency to develop operational and regulation strategies that will secure the sustainable development of strategically important water resources.

It is likely that the obligation to develop and document Catchment Abstraction Management Strategies will become an important driver for modelling projects.

1.2.3 References

Anderson & Woessner, 1992. *Applied Groundwater Modeling: Simulation of Flow and Advective Transport.* New York, Academic Press Inc.

2.1 The groundwater modelling process

This section deals briefly with why the Agency undertakes modelling projects and outlines the various phases of such projects. General descriptions of the groundwater modelling process are readily available (e.g. Anderson & Woessner, 1992; ASTM, 1994). The main components of this process are listed below and their relationships shown in Figure 2.1.1:

- Definition of the purpose and project brief
- Collation of data & formulation of conceptual model
- Development of the historical model
- Predictions & option appraisal
- Further operational use

For the purposes of managing tasks during a modelling contract, the three main components have been labelled Phases 1, 2 and 3, as shown in Figure 2.1.1.

Figure 2.1.1 shows that the groundwater modelling process is iterative in that the project does not pass through each stage only once, but previous stages are revisited as understanding improves. For example, the mathematical representation of the conceptual model usually challenges aspects of the conceptual model and prompts its revision. This illustrates that a modelling project involves much that is open-ended and not routine. In this way, it is similar to a research project where the problems which the work itself raises are difficult to quantify at the outset. This has implications for project management and procurement. When should we stop refining the model? When is it good enough to fulfil its purpose? How simple can the model be and still provide useful answers? What hydrological processes must be included and which can be ignored?

Unlike the guidance provided by Anderson & Woessner (1992) and ASTM (1994), these Guidance Notes focus specifically on the approach being developed by the Environment Agency for regional modelling as part of its water resources investigations.

Each of the components in the modelling process shown in Figure 2.1.1 is described briefly below. More information is given under relevant topics in Sections 3 to 6 of these notes. The tasks commonly undertaken during a modelling project are listed in Box 1.

2.1.1 Defining the purpose and project brief

A clearly identified purpose will make it easier to focus on what questions the modelling project is trying to answer, and what resources of time and money are likely to be required. It will also help clarify the confidence we require in our results which in turn influences all aspects of the modelling effort.

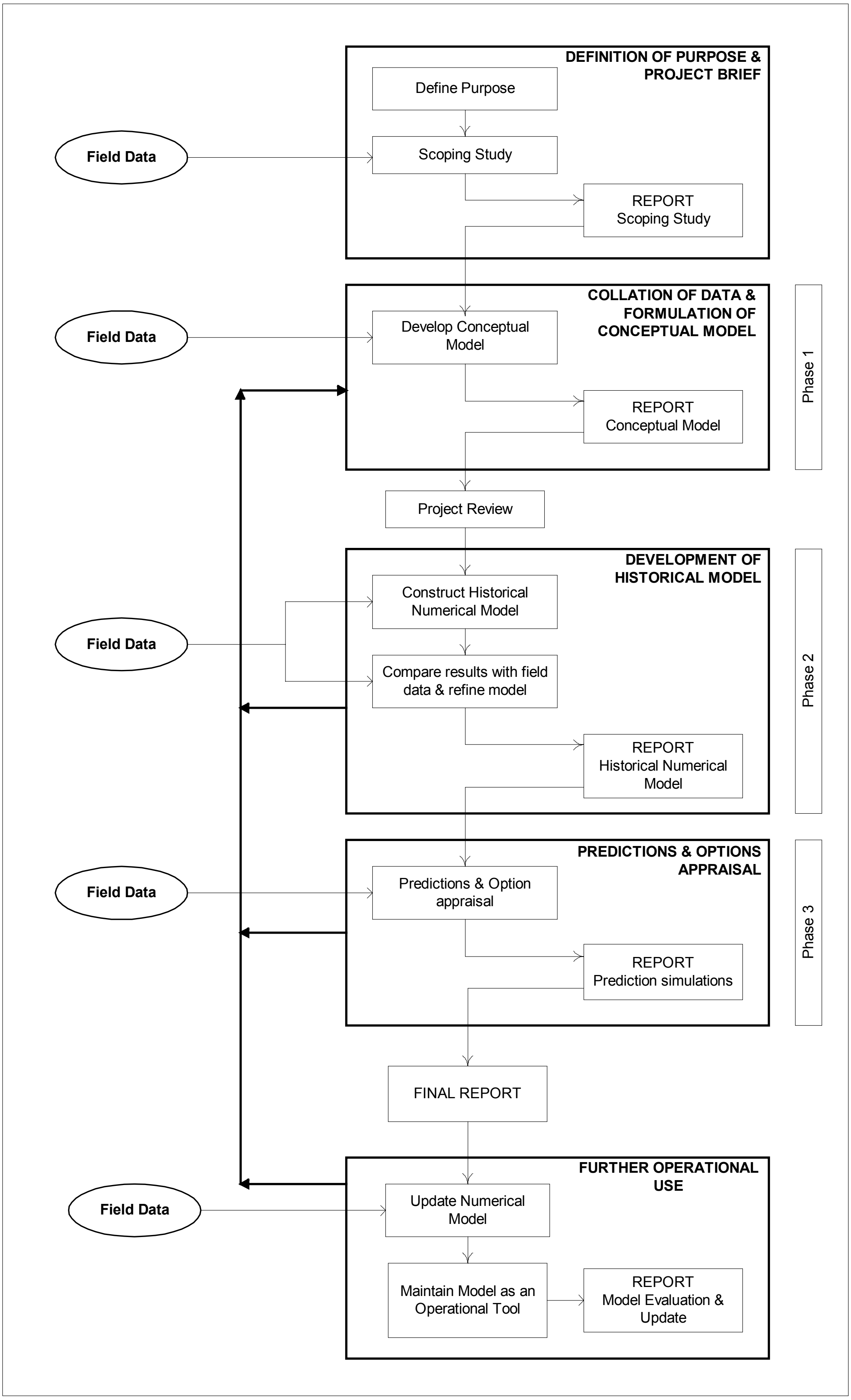


Figure 2.1.1. Groundwater Modelling Process

Box 1. Typical Tasks Undertaken During a Groundwater Resources Modelling Project

The following tasks are typical of those required during a groundwater resources modelling project.

Definition of purpose of modelling project

1) Identify the major issues in the area of interest
2) Define the purpose of the modelling study

Data collation and formulation of conceptual model (Phase 1 in Template Project Brief)

1) Inaugural meeting and visit study area with project team
2) Collate, quality assure analyse and present available data (including developing a database)
3) Critically review previous groundwater studies and models of the study area
4) Interpretation of geological data
5) Interpretation of hydrochemistry data
6) Groundwater level analysis
7) Calculation of effective rainfall
8) River-flow analysis
9) Calculate preliminary water balances
10) Develop conceptual models of surface water/groundwater system including:
    a) a definition of the extent of the study area and its subdivision into appropriate zones (vertically and horizontally) based on the hydrogeology
    b) a description of the hydrogeological conditions and flows at the boundaries of the study area
    c) an estimate of all inflows and outflows, and their variation in time
    d) an estimate of the plausible range of all aquifer parameters in each hydrogeologically distinct zone
    e) a description of the limitations of the current conceptual understanding and the major sources of uncertainty.
11) Propose whether/how numerical model should be developed and refined
12) Phase 1 report
13) Review of options for meeting project objectives

Development of historical numerical model (Phase 2 in Template Project Brief)

1) Construct model and carry out initial model runs. This will involve representing the key aspects of the conceptual models in the numerical model. In addition we will need to consider the initial conditions, the grid size and time step size, the numerical solver and its convergence criteria and the acceptance criteria (when is the model is good enough to fulfil its purpose?)
2) Refine model so that it can represent the observed behaviour of the groundwater/surface water system sufficient to answer the questions identified in the objectives of the project
3) Assess uncertainty using sensitivity analysis
4) Phase 2 report

Predictive simulations (Phase 3 in Template Project Brief)

1) Specify the options for future management of the system
2) Identify and carry out the predictive simulations
3) Assess influence of sources of uncertainty on predictive results
4) Phase 3 report followed by compilation of final project report

Further operational use

There are a variety of ways in which a model may be used after it is completed including:

1) Extend historical model as with new abstraction and recharge data
2) Compare predictions against observed response and re-evaluate conceptual model
3) Assess potential of using model for another different purpose
4) Reporting

The purpose of the model may not be clear or agreed at the beginning of a water resources study. This can be remedied by identifying the particular issues in the area of interest, the questions these raise, and the benefits the model study will bring in terms of answering these questions. For example, falling groundwater heads in a part of an aquifer raise questions about the sustainability of abstractions. For most projects a scoping study (Chapter 2) will be required to help identify the purpose and define the scope of work. For large projects this will probably be done externally and for smaller projects it can be done in-house.

The scoping study will produce a project brief for the main modelling study which defines the tasks and deliverables required.

2.1.2 Data collation & conceptual modelling

The first task in any groundwater modelling project is to collect and analyse the available data. This includes reports on the project area, papers in journals and University theses, as well as monitoring data such as groundwater and surface water abstraction records. At this stage, the importance of site visits (see elsewhere) should not be overlooked as these will give insights into the catchment behaviour and may enable some data collection to be undertaken.

The conceptual modelling and the refinement of the numerical model must be based on detailed quantitative analysis of field data. It should always be remembered that a model is only as good as the data upon which it is built.

In his paper on Groundwater at Risk, Rushton (1998) states:

"Aquifer systems are so complex that it is not possible to study every detail. This leads to the question of what needs to be included in an aquifer study and what can be ignored. For most aquifer systems there are a small number of crucial factors which must be examined in detail; if only one of these is ignored the conclusions may be seriously in error".

The objective of formulating a conceptual model is to identify and quantify the "small number of crucial processes" which will adequately represent how the real system behaves. This entails a simplification reality that involves hard hydrogeological thinking and takes up at least 50% of the modelling effort.

A conceptual model is a synthesis of the current understanding of how the real system behaves, based on *quantitative* analysis of the field data. Because conceptual modelling forms the foundation of any numerical modelling, time spent doing this well will save time during the numerical modelling. To avoid 'woolly thinking', the conceptual model must be quantified and tested (see Chapter 5) by using:

- Recharge calculations (requiring the use of a distributed recharge model)
- Water balances
- Exploratory or investigative modelling

It is vital that the conceptual model and the stages in its development are well documented since it is valuable, not only as a record of the hydrogeological reasoning behind the conceptual model, but also as a resource in its own right. This (Phase 1) report should clearly state all the assumptions being made about the system, together with the justifications for each assumption.

At this stage in the project, the options for achieving the objectives of the project should be reviewed. It might be decided, for example, that a distributed numerical model is not required to answer the specific questions to be answered by the project, and that a less sophisticated toll will suffice.

If numerical modelling is to be pursued, acceptance criteria for the historical numerical model should be proposed at this stage. The choice of model code (see Chapter 6) should not be finalised until the conceptual modelling has identified what key processes need to be represented.

2.1.3 Development of the historical model

The second phase is to represent mathematically the processes that have been identified in the conceptual model. This can be done analytically or numerically, and involves a further simplification of reality.

Analytical models such as Theis solve the groundwater flow equations exactly for all locations and times but only for highly idealised conceptual models (see Chapter 5). Numerical models (such as MODFLOW or MIKE-SHE) solve the groundwater flow equations numerically by dividing up space and time and interpolating linearly between adjacent points. This allows more complex features to be represented, such as aquifer properties which vary in space or boundary conditions which vary with time. The remainder of this section considers only numerical modelling.

Once a numerical model has been built, there follows a cyclical process of comparing the output from the model with the observed data and other information. When they differ, the conceptual model is re-evaluated and the numerical model revised. Although this is often referred to as *calibration*, this is a misnomer and *refinement* (Chapter 6) would be a more accurate description of what is required. The acceptance criteria for the model in terms of, for example, simulation of observed groundwater levels or baseflows, will have been agreed in the proposal for the model development included in the conceptual model report.

2.1.4 Predictions & analysis of results

When the historical model has been refined so that the user has confidence that it can adequately represent the past behaviour of the groundwater system, the model may be used for predictive runs. The results are analysed in the light of the assumptions made in the numerical model and by comparison with the conceptual model in order to inform a management decision.

Sensitivity analysis is required during both the historical and the predictive simulations to assess what influence various sources of uncertainty may have on the results.

2.1.5 Further operational use

Regional groundwater modelling projects can be expected to cost between £100,000 and £300,000 over 3-4 years. This is a significant investment of time and money. Ongoing benefits from a modelling project can be realised if the management tools are kept up to date. Therefore, both the conceptual model and the numerical model need to be evaluated and updated in the light of new field data and new insights into how the system is behaving. Again it is essential that these activities are written up.

Anglian and Midlands Regions have recently (1998 & 1999) been carrying out a comprehensive review and post-project evaluation of their existing models with a view to their future usefulness.

2.1.6 Reporting

Comprehensive reporting at completion of each of the five stages noted above is essential.

Reporting at the end of each phase and not just at the end of the project is essential to allow detailed review by Agency staff before committing to the next phase of work. This review provides the opportunity to check that the report adequately documents the work done, how it fits together and the implications for the next phase. Section 4 of the Guidance Notes covers this topic in detail.

The conceptual and numerical modelling reports form the main outputs of a modelling project.

2.1.7 Template Project Brief

The template Project Brief divides the conceptual and numerical modelling components of the modelling process into five project phases and provides details of the purpose, approach and outputs required for the tasks in each phase.

The relationship between the modelling process and the phases in the Template Project Brief is given in Table 2.1.1.

2.1.8 Field work

Field work to collect additional data is not identified as a separate single stage in Figure 2.1.1 because it may be undertaken at any time during the modelling process. Further field investigation may be required, for example:

- after the conceptual modelling and prior to any numerical modelling because the conceptual model cannot be sufficiently well defined;
- after the refinement to reduce uncertainty in the predictive simulations;
- as part of the post-project evaluation and updating and when a new purpose arises.

Table 2.1.1. Relationship between modelling process and project phases in Template Project Brief

The Modelling Process	Phases in Template Project Brief
Definition of the purpose	Not included – defined by Terms of Reference for a scoping study
Collation of data & formulation of conceptual model	*Phase 1* Data Collation & Formulation of Conceptual Model
Development of the historical model	*Phase 2* Development & Refinement of Historical Model
Predictions & option appraisal	*Phase 3* Modelling of Resource Options *Phase 4* Final Report *Phase 5* Training & User Support
Further operational use	Not included

2.1.9 References

Anderson & Woessner, 1992. *Applied Groundwater Modeling: Simulation of Flow and Advective Transport.* New York, Academic Press Inc.

ASTM, 1994. *Standard Guide for the Application of a Groundwater Flow Model to a Site-Specific Problem.* American Society for Testing and Materials. Reprinted from the Annual Book of Standards.

Rushton K.R., 1998. Groundwater at Risk – A Reflection. *Hydrology in a Changing Environment, Volume 2*. British Hydrological Society. International Conference, Exeter. Wiley. p 1-10.

2.2 Defining the Purpose of a Modelling Project

2.2.1 Role of groundwater modelling

The role of modelling work within a water resources investigation has been outlined in the Environment Agency Framework for Groundwater Resource Conceptual and Numerical Modelling (Environment Agency, 2001) and is summarised here.

Numerical modelling is being used increasingly to quantify the water resource availability of our complex, dynamic groundwater/surface water systems and to take account of the environmental impact of abstraction. However, to be credible, modelling tools must be technically valid and agreed representations of the real system. Therefore, one of the key objectives of any resource study is the process of developing a shared understanding (the conceptual model) of the essential flow mechanisms. Only then can the numerical model be used as a predictive tool to investigate different future conditions (e.g., new abstraction regimes and changes in climate).

2.2.2 Purpose and objectives of a modelling project

Within the framework of national and regional resource assessments/modelling strategies, each project needs to be fully justified and have specific and achievable aims and objectives to address identified issues e.g. over-abstraction causing saline intrusion or low flows in rivers. With the move towards integrated management of surface and groundwater catchments, the aims and objectives are likely to be wider than just water resources i.e. they will be multi-functional, and impact parties outside the Agency. Without a clear purpose, a project is very likely to be poorly defined.

In setting the objectives it is often useful to write a list of questions which need to be answered. To answer these, we need to understand the flow behaviour of the system. However, the very nature of hydrology and hydrogeology, i.e. their complexity, spatial and temporal variability, and frequent data deficiency, means it is impossible to ever *fully understand* a system. The conceptual model will inevitably be a simplification of reality and the limitations imposed in representing the key processes mathematically will involve further simplifications and idealisations. Therefore, to guide us in making appropriate simplifications, we must focus on the processes and parameters which are relevant to answering the specific objectives of the study.

The purpose of the modelling work and the specific modelling objectives should be defined in advance of a scoping study. For example, the overall purpose may be to assess the potential effect on river flows of redistributing abstractions. The specific objectives can often be listed initially as a set of questions which the project aims to answer. These should be directed at aiding operational decision making.

The River Itchen study illustrates the nature of modelling project aims and objectives. The Itchen is recognised as a SSSI and cSAC and therefore, under the Habitats Directive, competent authorities are required to undertake appropriate assessments of proposed developments that may have significant effects in habitat terms. A Steering Group, including competent authorities and various stakeholders, has been set up to determine a sustainable management strategy for the river. The groundwater modelling is on the critical path of the Itchen sustainability study and the groundwater model is pivotal to the resolution of some key issues.

The overall objectives for the model, as made explicit in the Agency's Itchen project document are:

- to produce outputs in support of the River Itchen sustainability study objectives;
- to be a water resources management tool;
- to assist with assessing abstraction licences under the Habitats Directive Review;
- to determine water resources balances for the Test and Itchen CAMS.

The specific objectives were expressed as a series of questions:

- do public water supply abstractions at Easton, Totford, Twyford and Otterbourne have an impact on river flow?;
- what is the impact on river flow of using all groundwater public water supply licences at their full licenced rate under a low flow scenario?;
- do other groundwater abstractions, identified in Habitats Directive Stage 3, have an impact on river flow?;
- what are the impacts of effluent discharges to the ground in low recharge and high recharge years?

In most cases it will be necessary for the main project to be preceded by a scoping study (see Chapter 2) to define clear objectives, identify data availability, set budgets and to establish the best approach for carrying out the main project. The scoping study will normally form the basis for preparation of the Project Initiation Document (PID) in addition to reference to the Agency's project management manual (Environment Agency, 1998).

2.2.3 The implications of models being purpose-specific

Modelling projects are framed under specific objectives which have a fundamental influence on the development and refinement of the numerical model. For example, a number of regional-scale models are currently (2001/2002) under development to study low flow problems in one or two watercourses (usually Chalk streams) in southern England. The targeted water course(s) are at the centre of the model domain, with usually two or three adjoining catchments between them and the edge of the model. At the refinement stage of these models, the stringency of the acceptance criteria, and therefore the degree to which the model simulates observed conditions (the *reliability* of the model), reduces away from the main centre of interest.

It is usually also true that, *de facto*, refinement of a model in the area of interest concentrates on the specific hydrogeological mechanisms and processes relating to the purpose of the modelling exercise. Hence, for models relating to low flow problems, model refinement within the area of interest will concentrate on simulating the mechanisms which operate during low flow conditions.

For these reasons, models should be used only with great caution for purposes outside the specific purpose for which they were developed. Specifically:

- *They should not be used for prediction simulations and subsequent decision making for locations/areas which are within the model domain but outside the area relating to the original purpose of the model.*

  For example, if a location or area which is the subject of a CAMS assessment or a wetland habitat investigation happens to lie just within the domain of a regional groundwater model, at some distance from the area relating to the original purpose of the model, the model should not be relied upon solely for the investigation. This is true even if the same hydrogeological mechanisms or processes which were the focus of the original purpose are involved.

- *They should not be used for prediction simulations and subsequent decision making, even within the area relating to the original purpose of the model, if different hydrogeological mechanisms and processes are involved.*

  For example, models constructed for the purpose of studying low flows in a Chalk catchment should not be used for studying groundwater flooding problems as they are unlikely to contain any representation, even in the area of interest, of any reduction in specific yield above the vertical interval of water table fluctuation.

If a hydrogeological assessment or investigation is required at any location, it should therefore be conducted as a separate project from the outset. This is not to say that products of a previous investigation (e.g. conceptual and numerical models) cannot represent an invaluable resource for the new project. For example, the conceptual understanding of the regional hydrogeology developed during a modelling project will be relevant for most locations within that region. It will usually be possible for a regional numerical model to be used as a starting point for a new model, but only following a new phase of conceptual modelling including identification and characterisation of the important hydrogeological mechanisms at an appropriate scale. Using this approach, the benefits of the original modelling study are realised in an appropriate way.

2.2.4 References

Environment Agency, 1998. *Project Management in the Agency*.

2.3 Initial scoping study

2.3.1 Purpose

Once the need for a groundwater resource study has been identified it is recommended that an initial scoping study is carried out, particularly for regional scale studies. The initial scoping study is the first step in getting the project started. It will normally form the basis of the Project Initiation Document (PID) for large projects and aid the preparation of the Project Brief for the main project if required.

The objectives and scale of a scoping study will depend on a number of variables such as the size of the project, the amount of work already carried out on the project and the proposed approach to the main part of the project. However, for the purpose of this general guidance the following objectives for the initial scoping study could be considered:

1. to clarify and agree the overall purpose and define clear, specific objectives for the main project;
2. to identify the main issues and drivers for the work (e.g. water resources assessment, assessment of impacts on surface waters, Habitats Directive, CAMS, Water Framework Directive, etc);
3. to identify the available data, both internal and external; how much, where and in what format it is stored, and its quality;
4. to identify critical gaps in the data and likely cost and timescale for obtaining these data;
5. to identify (and briefly review) relevant previous investigations and research;
6. to define the likely geographical extent of the study area and model domains;
7. to briefly summarise the current conceptual understanding of the study area and its surroundings and to identify any uncertainties;
8. to identify technical issues that need to be addressed by the model or which may limit the implementation of the model. It may be that a significant amount of technical work is required to assess these (e.g. the calculation of provisional water balances to check the conceptual model);
9. to identify and make contact with key interested parties, both within the Agency (from different functions and at area/regional level) and externally (major abstractors, environmental organisations, etc) in order to establish their expectations, relevant knowledge and ability to provide constructive contributions to the study and to determine whether there are any ongoing or planned studies or research programmes in the area;

2.3.2 Approach

For smaller, localised resource studies, or where the above issues can be readily addressed by individuals with the appropriate ‘local knowledge’, the scoping study can be carried out in-house. In these circumstances it is recommended that a small working group is established, involving appropriate regional and area hydrogeologists, hydrologists, ecologists and water quality staff.

For larger more complex projects, particularly those requiring extensive consultation and/or investigation into data availability, and where Agency staff resources are limited, the scoping study may be wholly or partially contracted out. However, if this approach is adopted, an external consultant will be unable to make certain key decisions relating to project management, liaison, timing and budgets and allowance for inputs from key Agency staff should be made.

2.3.3 Deliverables

The scoping study should aim to provide a scoping study report (addressing the above objectives). It should include:

1. an assessment of the need for the study and discussion showing how the objectives for the study will address these;
2. a listing of available data and information;
3. maps of the study area and key locations (e.g. extent of hydrometric network);
4. a provisional description of the understanding of the system with an assessment of key areas of uncertainty;
5. recommendations for field investigations as appropriate;
6. a bibliography;
7. recommendations for carrying out the main project;

In specifying the deliverables for the scoping study it is important to be clear whether any of the technical tasks (e.g. review of groundwater level data) are to be carried out at a preliminary, 'surveillance' level or whether they are to be deliverables that will contribute to the main project. The scoping study can also be designed to contribute interim guidance to licensing policy in the study area or inputs to other initiatives (e.g. CAMS) that are being carried out on a shorter timescale than the main study.

The main project deliverables are specified within the Project Brief. If a numerical model is to be developed, the acceptance criteria for the model will be specified once the conceptual model has been agreed (Chapter 6).

2.3.4 Timing & Resources

It is recommended that the Scoping Study is programmed for completion within 2-4 months. If contracted out a budget of between £15K and £30K will be required plus between 30 and 50 Agency man-days, depending on the size and complexity of the study area and the issues addressed.

2.4 The scale of a study area

Factors to be considered in determining the scale of study area should include:

- the scale of the issues under consideration;
- the location of hydrogeologically defensible boundaries;
- the scale of input data.

Clearly, the end use of a model is key to defining a suitable study area. Regional flow processes, such as river aquifer interaction and water resource assessment will require large study areas to ensure that the regional flow pattern can be investigated and represented adequately. Smaller scale processes, abstraction impacts on wetlands and contaminant movement, which are dominated by more localised flow processes may require smaller study areas. However, in both cases it will be important to use hydrogeologically defensible boundaries.

The key question when determining the size of the study area is: What affect do the boundaries I have chosen have on key outputs from the model? If the boundary could potentially have a large impact on the model output, and it is not hydrogeologically defensible (flow line or groundwater divide) a new, more remote boundary should be chosen. One of the first tasks when constructing a numerical model should be to test any uncertain boundaries in order to build confidence that the model area is appropriate for the question we wish to answer.

The final factor that should be considered is the scale of the input data. Although it is unlikely that the study area will be altered to suit the data we should consider how the data can be interpreted to best represent the area. If the data available is representative of a far larger area, e.g. MORECS potential evaporation $40km^2$, then we should consider how this source of data should be distributed across the study area. If the data is representative only of small sections of the study area we should consider how we use it, e.g. transmissivity from short term pumping test in a highly heterogeneous aquifer.

2.4.1 Regional studies

The study area must include all the major inflows and outflows which are likely to influence the aquifer response. This will often mean that the study area needs to extend into other aquifer units, although it may be possible to limit the data collection and use a coarser model mesh in these additional areas. Care must be taken in the use of groundwater divides since they are hard to define and they often move (perhaps only slowly) due to changed conditions. When flows occur from minor aquifers, some allowance should be made either using an estimated flow or a head dependent flow (see Chapter 4).

The need for a regional model is illustrated by the Southern Lincolnshire Limestone catchment (Fig. 2.4.1). It is essential to consider both the Glen and Slea catchments; the high transmissivities in the confined region (mostly in excess of 1000 m^2/d) mean that any changes in the abstraction patterns in one part of the catchment influence streamflows throughout the whole catchment. This was illustrated by the sealing or controlling of wild bores (uncontrolled artesian leakage points in the confined zone) in the Glen catchment, which led to an increase in river flows in both the Slea and Glen catchments (Johnson and Rushton 1999).

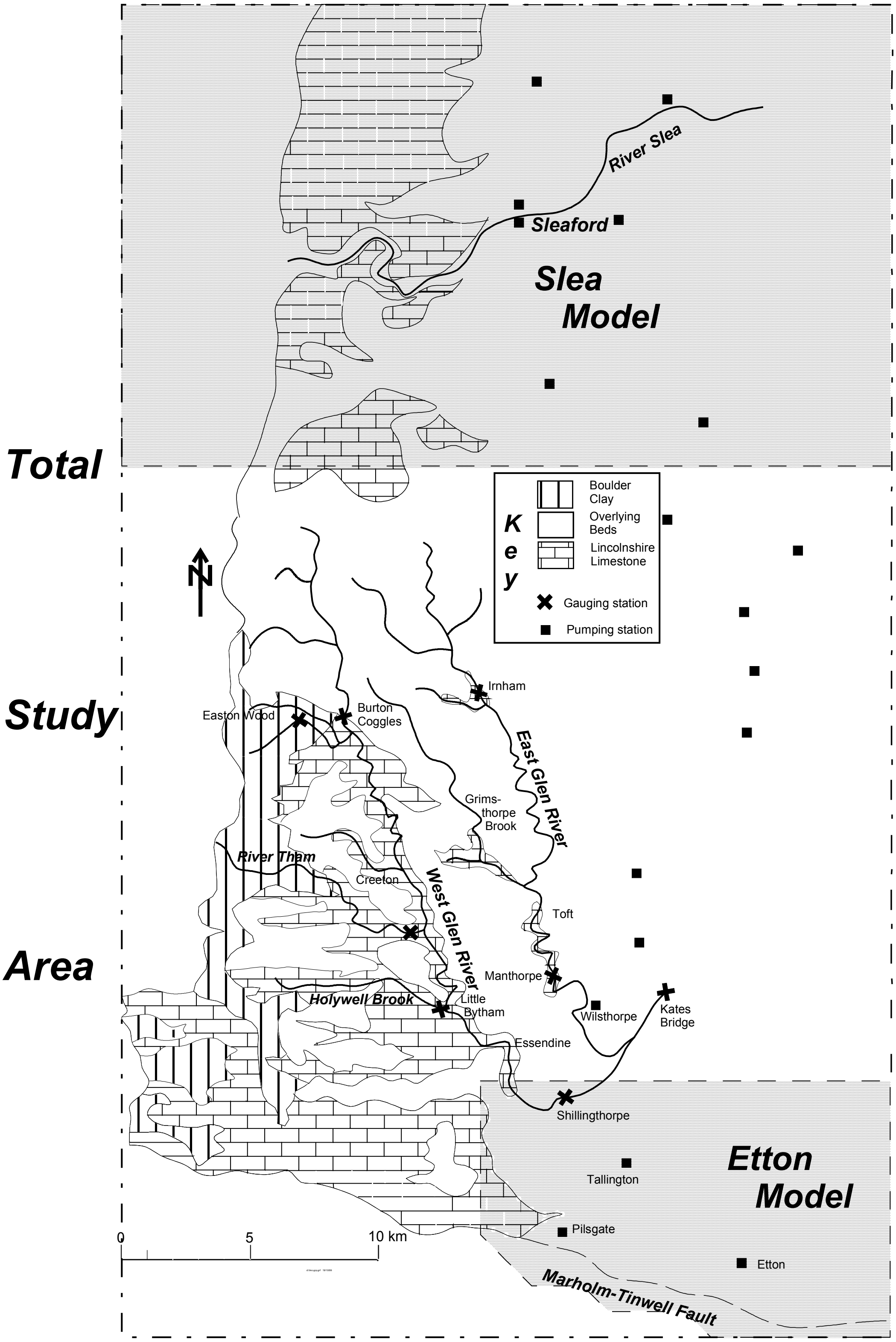


Figure 2.4.1. Southern Lincolnshire Limestone catchment showing the areas included in detail studies of the Slea catchment and the area around Etton pumping station.

2.4.2 Smaller scale studies

For studies where more local issues need to be addressed, both data collection and numerical modelling will be more detailed. Either smaller mesh intervals should be incorporated in the larger regional model, or a separate detailed model needs to be constructed with information from the larger model used as boundary conditions (see Fig. 2.4.1 for the areas of the smaller models for the Southern Lincolnshire Limestone catchment). If a smaller mesh is included in a larger model, care must be taken that the transfer from coarser to finer mesh is carried out gradually in a number of steps to minimise the numerical errors introduced. If a model representing a smaller area is used with boundary conditions taken from a larger model, most of the boundary conditions should be of specified flows to ensure that continuity of flow is satisfied. Unless careful checks are made to ensure that the flow conditions are transferred correctly from the larger to the smaller model, there is a risk that the predictions of the smaller model will be unreliable. The detailed study might also represent a smaller time period with shorter time steps.

2.4.3 Examples and further reading

Information and/or references are given below on a number of case studies which illustrate some issues related to the scale of modelling studies.

Studies of large areas include the Berkshire Downs Chalk (Rushton *et al*. 1989), the Fylde Sandstone aquifer (Seymour *et al*. 1998), the Nottinghamshire-Doncaster Sherwood Sandstone aquifer (Rushton *et al*. 1995) and the Southern Lincolnshire Limestone Catchments (Rushton and Tomlinson 1999).

Examples of more detailed studies include the Dover area of the East Kent Chalk, the Sleaford area of the Southern Lincolnshire Limestone and the Etton area of the Southern Lincolnshire Limestone.

- To understand the flow conditions in the vicinity of Dover, especially the surface water/groundwater interaction, the mesh in the regional model of the East Kent Chalk (Cross *et al*. 1995) was reduced from the standard mesh of 1.0 km to 250 m in the area of specific interest.
- Complex river-aquifer interaction occurs in the vicinity of Sleaford in the Southern Lincolnshire Limestone catchment; travel times of nitrates are also important. A separate more detailed model of the Sleaford area was prepared using boundary heads and flows deduced from the regional model; the area included in the Sleaford model is shown on Fig. 2.4.1. Because of the small distances between important features including springs, rivers and abstraction boreholes in the vicinity of the River Slea in Sleaford, the mesh spacing was reduced to 250 m.
- To the south of the Southern Lincolnshire Limestone is the Marholm-Tinwell Fault. Originally this fault was considered to be effectively impermeable but contaminants have moved across it from waste disposal sites to its south. The regional groundwater model has been used to provide boundary flows and heads for a more detailed contaminant transport model of the area likely to be effected by flows across the Fault (Fig. 2.4.1). Furthermore, the time step of the numerical models was reduced from 15 to 3 days for a specific investigation.

2.4.4 References

Cross, G.A., Rushton, K.R. and Tomlinson, L.M. 1995. The East Kent Chalk aquifer during the 1988-92 drought. *Journal of the Institution of Water and Environmental Management,* **9**, 37-48.

Johnson, D. and Rushton, K.R. 1999. The effect of borehole sealing on the Southern Lincolnshire Limestone catchment. *Journal Chartered Institution of Water and Environmental Management*. **13**, 37-46.

Rushton, K.R., Connorton, B.J. and Tomlinson, L.M. 1989. Estimation of the groundwater resources of the Berkshire Downs supported by mathematical modelling. *Quarterly Journal of Engineering Geology,* **22**, 329-341.

Rushton, K.R., Fletcher, S.W. and Bishop, T.J. 1995. Surface water and groundwater components of the Nottinghamshire Sherwood Sandstone aquifer system. *British Hydrological Society, 4th International Symposium, Edinburgh*, 2-17 to 2-24.

Rushton, K.R., Kawecki, M.W. and Brassington, F.C. 1988: Groundwater model of conditions in the Liverpool Sandstone Aquifer. *J. Inst. Wat. & Env. Man.,* **2**; 67-84.

Rushton, K. R. and Salmon, S. 1993 Significance of vertical flow through low-conductivity zones in Bromsgrove Sandstone Aquifer, *J. Hydrol*. **152,** 131-152.

Rushton, K.R. and Tomlinson, L.M. 1999. Total catchment conditions in the Southern Lincolnshire Limestone, UK. *Quarterly Journal of Engineering Geology*, **32**, 233-246.

Seymour, K.J., Wyness, A.J. and Rushton, K.R. 1998. The Fylde aquifer - a case study in assessing the sustainable use of groundwater resources. *Hydrology in a Changing Environment*, Proceedings of the British Hydrological Society International Conference, vol. II, Wiley, 253-267.

2.7 Outputs and documentation

2.7.1 Why?

- *To communicate.* During the process, ideas are communicated between interested parties, facilitating a much wider consideration of the issues. The findings of the study can be communicated to the various stakeholders. Developments and experience (knowledge) are transferred to the wider community.
- *To create a permanent record.* All of the above can be achieved by oral communication. Documentation is permanent, meaning that the full benefits of the project are available after those involved have forgotten or moved on.
- *It is an invaluable discipline.* It causes us to formalise our thoughts for wider exposure, forcing us to identify and address any inadequacies in our reasoning. Sometimes it is recognised that these inadequacies exist but, for whatever reason, the discipline to confront them is lacking. Writing things down provides this discipline and it should be used at every appropriate opportunity.

For these reasons, documentation and good reporting is vital to the successful development and handover of a modelling project. However, in order to realise the value of a report it needs to be read, explained and discussed. These activities take time and patience. Reviewers need to allow enough time for review/digestion and are likely to be better able to assimilate a report if they have been actively involved in previous progress and technical development meetings and/or work. Writers must not assume that their reports will have been read or entirely understood by reviewers (particularly any badly written, long and boring bits!). They need to put in the extra time and effort to provide pithy summaries and to present, highlight and explain the main findings and assumptions contained within the report, emphasising key uncertainties and potentially technically contentious issues to promote debate and consensus. It is important to recognise that all those involved will bring their own interests and prejudices to these activities.

As a consequence, several drafting iterations may be required at the end of a modelling study to produce a Final Report which will stand the test of time. Other reports written at the end of Phases within the development of the study should not be confused with this Final Report - they all represent (to some extent) 'work in progress' and probably do not warrant as high a level of typographical, grammatical and presentational scrutiny!

2.7.2 What?

Given the above listed of functions for documentation of the modelling process, it should come as no surprise that *just about everything* should be documented. In addition to the formal reporting obligations, the importance of process documentation and working documents should be noted. These documents should provide a narrative (or audit trail) through the entire process, such that a third party can revisit and check the reasoning behind all decisions.

2.7.3 Forms of documentation

Workplan

A workplan (or Project Initiation Document) must be produced at the start of the project. It should be agreed with all contributors to the project before work commences. It should include:

?? Project type, background, issues and objectives;

?? Finances (source and organisation);

?? Project team (including organisation chart, etc);

?? External organisations and supplies;

?? Work programme (often with Gantt chart or similar);

?? Input data and output requirements;

?? Quality control and assurance procedures;

?? Project records and documentation;

?? Special/novel techniques to be used;

?? Risks and issues logs.

Reports

Reports are the formal documentation of the process and, whilst including some detail on the process, tend to concentrate on the results and conclusions of the study. The series of reports produced during a project will usually include the following: the scoping study report, the project specification, the data catalogue and database, the conceptual model report, the numerical model report, the final project report.

Reports often have a wider use than the original target audience. For example, the conceptual model report for a regional study which has been developed by water resources staff will be referred to by water quality, waste, and licensing staff and by new water resources staff because it provides:

?? essential information for licensing decisions (cross-sections, water balances);

?? the input to the conceptual models being developed for local issues (impact on wetlands/rivers, SPZ, contaminant transport);

?? a review and reference point for previous work;

?? a synthesis of current understanding in one document.

Publications and presentations

To communicate significant findings from the study to an appropriate target audience, e.g. significant technical discoveries/developments to the wider scientific community.

Process documentation and working documents

As noted above, these documents should provide a narrative (or audit trail) through the entire modelling process. Examples include:

Working notes and diagrams. E.g. scribblings, notes, working diagrams, exploratory calculations, etc.

Modelling log. Should include enough information to repeat any model run, and should include justification (and reference to related material) for any changes made to the model (i.e. what the run was seeking to investigate), a list of the input model files used (highlighting those which have been modified) and output files generated, and a brief summary of the results (were changes as expected/significant, etc?).

Project meeting documentation. E.g. Formal/informal presentation materials, detailed minutes of meeting discussions. Experience has demonstrated that meetings are often a forum for *hard* hydrogeological thinking amongst the technical contributors to the project, and therefore their thorough documentation is important. Documenting decisions reached and proposed ways forward is often best done at the meeting itself (on a flip chart), particularly with respect to contentious technical debates.

User manuals & training materials

It is much easier to hand a model over at the end of a 'project' if the users, computer hardware and uses (i.e. applications of the model) have been clearly established at the beginning of the project. It is then possible to target the model design appropriately from the outset, to involve the future users in its construction and refinement, and to prepare user manual and training exercises/materials pitched at the right level.

User Manuals are often most effective if they also form the basic material for a handover training session or sessions which focus on how to get the model to do what you want, rather than on the guts or theory of its calculations. Important topics should include:

- ?? how to update the simulation as new data come in;
- ?? how to run scenarios;
- ?? how to critically review results and build in refinement or changes reflecting improved understanding related to new information.

File naming conventions, keeping track of quality with run logs, and flow diagrams of input, executable and output files, should all facilitate the controlled use of the model. An appreciation of the limitations of its application is also essential - i.e. the spatial and temporal scales at which it cannot provide useful answers, the magnitude of proposed stress changes for which it is worth 'bothering with the model' (i.e. larger abstraction licence applications, not tiny ones), processes which have not been incorporated into the model and which cannot therefore be investigated.

Agency staff should be encouraged to develop 'hands-on' experience with the model during the hand-over period, and an adequately funded ongoing support arrangement should be made with the developers of the model.

2.7.4 Electronic deliverables

During a large regional modelling project, a considerable amount of digital output will be generated. In order to realise the maximum benefit from the project, it is vital that these digital outputs are handed over to the Agency in agreed, useable structures and formats.

A simple, readily understood, file-naming convention should be adopted throughout a project.

A single electronic deliverable should be produced that is properly quality assured. It is very useful if this deliverable has an extensive set of 'README' files detailing the exact content and purpose of every single file. The Agency should quality assure this deliverable and request further deliverables if it is found to be incomplete, or that files are corrupted. It is important that relevant Agency personnel take responsibility to familiarise themselves with the electronic deliverables so that they can use them to maximum effect in the future.

2.7.5 Final thoughts

The following facts indicate that the documentation process has received insufficient attention in previous Agency modelling projects:

- The survey of existing Agency models undertaken as part of the Strategic Review of Groundwater Modelling R&D Project revealed that documentation at all stages in modelling projects has often been inadequate. The main issues which the project is addressing or the conceptual ideas are frequently not documented adequately, and therefore remain in the heads of the Agency or contractor staff concerned. This can result in models being either completely unusable or requiring enormous effort to get going again. Inadequate documentation can also mean that models picked up in this fashion are inadvertently used incorrectly, often because certain features have been hard-coded, or other 'non-standard' procedures have been followed which are not immediately apparent.
- Experience has revealed that the time allotted in modelling project proposals to preparing documentation is often insufficient.

2.6 Project management

2.6.1 Introduction

Major groundwater resource assessments will usually cover large areas of aquifer, possibly crossing from one Agency Region to another. The size and complexity of these projects will normally necessitate a significant part of the work to be carried out by external contractors. However, it is unreasonable to expect contractors to have the local knowledge and experience of either Agency staff (at Regional or Area level) or water company hydrogeologists. Furthermore, most aquifer units will have been subject to previous investigation by predecessor organisations to the Agency, particularly from the time of the water authorities prior to 1989. It is important not to waste time and resources 'reinventing the wheel'.

These guidance notes on management of a groundwater modelling project should be read in conjunction with the Template Project Brief (Appendix A) and Agency project management procedures and guidelines (Environment Agency 1998).

The role of project manager is to ensure that:

1. The technical objectives are met to a standard acceptable to both the Agency and others potentially affected by the outcome (the acid test being 'will the decisions made as a result of the investigation withstand scrutiny at a Public Inquiry?').
2. The study is completed on time, within budget, and in compliance with Agency financial procedures.

At the risk of stating the obvious, it is difficult to over-estimate the importance of the Project Manager’s role.

2.6.2 Time records

The project manager has the responsibility to ensure that records are kept of time spent by Agency staff and contractors on the various tasks in the project. This will not only aid the post project appraisal, but also aid realistic planning of future projects.

2.6.3 Approach

A collaborative, multi-disciplinary approach is recommended, involving appropriate specialists and all the key interested parties. This is primarily so that individuals and organisations reach agreement on, and gain ownership of, the conceptual and numerical models developed through sharing their knowledge, data and experience to unravel how the flow system is behaving. This is particularly important if there is subsequent discussion over the implications regarding resource allocation and impact of abstraction.

Groundwater resource assessments require a combination of geological, geophysical, geochemical, hydrogeological, hydrological, ecological and numerical modelling skills.

2.6.4 Project staffing

The effectiveness of project execution is sensitive to the sourcing of personnel to fulfil the functions noted in Table 2.6.1:

– Project management should be carried out by Agency staff from the Region or Area office in whose jurisdiction the project area lies. It is expected that these staff will have the most intimate knowledge of the issues and will often be involved in the initiation of the project.

– Technical supervision should also be undertaken by the Agency, although its more specialist nature could mean that Agency personnel outside the Region may have to be brought in. For example, temporary secondment from another office might be possible.

– The modelling function is the most specialist, and a higher degree of flexibility might be required in order to secure appropriate personnel. The Agency is aiming to develop its in-house capability in modelling and at least one Agency person should be on the modelling team. It is hoped that this person will run and update the model in the future with a minimum of contractor support.

– Technical review will usually be undertaken by other modellers within the Agency and/or external advisors such as staff from academic insitiutions.

Table 2.6.1. Roles and areas of responsibility

	Role	Responsibility
1	**Project Management**	• Ensuring that the project is running to programme and budget • Resolving contractual and liaison difficulties • Providing ongoing review of progress
2	**Technical Supervision**	• Ensuring that the technical team undertakes the work in accordance with best practice standards • Ensuring the work meets the Agency's objectives
3	**Modelling**	
	3a Supervision	• Management of the modelling team • Ensuring outputs meet the objectives of the Project Brief
	3b Technical Team	• Delivering the outputs required by the Project Brief
4	**Technical Review**	• Independent review of project • QA/QC of outputs • Technical advice and backup

The resources necessary (c. £250,000 [2002] and 200 or more Agency man-days over 3 years) for a large regional project should not be underestimated, particularly as Agency staff will have other operational commitments. Possible options for increasing resources in the short-term are to bring in contract staff for particular project tasks, or to temporarily replace Agency staff with a contractor while they are assigned to the modelling project. Systems must be established (e.g. peer and expert review) to ensure that the standards for in-house projects are the same as those for contractors.

2.6.5 Project Structure & Phasing

Resource investigations should be carried out in a staged manner. Generally the main project will be preceded by a scoping study (see Chapter 2) which should define precisely the issues, the objectives and the scope of work. The main project involves: the collation and analysis of the available data and the development of a conceptual model (Phase 1 in the Template Project Brief), the construction of the historical numerical model (Phase 2), predictive simulations (Phase 3), and compilation of the final report and handover (Phases 4 and 5).

It is wise to plan for a period at the end of the conceptual modelling (Phase 1) when the report is reviewed, understanding is discussed and tested, and an assessment is made on whether it is appropriate to progress to detailed numerical modelling (Phase 2).

Possible reasons for not progressing to detailed numerical modelling include:

- the conceptual model is sufficient for decision-making purposes;
- there is insufficient data or understanding of the system.

Splitting the project allows additional fieldwork and investigations to be carried out. These can address deficiencies in information or understanding identified at the end of the conceptual modelling, and the results can be implemented before proceeding to numerical modelling.

Anglian region have let a term contract to cover all of their groundwater resource investigation and modelling needs over a five year period. Again, there are advantages and disadvantages with this approach.

2.6.6 Project Liaison

Given the importance of effective communication throughout the project it is recommended that three main groups are established: a Project Steering Group, a Project Board and a Technical Working Group. The exact composition of each group and the frequency of their meetings will vary from project to project. Guidance is given on Table 2.6.2.

It is valuable to visit the contractors office to review work in progress. Minutes of meetings, progress reports and drafts of project reports should be circulated to the key participants, and feedback incorporated in the final report. A realistic estimate of the time required for this ongoing consultation should be included explicitly within the project budget.

2.6.7 Post Project Appraisal

A thorough review of the process and outcome(s) of the project is a requirement of the Agency's project management procedures. Issues covered should include:

- were the project objectives met?
- what was done well/what was not done well?
- where and why were there delays?
- what were the costs: budgeted v. actual?
- what were the time inputs: budgeted v. actual?
- how did the contractor perform:
  - ~ quality of output?
  - ~ flexibility during the contract?
  - ~ value for money?
- how did the Agency perform?
- what will we strive to do better in the future?

Information from such a review exercise is invaluable, not only within the individual region but also across the Agency's groundwater modelling community, in refining the Agency's approach to future modelling projects. The project manager should make this information available to colleagues in the Agency's groundwater modelling community through modelling seminars run by National Groundwater and Contaminated Land Centre.

Table 2.6.2. Project management groups

Forum	Purposes	Suggested Membership	Meeting Frequency
Project Steering Group	• to gain wide ownership by stakeholders • to inform of aim, progress and outcome of study • to identify data sources and points of contact for liaison between contractor and Agency areas/others	Agency • Area Water Resource Team Leaders (or licensing & hydrometry staff) • Area FCR staff (if low flow issues) • EP staff (if quality issues) • Regional & Area hydrologists/hydrogeologist Contractor • Project Manager/Director Wider stakeholders • Water Utilities/Major Abstractors • Conservation Organisations • Local Authorities • Local Residents • Agricultural Organisations • Etc…..	Start and end of each Phase
Project Board	• to ensure programme is running to programme and on budget • to resolve potential contractual, or liaison difficulties • to provide ongoing review of progress	Agency • Project Manager (lead region*) • Project Executive • representative of other region* • senior hydrogeologist & hydrologist Contractor • Project Manager/Director	Monthly
Technical Working Group	• to share knowledge and ideas on specific technical aspects	Agency • Project Manager • Regional & Area hydrologists, hydrogeologist, ecologists • Agency modeller External Reviewer** Water Utilities/major abstractors • hydrogeologists Others • ex-Agency/predecessor hydrogeologists/hydrologists Contractor • Project Manager • hydrogeologist/hydrologist/modeller	Every 6 to 10 weeks

* If multi-regional coverage
** Appointed by Agency via Project Board

2.6.8 References

Environment Agency, 1998. *Project Management in the Agency*.

2.5 Procurement

2.5.1 Introduction

Procurement is dealt with Regionally. The accumulated experience of other Regions on contractor selection and tender evaluation can be obtained via the Senior Modeller at the National Groundwater and Contaminated Land Centre or the Regional staff themselves. This information should be contained in Post Project Appraisals.

2.5.2 Contractor Selection and tender evaluation

Selection of the right contractor is important to ensure a productive and successful outcome to a resource study. Considerable time, effort and expense can be wasted in managing projects if contractors underbid for work and do not appreciate the very high time input and commitment which is inevitably involved in collecting, collating and analysing vast amounts of data from disparate sources, often in different formats. This should be made as clear as possible in the Project Brief; hence the need for the initial scoping study. Furthermore, it is essential that contractors have the required knowledge and experience, are flexible in their approach and are able to rigorously analyse information and concepts, and are prepared to be receptive to the views of other members of the project management groups.

Guidance on contractor selection and tender evaluation is available from Regions that have carried out similar resource studies. Tendering procedures should be agreed with Regional Procurement sections to ensure they comply with Agency rules. Bids that do not fulfil these criteria or which may jeopardise a fair comparison during the evaluation of bids should be rejected as non-compliant after consultation with Procurement.

The increasing use of national procurement frameworks, e.g. NEECA (National Engineering and Environmental Consultancy Agreement) and regional hydrogeological call-off contracts, provide alternative ways of engaging consultants for modelling projects. These have advantages in terms of ease of tendering, but it is essential to ensure appropriately experienced individuals are available within the companies concerned. Experience of using this approach is increasing, and lessons will be learned over time about the pros and cons.

2.8 Quality Assurance and Control

2.8.1 Introduction

Quality assurance and control (QA/QC) has been, and is being, organised in a number of different ways during recently completed and ongoing Agency modelling projects. The advantages and limitations of these different methods are still being evaluated, and therefore it is not appropriate at this stage to give detailed recommendations.

In order to encourage consideration on how QA/QC can be effected during a modelling project, a number of fundamental principles are presented below. Feedback, including general thoughts and experience, is encouraged on this topic.

2.8.2 Principles

In relation to modelling projects, quality assurance and control is:

> *a system to avoid technical principles or practices, mistakes or misunderstandings remaining unidentified for significant periods of time in project terms.*

It is therefore an integral part of project management.

Important considerations in relation to QA/QC include:

- it must be organised such that the contractor is not delayed;
- appropriate personnel should be allotted to each review task;
- outside contractors must have sufficient internal QA/QC which should be costed explicitly in the proposal;
- it should be as simple as possible whilst serving its purpose.

3.1 Review of Literature, Previous Investigations and Modelling

A great deal of useful information is generally available in reports and other forms of literature dealing with the study area. Not only is the review important for the current project but it will also provide a valuable long term resource for the Agency. Therefore the initial purpose of the literature review is to provide a comprehensive summary of the contents of all the literature.

For most studies information is available from a wide variety of sources such as:

- papers in published journals;
- geological memoirs;
- Water Company and Agency reports (and those of the predecessor organisations);
- University theses and reports;
- reports of contractors;
- maps (geological, hydrogeological, topographical, soils, mineral assessments, etc.);
- computer programs;
- documentation supporting licence applications.

The main tasks in a literature review include:

1. Providing a list of all the available literature and other forms of information with full details of the authors, source, etc.
2. Preparing a brief summary of the contents of each item; the summary should be 100-250 words in length and may include an important diagram. Information from (1.) and (2.) should be included in an Appendix.
3. Provide a copy of all reference material in a separate volume.
4. For references which have a particular relevance to the current study; the important information or insights should be presented in the main text.
5. Having presented the important information, critical yet constructive comments should be added. In preparing comments it is important to recognise that:
    - Significant developments have been made in recent years in many of the disciplines associated with groundwater studies. Although the contents of a report or paper may appear to be out-of-date by current standards, there may still be valuable information in the document.
    - All important information must be reported, even if the reviewer does not agree with the findings.
    - Reasons must be given for rejecting or ignoring previous work. The aim of each study is to contribute further to the understanding of the aquifer system; no study ever provides the final answer.

Particular skill is required when reviewing previous *major* studies. The *first part* of the review must list all the main issues which are presented in the report. The objectives of the study, the achievements and the conclusions should be presented. It may be helpful to use tables to summarise factual information such as number and quality of lithological information from boreholes, number and reliability of pumping tests, number of rain-gauge stations and length of record, etc. When groundwater modelling has played an important part, a reasonsable summary of the model, the results and comparisons with field data should be presented. The *second part* of the review should be a critical, but constructive, assessment of the contributions made by this study.

It will be necessary to re-examine and perhaps revise some of the contents of the literature review as the study proceeds; this is likely to be of particular importance during the development of the conceptual model and the refinement of the mathematical models.

It is important that a relatively senior and experienced member of the team is assigned to the literature review. It is hoped that such a person will have an appreciation of wider issues, such as the development through time of hydrogeological knowledge and techniques, so that the literature review will be informed and objective with regard to the relative merits of various sources of literature.

3.2 Site Visits

It is likely that a number of site visits will need to be undertaken during conceptual and numerical modelling, to enable familiarisation with the geography, topography, hydrology and geology of the study area and to enable the conceptual understanding of a groundwater unit to be tested against field observations and evidence. It is important to consider repeat site visits during different weather conditions and seasons to record changes in relevant features, such as surface water flows, crop cover, etc.

Site visits range in time and organisational requirements from simple walkover surveys, where mainly qualitative observations are made, through to prolonged field campaigns where the emphasis is on the collection of quantitative information. Some of the items that may need to be identified during these investigations are discussed below.

3.2.1 Qualitative information

Before any site visit is undertaken, it is normally good practice to undertake a desk study of an area so that a basic understanding of the hydrogeology can be acquired. This understanding can then be tested against field observations.

Take photographs

Photographs, with accompanying notes, provide the best possible *aide memoire* when reviewing and interpreting the information gained during a field visit. They can also be used as direct evidence when unusual features or conditions are observed during a site visit, and they have great descriptive value in the documentation of a conceptual model.

Digital cameras have increased the convenience of the photographic process to a large degree in this context as the quality of the photographs can be assessed immediately after capture. The photographs can also be integrated rapidly into discussion documents and reports.

The following photographs and interpretive notes, by Vin Robinson of Thames Region, give an indication of the potential value of photography in helping to document significant events witnessed during field visits:

> *The photographs were taken on a field trip to document some active swallow holes on the Chalk with BGS staff from Wallingford. These swallow holes are typically on sloping ground below ridges capped with tertiary strata. After heavy rain, water flows off these strata and from minor aquifers within these Tertiary strata. Temporary streams flow away from the ridges (Photo 1) across sloping ground and on to unconfined Chalk or Chalk just under the edge of the Tertiary strata. There the flow disappears down numerous holes in the beds of the watercourses (Photo 2) or into depressions with holes in the base, thus recharging the Chalk with the entire stream flow. Usually there is no water course beyond the last depression. Sometimes these operate for just a few hours.*
>
> *Where there are larger streams with large catchments, large areas of swallow holes exist in large depressions. At times of extended periods of heavy rain, often the flow is such that the swallow holes and depressions fill up faster than the inflow to the Chalk, and form a lake (Photo 3). These lakes then overflow and flood fields and flow into land and roads down valley (Photo 4). Much of*

this recharges the chalk over a wider area or occasionally reaches the perennial surface water system.

These sites and this mechanism are much more common than would be expected, but the short duration of the events means that they are not often recorded.

Talk to the locals
Speak to the local people with regard to all the issues detailed below.

Soils
- Observe in valley, valley sides and interfluves.
- Where do low permeability soils occur? Have solution features developed in topographic depressions?
- Are land drains installed (clay or plastic pipes entering large cut drains) indicating that farmers find it difficult to drain the soils, therefore suggesting that the soils are of low permeability. Land drains can lead to interflow resulting in flow into streams over a period of c. 10 days after a rainfall event (Environment Agency R&D Project, 2002).

Geology
The majority of geological information on an area is gained during the desk study, however the boundaries of various deposits can often more accurately be mapped in the field. Keys to geological mapping may be:

- Observing the general topography of an area which is often influenced by the geology (harder and softer strata, structure, etc) at a number of scales.
- Observe brash deposits in ploughed fields to identify likely soil thickness (bedrock is often assumed to be within 1m of the land surface when significant brash is present).

Surface water/groundwater continuity
- Observe and note stream bed gradients, stream bed materials and the relative elevation of the streambed and streambank.
- Use an auger to estimate bed thickness (i.e. thickness of the alluvial deposits, etc).
- Describe stream bed sediments and if possible obtain a sample for grain size analysis.
- Assess stream flow accretion along the river and identify areas where the stream is gaining or losing flow. Compare these with soil types and geology, topography, groundwater levels, artificial influences (abstractions, discharges, quarries, land and road drains).
- Identify seasonal groundwater level fluctuations along the river as well as river stage elevation, pond heights etc (using historic observations).
- Investigate the source of surface ponding (natural water table, perched water tables, etc)
- Observe seepage lines on stream banks, indicating efluent aquifer/influent stream.
- In wet periods, observe flush/spring lines by looking for topographic hollows (drainage lines) and changes in vegetation type.

Vegetation (including crop) distribution
- Ask farmers where they grow different crop types and why. This will often be due to the different nutrient and water needs of the crop and so provide important information on soil types.

- Locate spring and flush lines by observing lush vegetation (land is often overgrown due to soft soil and difficulty in cultivating).
- Observe crop health and density on crests and drainage lines:

  Healthy crops on crests but not drainage lines, suggesting thicker, low permeability soils.

  Un-healthy on crest, healthy on drainage lines, suggesting shallow, higher permeability soils.

3.2.2 Quantitative investigations

Soil augering

- Drill auger holes to: a) obtain a soil profile, identify low permeability horizons.
- Carry out auger hole test (falling/rising head test) to obtain information on the hydraulic conductivity of soils (particularly river bank deposits).

Hydraulic conductivity

The hydraulic conductivity of soil/drift deposits can be obtained by:

- Undertaking auger hole tests
- Rising/falling head tests on observation and production boreholes.
- Obtain specific capacity for wet dry years by observing operational pumping yields and levels.
- Identify infiltration capacity using double ring infiltrometer.

Stream flows

- Estimate river flows by choosing straight reach of river, identify cross sectional area (A, m^2) and profile and using float, (stick, orange) measure stream flow velocity over a set measured length (V, m/sec). Deduce flow volume ($Q=A*V$,m^3/s).
- Carry out spot gauging of flows to obtain an accretion profile for rivers and streams in the investigation area. The spacing of locations for spot-gauging should be decided with reference to the known importance of the reach in terms of accretion/decretion.
- Produce Winterbourne Signature for rivers that dry, by identifying the reach where rivers start and cease flowing and plot these locations graphically with river reach (Y scale) and date (X scale) to identify the winterbourne trends for a river over time. Information such as geology and major abstractions/discharges can be plotted on the Y scale to help interpret the observations.
- Conductance values can be deduced using current meter and stream area information.

Springs

- Location of springs may be observed in cold or hot weather using an accurate thermometer to locate changes in temperature in stream's ditches and ponds. Other hydrochemical measurements may also be used to differentiate in the field between surface and groundwater, although this can be difficult where the stream has a high baseflow index and most of the stream flow is derived from groundwater.

Groundwater levels

- Locate observation boreholes in the study area, confirm aquifer being monitored and collect water level data that can be used to produce piezometry maps and can be compared with accretion profiles. Groundwater fed ponds can also be a useful source of groundwater level information, although some display a lag caused by low conductance materials at their base.
- Produce long and cross sections through the catchment using groundwater data in order to characterise the head distribution.
- Identify points/lines at which there are significant changes in the groundwater head gradient. Investigate the causes of these changes, e.g. are they coincident with a change in hydraulic properties, or with a structural geological feature (e.g. faulting)?
- Shallow dip wells/piezometers can be installed in any auger holes drilled, to observe the height of the shallow water table, particularly next to streams, springs or wetlands.

Topographic levels

- Survey river bed and spring locations to Ordnance Datum to enable interpretation of accretion profile, topography, groundwater levels and stream flows (gaining or losing). This data may already have been collected in relation to surface water management issues.
- Confirm the elevations of surface water and groundwater level monitoring sites.

3.2.3 References

Environment Agency, *in press* (2002). 'Investigating the effects of land drainage activities on natural recharge to groundwater'. *R&D Technical Report W6-076.*

Photograph 1

Photograph 2

Photograph 3

Photograph 4

3.3 Collation and Preliminary Analysis of Data

3.3.1 Purpose & Importance

The purpose of this task is to gather together, probably within a project database, all available and relevant data. The database will provide the basic information that is used to develop an understanding of the groundwater/surface water system (the conceptual model) and to aid with the construction and testing of the numerical model. It will also facilitate identification of areas of data deficiency, enabling actions to remedy the deficiencies to be planned. Furthermore, the production of a comprehensive, quality assured digital database together with the documented conceptual model will form an enduring source of reference, of value within and outside the Agency, well beyond the life of the project.

3.3.2 Scope and Data Sources

The task involves seeking out, pulling together, validating and storing a vast amount of information from a large number of disparate sources. The information will be of varying quality and held in a wide variety of formats. The main types of information required are clearly set out in Task 2 of the Template Project Brief (Appendix B). They can be summarised as geological, hydrogeological, hydrometric, soil type and land use, and abstraction/discharge records.

Where there have been significant changes in land use patterns and/or there is a long history of groundwater development it will be necessary for these influences to be taken into account in the groundwater resource assessment. This will involve searching for information which pre-dates Agency records; the skills of an archivist and possibly an industrial historian could be useful.

Agency Records

Accurate abstraction and discharge data are fundamentals for historical simulations. Abstraction data from April 1998 onwards is held on the National Abstraction Licence Database (NALD). Historical abstraction data prior to April 1998 is held on local Regional archives, for example the LADS Historical Archive (LADSHA) in Midlands Region.

Hydrometric records, particularly river flows, may be required if the records have not been reviewed for a long period.

Abstraction and discharges may not have been measured continuously and there may be significant gaps in the data, which need to be filled. There is an Agency R&D Project addressing this issue, W6-042, "Development of Methods for Estimating Missing Artificial Influence Data".

BGS

Published geological maps, memoirs and BGS databases (e.g. well records at Keyworth and Wallingford, and the Aquifer Properties Manual) are accessible to the Agency and consultants. Caution needs to be applied when using geological maps as surveys can date from early in the last century. It is usually profitable to contact the appropriate regional BGS geologist for the study area to establish the status of the published survey. BGS Wallingford also hold abstraction records pre-dating the introduction of licensing in 1963 and details of old abstraction boreholes in the form of 'Wartime Pamphlets'. It should also be remembered that certain BGS geoscientists are in an almost unique position to provide information which can add crucial insights into the groundwater flow mechanisms.

It is recommended that discussions with BGS geophysicists, as well as field mapping teams, are carried out by the Agency Project Manager at the scoping study stage to establish the potential benefits of sharing information and liaison as conceptual understanding evolves.

BGS hydrogeologists may have carried out relevant research as part of their core programme which could make useful contributions to understanding the groundwater system; for example, their hydrogeological re-mapping of the Chalk and their baseline geochemical studies have proved useful in understanding the age and origin of groundwaters. The move by the BGS to digital mapping and databasing enhances the usefulness of their geological information for modelling projects.

Other Sources
BGS archives only represent a part of the relevant data sets and previous research which may be relevant to a groundwater resource study. Investigations by the Agency's predecessors, particularly the old water authorities, should provide an essential foundation. Site investigation companies, large consultants and local authorities are likely to hold information on shallow ground conditions, including permeability values and groundwater levels in superficial deposits. Also, PhD and MSc theses can prove to be invaluable references. Local interest groups (caving, mining, archaeology or historical) may be worth contacting.

3.3.3 Data Acquisition

In general it is recommended that the Agency purchases data sets required for the individual resource assessments; they are likely to be of value in fulfilling other duties of the Agency and enhance existing archives. It should be noted that licence agreements with the data providers, e.g. the Met' Office, may limit use to specified users/projects. Purchasing agreements for full regional or national data sets may be in place with the major suppliers/holders (e.g. LANDIS), or reciprocal arrangements may exist for data exchange, e.g. BGS lithological logs. The potentially high cost of acquiring such data needs to be taken into account at the project planning stage.

3.3.4 Quality Assurance & Validation

The process of collating and critically reviewing data sets for the resource assessment provides a unique opportunity to identify and query errors, gaps and deficiencies in the source data. Access to the raw data may be necessary to resolve uncertainty. Ideally the consultant should liase directly with the holders of these data sets. An audit trail should be provided to document errors and feed these back into the original archive, to avoid either duplication of effort in the future or maintenance of conflicting data sets. It will be important to define clearly the Agency's and the consultant's roles and responsibilities in completing this task.

3.3.5 Databases

With the move towards standardisation (harmonisation) of Agency software packages, unless there is an overriding justification the consultant should use preferred software, e.g. ACCESS and HYDROLOG™ at present. This will allow onward compatibility and processing for purposes other than the specific modelling contract.

It is also important to state when data is missing.

The need for developing clear, consistent and accessible databases for such resource studies has been recognised across the Agency, and the links with BGS databases are under discussion.

3.3.6 Size of Task

It is easy to underestimate the complexity and time consuming nature of the data collection and collation process. For example, it took almost 12 months and over 3 man-years, costing £90K, to carry out Phase 1 of the Wirral and West Cheshire Aquifer Groundwater Resources Study.

The size and duration of the task should be defined as closely as possible during the scoping study, but flexibility (time and resources) to accommodate extra, unexpected information should be maintained.

Data collation and processing requires tenacity and attention to detail, attributes which should be considered important factors in contractor selection. However, given the financial and time constraints on completing this stage of the project we may need to be selective in the detail and type of data collected, whilst maintaining rigorous standards of quality assurance and analysis.

3.3.7 Typical complications

Experience of recent modelling contracts has highlighted the following aspects as being particularly time consuming :

- Well records:
  - differences of numbering systems for borehole records held at BGS Wallingford and Keyworth and within the Agency;
  - erroneous or conflicting grid references and construction details.
- External data acquisition:
  - availability (delays in making it available) , format, and duration of record.
- Abstraction records:
  - differences in units (imperial/metric), licensed vs. actual, daily/monthly/annual records may be incomplete;
  - format particularly historic archived data: digital, paper, computer printout, original annual returns, microfiche);
  - ambiguous or erroneous well datums (artesian heads, m b Datum/m AOD);
  - limited duration (last two decades) – BGS Wallingford have *some* pre-licensing (1963) data;
  - lack of records in licence-exempt areas.
- Hydrometric data (climatic, groundwater and surface water):
  - format, validity, duration of record;
  - discharge consent (return) flow data generally not recorded.
- Aquifer properties:
  - reliability and format of pumping test analyses and reports.

3.4 Hydrochemistry

3.4.1 Application of hydrochemical methods

The application of hydrochemical methods in hydrogeological investigations is particularly valuable in regions where there is an absence of detailed hydraulic data, for example pumping test data, for determining aquifer conditions. Groundwater chemical distributions are a function of recharge composition, velocity pattern, water-rock interaction and dispersion. Hence, an interpretation of chemical distributions can provide information on recharge sources, recharge areas, residence times (and therefore velocity) and aquifer to aquifer and aquifer to aquitard transfers. The advantages of using hydrochemical data are that the data are independent of those needed for flow modelling and direct information can be gained on the likely behaviour of regional water quality evolution. In addition, groundwater dating methods (carbon-14, tritium, CFCs and, for the future, tritium-helium) and stable isotope methods ($\delta^{18}O$ and $\delta^{2}H$ of water, $\delta^{15}N$ and $\delta^{18}O$ of nitrate, $\delta^{34}S$ and $\delta^{34}O$ of sulphate) can contribute understanding of past and present recharge conditions, groundwater flow rates and the identification of recharge sources. In addition, specific inorganic species with a known history of usage in a region can be used in dating waters, for example boron where sewer leakage is expected, chlorinated solvents and BTEX compounds in urban and industrial areas and pesticides in rural areas.

3.4.2 Hydrochemical distribution and water types

Several published studies (for example, Downing et al. (1979) and Edmunds *et al*. (1987) in the London Basin and Berkshire Chalk aquifers, Edmunds & Walton, (1983) in the Lincolnshire Limestone aquifer and Wilson et al. (1994) in the East Midlands Triassic sandstone aquifer) demonstrate the classic sequence of hydrochemical evolution of groundwater in the direction of groundwater flow and exemplify the relationship between hydrochemical water types (or facies) and hydrogeological conditions. In general terms, areas of modern water with evidence of contamination from surface sources (nitrate, CFCs, VOCs, tritium) or regions that have chemically oxidising conditions (high dissolved oxygen content and partial pressure of carbon dioxide) are likely to be areas of unconfined groundwater conditions. Conversely, uncontaminated groundwaters exhibiting baseline hydrochemical characteristics or having chemically reducing conditions (high dissolved iron concentrations and enhanced N_2/Ar ratios as evidence of redox reactions, often catalysed by bacteria) can usually be equated with confined groundwater conditions. The mapping of distributions of water types across an area from the interpretations of individual site water chemistries is normally done manually using all the available information, chemical and other, as explained by Lloyd and Heathcote (1985). Rule-based approaches which can easily be applied using a GIS have also been used but these make further assumptions.

As an example of the water typing approach, Fig. 3.4.1 is a conceptual hydrochemical model for the Bure catchment in north Norfolk (Hiscock, 1993). The Chalk aquifer of northern East Anglia is covered by extensive Quaternary deposits that have a significant influence on groundwater conditions that are difficult to explain on the basis of the often sparse pumping test data and the widely spaced array of monitoring points. Further to the initial conceptual model, Hiscock *et al*. (1996) demonstrated the limited vertical development of the Chalk aquifer in interfluve areas. Using a combination of stable isotope data ($\delta^{18}O$ and $\delta^{2}H$ of water), magnesium:calcium ratios and electrical conductivity data based on analyses of depth samples and geophysical borehole logging, the effective Chalk aquifer was shown to be limited to the upper 50 – 60 m in the west of the region and as little as 25 m where the

Palaeogene boundary is met in the east. Combined with further information from carbon-14 data and tritium analyses (Fig. 3.4.1), confined groundwaters in the interfluve areas were shown to have old groundwater ages and isotopically depleted stable isotope signatures suggestive of groundwater recharge under much cooler climatic conditions than present. In contrast, regions of unconfined Chalk in river valley zones were shown to contain modern groundwater with contaminants such as nitrate and also having a measurable tritium content. The overall understanding of the groundwater flow mechanism based on the hydrochemical interpretation is that limited direct recharge occurs to the Chalk aquifer in the interfluve areas and, instead, modern recharge moves horizontally through the overlying glacial deposits to the valley zones where direct recharge to the more transmissive Chalk can occur.

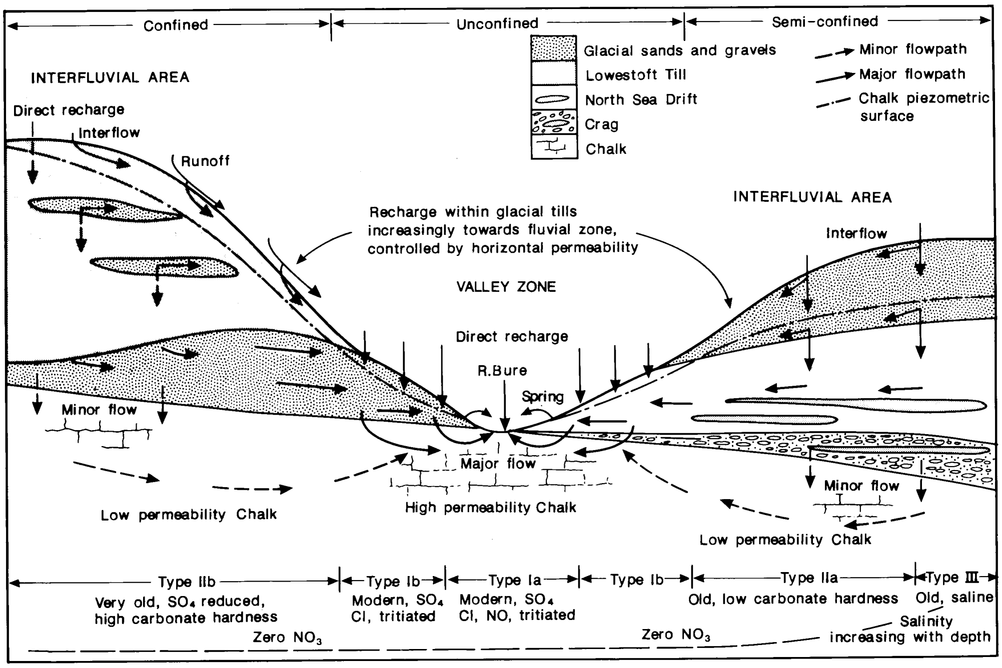


Figure 3.4.1. Conceptual hydrochemical model of the Chalk aquifer system of the Bure catchment, north Norfolk (from Hiscock, 1993).

Hydrochemical methods applied to understanding recharge and groundwater flow patterns will work best where there is large-scale heterogeneity compared with borehole spacing and where the main chemical variations are horizontal rather than vertical. Large changes in chemistry, for example due to variations in reactive components in the aquifer, or due to flow from one rock type to another, or large and sudden changes in recharge water chemistry will also assist interpretation. In the context of British aquifers, those aquifers covered by glacial deposits (the Chalk of East Anglia and the Triassic sandstones of the North West, Yorkshire and parts of the West Midlands) and those having a change from unconfined to confined conditions (Humberside Chalk, Lincolnshire Limestone and the East Midlands Triassic sandstone) can be expected to show good contrast in chemical distributions. On the otherhand, sand and gravel aquifers (for example in the Trent Valley), unconfined Chalk (Brighton Block), unconfined Triassic sandstone (parts of the West Midlands) and unconfined Carboniferous Limestone (Mendip Hills) are unlikely to show contrasting chemical distributions.

3.4.3 Examples of the application of hydrochemical data in groundwater modelling

Hydrochemical data can be used in both senses of groundwater modelling, that is for testing conceptual models and also as part of the refinement process for more advanced applications involving model predictions. Additionally, information on groundwater recharge rates and groundwater flow velocities derived from stable and radioactive isotope data can be used to postulate aquifer evolution over much longer timescales than is possible with relatively short-term instrumental records of groundwater head. This aspect of testing past recharge and boundary conditions provides for palaeohydrogeological reconstructions and the possibility of predicting future environmental conditions.

In their study of land drainage and saline intrusion in the coastal marshes of northeast Norfolk, Holman & Hiscock (1998) attempted an explanation for the apparent differences in the extent of saline intrusion in the locally important Norwich Crag aquifer as controlled by drainage levels. Drainage levels are maintained by surface water pumping and effectively determine the water table elevation in this low-lying district. Because of little previous hydrogeological investigations in the sand and gravel Crag aquifer, very limited groundwater level data existed with which to provide a conceptual model of the link between surface water and groundwater. By using spatial information gained from surface geophysical methods to map the apparent ground conductivity using electromagnetic and vertical electrical resistivity soundings, knowledge was gained of the subsurface salinity. This information was then used to constrain a density-coupled, vertical section groundwater model. Fig. 3.4.2 is a plot of the salinity contours for the case of the main drain in the coastal marsh being maintained by pumping at a lower level than the inland drainage level, with the main drains represented as fixed head cells. The modelled salinity distribution matched the situation on the Brograve marsh where low groundwater levels, as maintained by drainage pumping, serve to limit saline intrusion into the Crag aquifer.

Another example of the effective use of hydrochemical data in constraining conceptual model development is provided by Atkinson & Davison (2002) who attempted a simple steady-state model of the Carboniferous Limestone aquifer of the Bristol-Bath structural basin. Various thrust faults are conjectured to potentially disrupt the hydraulic continuity of flow within the 'Mendip Model' (Andrews *et al*., 1982) used to explain the thermal springs at Bath and Hotwells, near Bristol. As shown in Fig. 3.4.3, by using a mixing ratio of 1:2.3 between the locally recharged cooler groundwater and the deeply circulating thermally heated water based on the major ion chemistry, and comparing the ratio between regional transmissivity and the transmissivity of thrust zones, a number of geological scenarios were rejected in favour of the base model which assumed hydraulic continuity across the basin.

The modelling of aquifer evolution over longer periods than present-day provides insight into the development of aquifer permeability as determined by climatic controls on recharge and changes in the hydrologic base level. For the long-term disposal of wastes and the assessment of groundwater resources under different future climatic states, modelling of palaeohydrogeological conditions provide a proxy for future environmental conditions. One example of such a palaeohydrogeological model is presented by Hiscock & Lloyd (1992) for the South Humberside Chalk aquifer in which the permeability development was modelled since the Ipswichian interglacial, 140,000 years ago. This period includes the Devensian ice age when the base level reached a minimum of 120 m below sea level. Brackish to saline waters of probable Ipswichian origin exist at depth in the confined section of the aquifer beneath the cover of Devensian Till (Howard, 1985). The existence of a saline water body in the Chalk aquifer was a critical part in the modelling of the aquifer evolution and led to the conclusion that little groundwater flow and flushing of saline water occurred during the cold Devensian period when permafrost conditions prevailed. The present-day model also required saline water to be maintained at depth in the Chalk aquifer as shown to exist by geophysical borehole logging. To achieve this, a fixed saline head boundary was required at the base of the density-coupled model domain and was interpreted as providing evidence for long-term upward groundwater flow from the underlying Lower Cretaceous and Upper Jurassic formations.

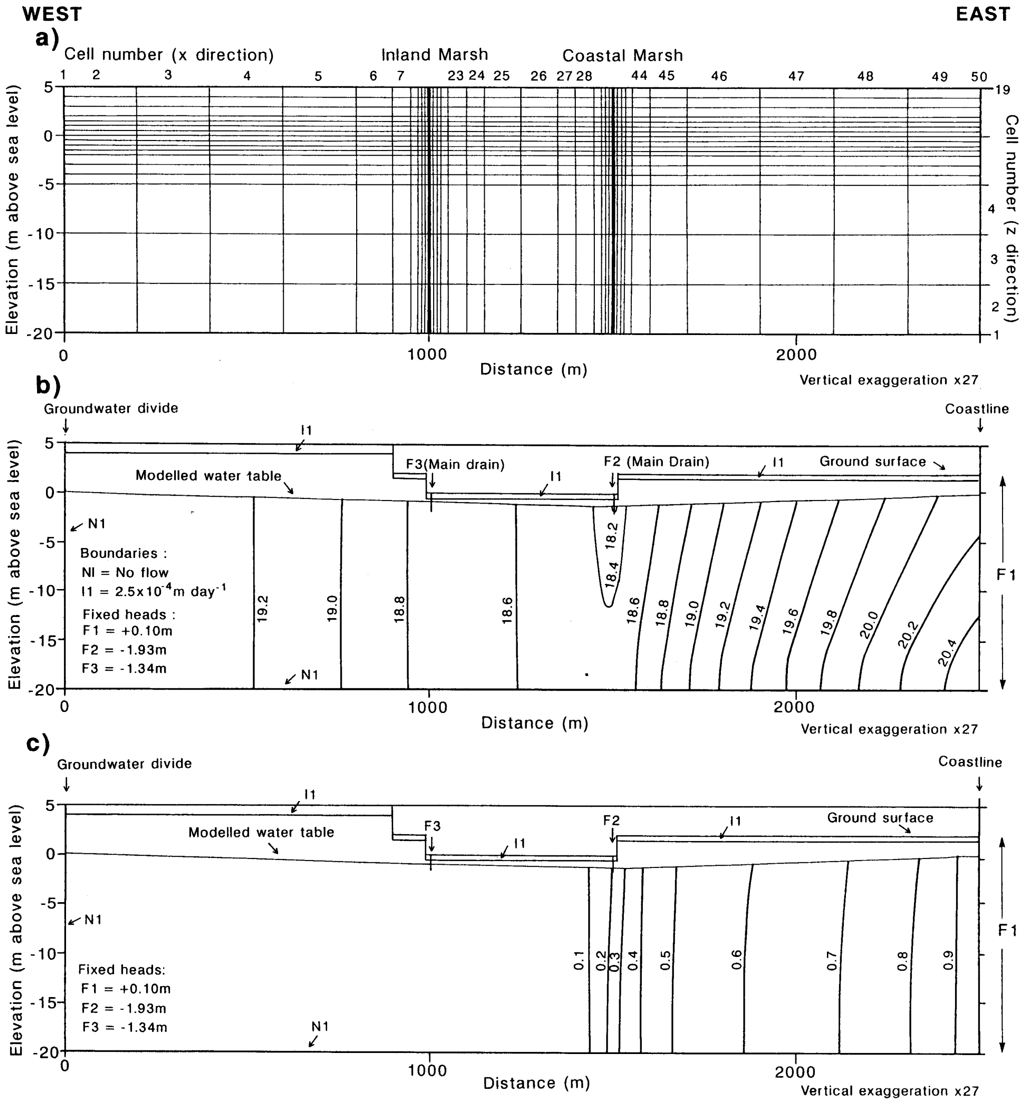
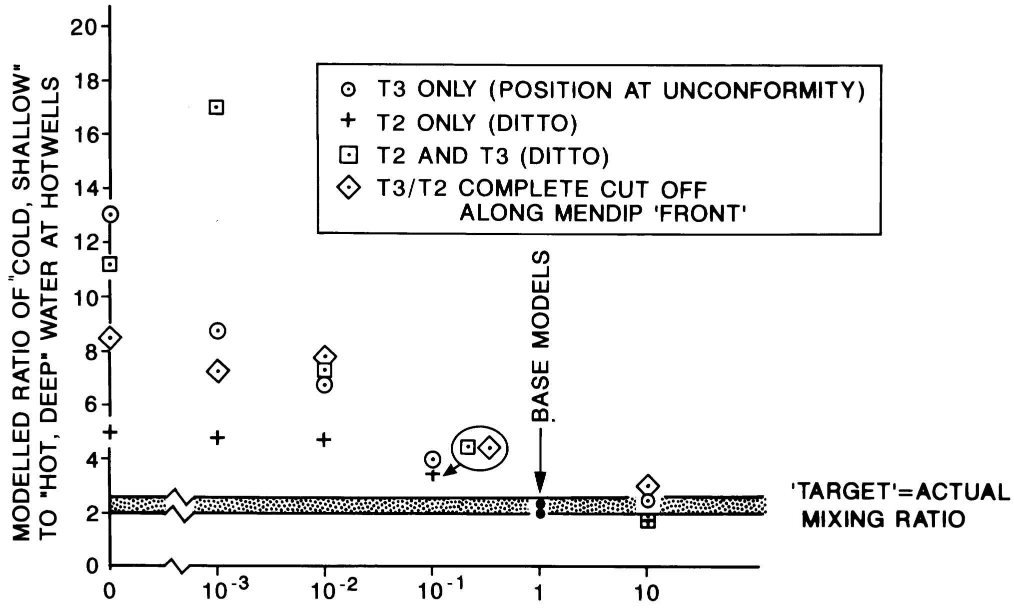


Figure 3.4.2. Set-up and results of solute transport modelling of saline intrusion in the Crag aquifer of the Thurne catchment, north-east Norfolk. Discretisation of the finite difference grid is shown in plot (a). Contours of equal hydraulic head and salinity distribution for a simulation with an infiltration rate of 2.5 x 10^{-4} m day^{-1} and horizontal and vertical hydraulic conductivity values of 10 and 1 m day^{-1}, respectively, are shown in plots (b) and (c) for the case where the seaward main drain (fixed head cell, F2) is maintained at a lower hydraulic head than the inland drain (fixed head cell, F3) (from Holman & Hiscock, 1998).

COMPARISON OF MODEL PREDICTIONS WITH
ACTUAL MIXING OF 'COLD' AND 'THERMAL' WATERS
AT HOTWELLS, BRISTOL



RATIO OF TRANSMISSIVITY IN THRUST ZONES
TO REGIONAL VALUE

Figure 3.4.3. Model predictions of the effects of the various thrust configurations (T2 and T3) upon mixing proportions of 'deep thermal' and 'shallow cold' waters at Hotwells Springs, as a function of the ratio between regional transmissivity and the transmissivity of the thrust zones. The only models to predict the correct mixing proportions are those in which thrust transmissivities are either equal to or greater than the regional value (from Atkinson & Davison, 2002).

3.4.4 Hydrochemical data uncertainty

The use of hydrochemistry in conceptual modelling is not without difficulties. The large number of linked hydrochemical processes means that there is much more scope for error than in flow interpretation. There is often a lack of data on processes and historical input quality that make interpretation difficult and there is a dependence on velocity distributions about which little is known in the UK. Also, all groundwater samples and hydrochemical interpretations are affected by the sampling device and the number of samples needed to resolve patterns within a region. To overcome heterogeneity, probably greater than 100 sample sites within a 20 x 20 km region is required to obtain a useful interpretation. This sampling density will usually require a combination of the Environment Agency's base data supplemented by special sampling.

Groundwater samples are often from pumped boreholes but it must be recognised that there can be large differences in the ages of water entering the borehole at different depths and therefore large differences in the water quality. If the effects of time-variant regional groundwater flow are considered then it is possible that water entering the borehole at any given depth is no longer necessarily of the same age, and can be of very different ages depending on flow paths reaching the borehole. Unpumped borehole samples often exhibit vertical flows and this is another cause of error in permitting deep water to be transferred into the upper part of an aquifer, or vice versa.

Other problems relating to groundwater sampling include chemical interactions with the borehole casing (Song & Atkinson 1991) and drilling-induced effects. In order to reduce data uncertainty and errors in interpretation, careful records of site details (geology, depth, casing, flows, pumping rates, times of pumping, etc.) should be kept. If recharge calculations are to be undertaken, then additional rainfall chemistry and possible porewater samples will be required and this data collection will require specialist methods.

3.4.5 References

Andrews, J.N., Burgess, W.G., Edmunds, W.M., Kay, R.L.F. & Lee, D.J., 1982. The thermal springs of Bath. *Nature*, **298**, 339-343.

Atkinson, T.C. & Davison, R.M., 2002. Is the water still hot? Sustainability and the thermal springs at Bath, England. In: Hiscock, K.M., Rivett, M.O. & Davison, R.M. (eds), *Sustainable Groundwater Development*. Geological Society, London, Special Publications, **193**, 15-40.

Downing, R.A., Pearson, F.J. & Smith, D.B., 1979. The flow mechanism in the Chalk based on radio-isotope analyses of groundwater in the London Basin. *Journal of Hydrology*, **40**, 67-83.

Edmunds, W.M. & Walton, N.G.R., 1983. The Lincolnshire Limestone - Hydrogeological evolution over a ten year period. *Journal of Hydrology*, **61**, 201-211.

Edmunds, W.M., Cook, J.M., Darling, W.G., Kinniburgh, D.G. & Miles, D.L. (1987). Baseline geochemical conditions in the Chalk aquifer, Berkshire, U.K.: a basis for groundwater quality management. *Applied Geochemistry*, **2**, 251-274.

Hiscock, K.M., 1993. The influence of pre-Devensian deposits on the hydrogeochemistry of the Chalk aquifer system of north Norfolk, UK. *Journal of Hydrology*, **144**, 335-369.

Hiscock, K.M. and Lloyd, J.W., 1992. Palaeohydrogeological reconstructions of the north Lincolnshire Chalk, UK for the last 140,000 years. *Journal of Hydrology*, **133**, 313-342.

Hiscock, K.M., Dennis, P.F., Saynor, P.R. & Thomas, M.O., 1996. Hydrochemical and stable isotope evidence for the extent and nature of the Chalk aquifer of north Norfolk, UK. *Journal of Hydrology*, **180**, 79-107.

Holman, I.P. & Hiscock, K.M., 1998. Land drainage and saline intrusion in the coastal marshes of northeast Norfolk. *Quarterly Journal of Engineering Geology*, **31**, 47-62.

Howard, K.W.F., 1985. A multistage model for the development of hydrochemical zonation in Chalk groundwaters. *Ground Water*, **23**, 4-9.

Lloyd, J.W. & Heathcote, J.A., 1985. *Natural inorganic hydrochemistry in relation to groundwater: an introduction*. Clarendon Press, Oxford.

Song, L.-H. & Atkinson, T.C., 1991. Chemical reaction between concrete and natural groundwaters and its implications for the commissioning of observation boreholes in the Chalk. Quarterly Journal of Engineering Geology, **24**, 221-229.

Wilson, G.B., Andrews, J.N. & Bath, A.H., 1994. The nitrogen isotope composition of groundwater nitrates from the East Midlands Triassic Sandstone aquifer, England. *Journal of Hydrology*, **157**, 35-46.

4.1 Conceptual modelling

4.1.1 What is a conceptual model?

A conceptual model is a description of how a hydrogeological system is believed to behave.

It has a number of important characteristics:

1. It concentrates on the features of the system which are important in relation to the purpose of the project. In this regard, it is a simplification of reality;

2. It must be based on evidence;

3. Its essence is: observations, explanations, working hypotheses and assumptions;

4. It must be written down;

5. It must be tested.

Some of these characteristics are explored in more detail below:

– *It concentrates on the features of the system which are important in relation to the purpose of the project. In this regard, it is a simplification of reality.*

  The following quotes (italics) are taken from Rushton (1998):

  Aquifer systems are so complex that it is not possible to study every detail. This leads to the question of what needs to be to be included in an aquifer study and what can be ignored.

  Which elements of observed behaviour must the model be able to simulate? For example, for a groundwater resources model in a coastal area, the focus might be on the larger water resources question of whether any saline water is entering the aquifer or not, and if so how much. In this context, if it is not important that the model simulates the detail of saline water sinking below freshwater, it might be appropriate to ignore the effects of variable density associated with saline intrusion in order to simplify the mathematical representation.

  For most aquifer systems there are a small number of crucial factors which must be examined in detail; if only one of these is ignored the conclusions may be seriously in error.

  How do we identify these crucial factors? Considering the purpose of the study will help. For example, if the coastal model mentioned above is a small Caribbean island, then it will be important to establish the relative positions of the freshwater lens and the underlying saline water in order to know how much freshwater can be pumped without leading to water quality problems. For this purpose we should not ignore density differences. Hence writing down the purpose and specific objectives of your model is invaluable in focussing effort on the right factors.

– *It must be written down.*

The act of documenting, i.e. writing down, our conceptual models has the following advantages;

- it forces us to formalise our thoughts, and thus to identify and address any weaknesses in our reasoning such as unjustified assumptions (or plain mistakes!);
- it facilitates communication of our formalised thoughts so that others can discuss and challenge them;
- it provides something which we can test for validity.

– *It must be tested.*

We may think there is only one explanation for the observed behaviour but experience shows that we are usually wrong. Post-project evaluations of groundwater models in the US show that the most common cause of error is use of the wrong conceptual model (Anderson and Woessner, 1992, p.293). This is why testing is an essential part of the development of our conceptual model. It forces us to re-evaluate our current hypotheses and look for alternatives. Hence, an untested conceptual model is useless because it is almost certainly misleading. Continued testing leads to increasing confidence that our conceptual model is an adequate description of the real system.

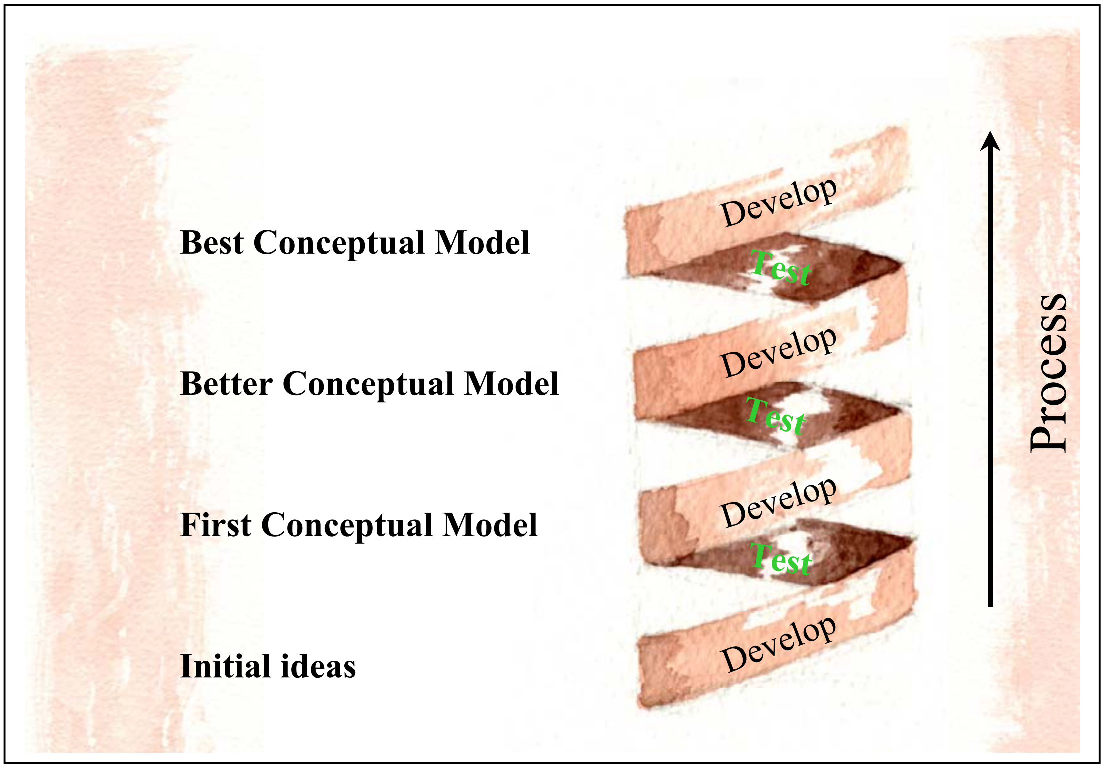


Figure 4.1.1. The development process for a conceptual model

4.1.2 How is it developed?

Modelling, and especially conceptual modelling, is an iterative or cyclical process of development and testing, as illustrated in Figure 4.1.1:

- We start with our initial ideas and write them down (e.g. observations, hypotheses, areas of uncertainty);

- We test the model, for example we can do some crude water balance calculations with long-term average recharge values, river flows, groundwater flow using Darcy's law, and storage changes based on long-term changes in groundwater level;
- Based on the results of the testing we re-evaluate the model, reject some hypotheses, keep some, and develop some new ones;
- We return to the start of the process: we write our first conceptual model down, we test it........, etc.

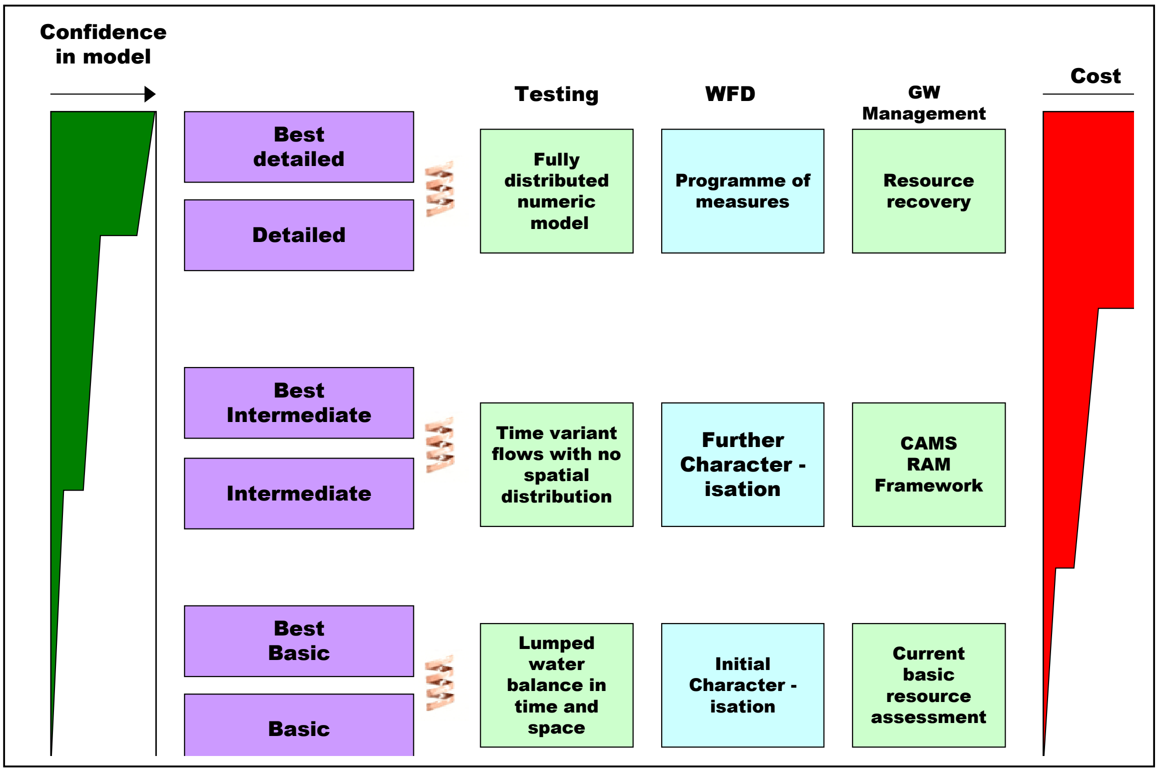


Figure 4.1.2. Tiered approach to conceptual models

Conceptual modelling is continuous and cyclical – it's a process, not a finished product. The degree of development of the conceptual model is determined by the sophistication of the tools used to test it. Figure 4.1.2 shows a hierarchy of model development, with associated tools for testing and appropriate uses for the models:

– **Best basic.** Lumped long-term average water balances gives us a "best basic" conceptual model. It will be adequate for initial characterisation within the Water Framework Directive (WFD) or a very basic groundwater resources assessment.

What if this understanding of how the system works is still too uncertain to answer our questions about whether the resource is over-abstracted or about the quantitative status of the groundwater system?

– **Intermediate.** We need a better conceptual model. Significant advances are required with different types of data (e.g. time-variant heads and flows) and different testing tools (e.g. spatially lumped, seasonal water balances, water balances for sub-catchments [semidistributed], or analytical equations [e.g. Jenkins for impact of abstraction on river flows]).

This scale of development leads to:

- increased confidence - further characterisation (WFD), level of confidence appropriate for many of the Agency's Catchment Abstraction Management Strategies (CAMS);
- and increased costs.

This conceptual model is still likely to be too uncertain for defining a programme of measures under the WFD or for negotiating reductions in abstraction to improve stream flows (resource recovery).

– **Detailed.** Hence we need a more detailed method of testing to improve confidence, usually a spatially distributed and time-variant numerical model.

4.1.3 The conceptual modelling process

Data Analysis

The various data sets should initially be considered, rigorously checked and analysed in their own right and presented independently. This should ensure that all the relevant information is reviewed in an unbiased way, minimising the prejudice that can easily grow from the review of previous work both within the study area (i.e. part of the literature review) and elsewhere (i.e. the experience of the team carrying out the work).

It should be possible to progress the analysis of each of the data sets (geology, meteorology, artificial influences, river flows and groundwater levels) in parallel. Each set can be represented by its own section in the report with associated time series and GIS or other spatial plots. Workers should attempt to maintain an 'open mind' throughout these tasks, seeking to subject the data to objective analysis, plotting and comparing information on consistent scales, identifying and describing differences and patterns of responses as they emerge. Subjective assumptions and conclusions should be challenged throughout.

Data Integration

Although a rigorous approach to each data set is an important starting point, the development of a sound conceptual model depends on achieving an integrated understanding of all available evidence.

Interrelationships between the many data sets need to be explored. A list of possible data to consider together is presented in Table 4.1.1 although data availability, the purpose of the model, and time may constrain what can practically be achieved. A prioritised and pragmatic approach is recommended which focuses on data of most significance to the purpose of the modelling study.

The conceptual model(s) derived to explain the data will usually be associated with considerable uncertainty and can be expected to evolve and change through the modelling process. In contrast, integrated data presentation formats should be kept as free from inference and interpretation as possible and may therefore have a much longer 'shelf life', providing benefits which extend beyond the modelling study itself.

Table 4.1.1. Data Integration – Analysis and Presentation

System understanding to be developed	Datasets which can be compared	Examination Mode
Runoff response, evidence of interflow and aquifer discharge	Rainfall, effective rainfall, river flow and groundwater baseflow	Time series
Recharge processes	Drift geology, soil types, land use, effective rainfall and groundwater levels	Time series, Plans
River-aquifer interaction and stream flow depletion due to groundwater abstractions	Piezometric surface, river bed/ground surface elevations, river flow, groundwater abstraction locations	Section & Accretion Profile
Areas of confined aquifer, inter-aquifer communications	Geology and water table/piezometric surface	Plan, Section
Groundwater flow directions, transmissivity	Piezometric surface elevation, groundwater abstraction locations and pumping test results	Plan
Evidence for hydraulic conductivity or specific yield as a function of depth	Groundwater level and river flow variations plus geophysical logs indicating zones of enhanced hydraulic conductivity	Time series
Evidence for the recent actual operational control of impoundments and abstraction licences and the impact of these constraints on river flows	Daily (or 15 minute) river flow, surface water abstraction returns (& surface water discharges), reservoir operational rules	Time series
Understand distribution of existing licensed stress on groundwater resources	Licensed groundwater abstraction rates and recharge	Schematic plan (overlapping circles)
Evidence for the impact of recent actual surface water influences on river flows	Surface water abstractions/ discharge locations, spot flow gaugings	Section & Accretion Profile

4.1.4 The Phase I report

Contents

The Phase I report is here assumed to include the presentation and integration of data analysed for a study, as well as the description of the conceptual model itself (see Box 1 for suggested contents). The report may also include proposals to test the concepts through exploratory modelling before development any more detailed numerical model.

Box 4.1.1. Suggested contents of the Phase I report

- Introduction to the aims and objectives of the modelling study.
- A summary of previous work carried out in the area, emphasising the key literature which has developed conceptual understanding.
- A number of Sections describing the individual data sets in their own right (including geology, meteorology, artificial influences on the hydrometric cycle, river flows and groundwater levels).
- A comprehensive integration of these data sets to develop and support one or more alternative conceptual models.
- The estimation of recharge and the calculation of water balances as part of the testing and development of conceptual understanding.
- Proposals for (and possibly results of) further testing and evolution of the conceptual model through exploratory or full modelling.

Presentation of the conceptual model

The textual description of the conceptual model will focus around figures covering the following topics:

- Integrated data maps showing geology, water table/piezometric surface for main aquifer units, abstractions and discharges (surface and groundwater), river gauging stations, impoundments, transfers, spot measurements and catchments;
- Integrated river profiles showing geology, water table, and flow accretion for the main rivers;
- Comparison of groundwater level and river flow hydrographs (with groundwater baseflow separated), with rainfall and effective rainfall time series, typically the major rivers and selected tributaries to indicate particular processes;
- Maps showing distribution of potential and actual recharge;
- Maps showing the zoned distribution of aquifer properties;
- Diagrams of the groundwater - surface water flow system and processes, with maps of conceptual 'domains' where groups of processes are similar, if relevant;
- Cartoons showing system/sub-system behaviour.

Examples of sketches, drawings and sections illustrating conceptual understanding are provided below for groundwater-dominated catchments where the issue of groundwater - surface water interaction is of particular importance:

- Figure 4.1.3 is an integrated profile along the River Mimram, one of the main tributaries to the River Lee. This includes geology, groundwater levels, river or ground elevations, the location of abstraction and observation wells and river flow accretion profiles from spot gaugings annotated with tributary and place names;
- Figure 4.1.3 also shows time series plots of rainfall, river flow, separated baseflow and groundwater levels. These are plotted against fixed scale axes to facilitate comparison of timing and amplitude;

- Figure 4.1.4 is a schematic block diagram summarising the key flow processes of the hydrological cycle of the River Stour catchment in the West Midlands. It illustrates the complex relationships on this highly urbanised sandstone aquifer which has a long history of groundwater abstraction;

- Figure 4.1.5 shows overlapping 'recharge circles' for groundwater sources in the Chalk of the Upper Lee catchment, superimposed onto a map of conceptual transmissivity zones. The area of each circle has been calculated to provide the annual licensed rate of abstraction from each source, based on the long term annual average recharge. By shading according to the number of overlaps, this type of map provides a simple but visually effective illustration of the commitment of recharge resources to abstraction. The real distribution of drawdown associated with the abstraction will, of course, be much more complex than the overlapping circles and will be influenced by the distribution of transmissivity, as included on the sketch map. However, the circles are useful as a source-focused integration of recharge and abstraction rates which do not require the delineation of groundwater management units for water balance purposes. Overlapped areas represent areas where there is local stress on groundwater resources that may require water to be drawn from long term storage or from unshaded areas.

- Figures 4.1.6 and 4.1.7 emphasise that conceptual sketches do not have to be professionally drafted to be useful. Figure 4.1.6 contrasts groundwater-surface water interaction processes along the River Mimram (as in Figure 4.1.3) in a dry summer and a wet winter. Changes in the pattern of river flow accretion, drawdown related to abstraction and regional groundwater contours are important features which have helped draw out understanding of how this Chalk river 'works'. Figure 4.1.7 is a sketched cross section along the Rivers Alre and Itchen on the Hampshire Chalk which schematically illustrates the flow of water into, through, and out of a high transmissivity fissured zone considered to be key to an explanation of observed river flow accretion.

The text and figures describing the qualitative aspects of how the system works should, as far as possible, be accompanied by simple quantitative calculations to show that the process explanation can account for observed flows and heads on the basis of credible aquifer parameters. Such calculations might include water balances, simple groundwater flow estimates or lumped parameter models.

The conceptual model report should identify possible uncertainties in understanding and should also attempt to identify alternative conceptual models which can be tested during exploratory modelling. A conceptual model description is a perception of the system, based on incomplete data which, especially in the early stages of a project, will have been incompletely evaluated. It is quite possible that it is not the only description of the system which is consistent with the data. Other descriptions may vary in parameter combinations or in the processes included. These alternatives give rise to conceptual uncertainty.

4.1.5 Conceptual Models are Derived by People

Attempts should be made to provide, where possible, standard methodologies for data analysis and integration, for example calculation of baseflow from a surface water hydrograph. Such guidance is helpful to achieving thorough and quality assured outcomes and avoiding basic mistakes.

It is important to recognise that conceptual modelling involves 'detective work' and some intuitive leaps in ideas: *its as much an art as a science!* Such models are usually best developed by a team of people and therefore the 'softer' processes of communications, consultation, review and facilitated involvement are also vital in achieving a credible understanding with which everyone agrees.

For large regional models, this process is likely to involve the following people:

- The Agency's project manager;
- The Agency's 'Local People with the Knowledge' (e.g. hydrogeologists, hydrologists etc);
- Stakeholders including water companies and others, some of whom may also have extensive local experience of the aquifers;
- The people 'Doing' most of the work (Agency or Consultant or both); and
- Peer Reviewer(s) – Agency or external

Meetings, reviews and workshops need to be carefully planned to involve the right people, benefit from their experience (i.e. get everyone to contribute) and maintain consensus towards a mutually agreed model. Such a process takes time and requires the commitment of those involved which can sometimes clash with the desire to 'get some results quick'.

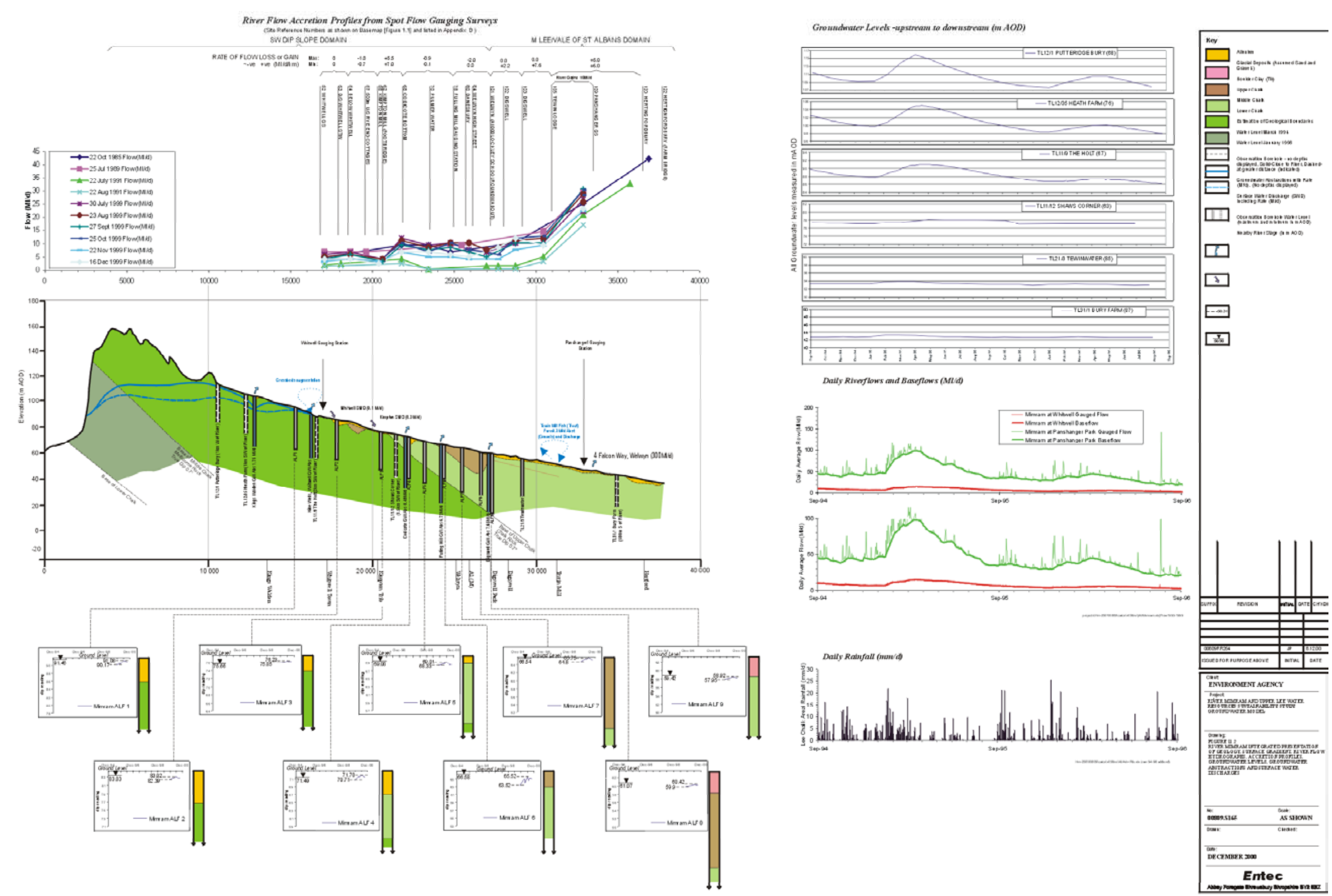
In scheduling a study, it is advisable to assume that key deliverables such as the conceptual modelling report will take at least 3 review iterations to move the project forward; this was the case for both the West Midlands and Upper Lee studies. It can be helpful to stagger the delivery of such large reports in order to ensure timely review and reduce the number of dead ends pursued (e.g. release data analysis, integration and conceptual model sections separately, as they are completed).

Finally, it is important to manage expectations amongst all involved as to what can be achieved. In some studies, the problems and uncertainties associated with a conceptual model and subsequent numerical model may not be resolved by the end of the 'project period', despite the best efforts of all involved. The models developed for both the Upper Lee and West Midlands Studies do not provide completely adequate simulations of observed flows and heads because the project teams involved decided that, within the constraints of a 'finite budget', there should be no unjustified parameter 'tweaking'.

4.1.6 References

Rushton, KR. 1998. Groundwater at risk – a reflection. In Wheater, H and Kirby, C (Eds.), *Hydrology in a changing environment, Vol. II.* Proceedings of the BHS International Conference, Exeter, Wiley, p 1-10.

Figure 4.1.3 Example of Integrated Presentation of Geology, River Flow Hydrograph, Groundwater Levels and River Flow Accretion (from the Upper Lee Study)



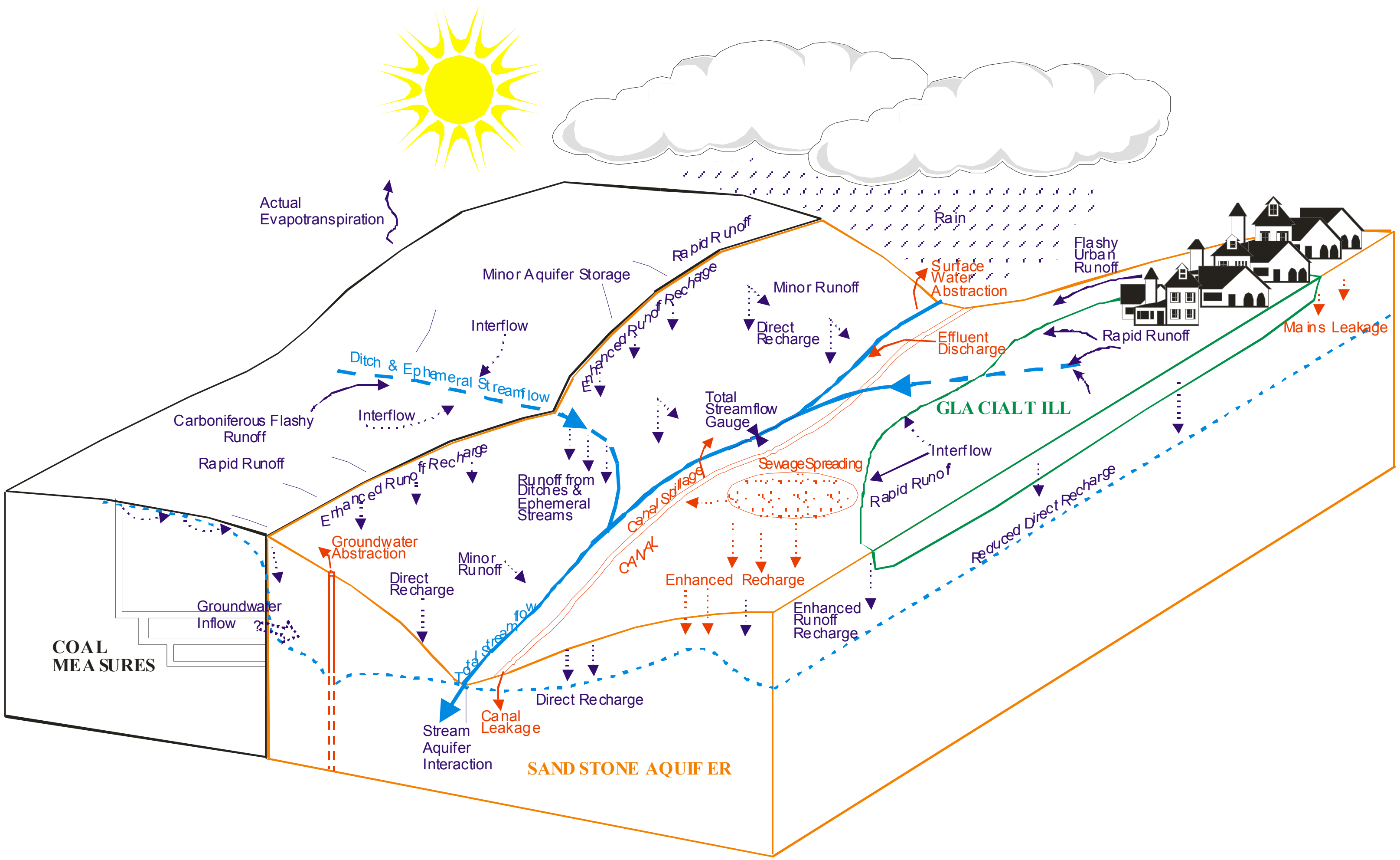


Figure 4.1.4 Example of a schematic sketch of the natural and artificial components of a catchment hydrological cycle (from the West Midlands study,)

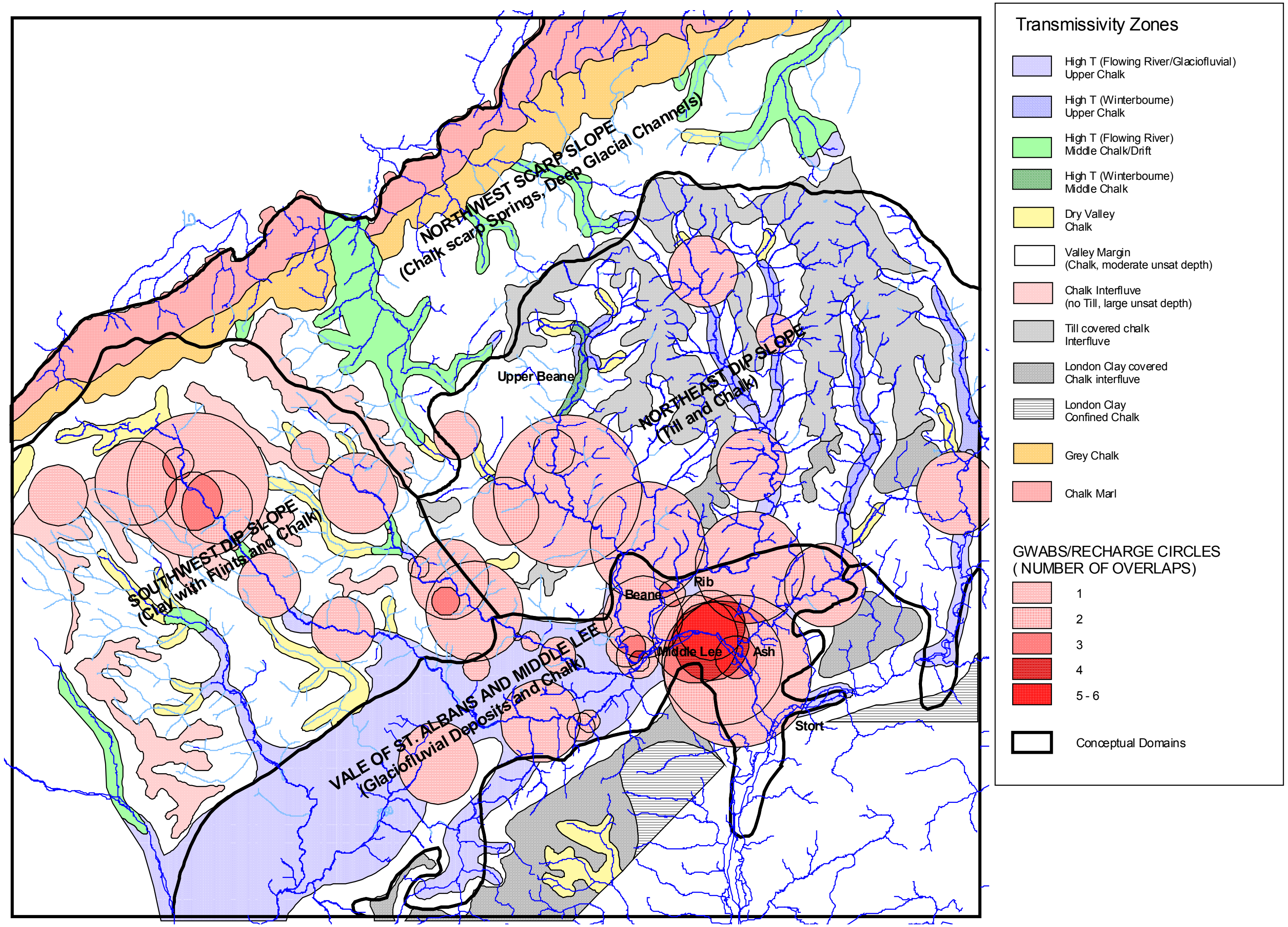


Figure 4.1.5 River Lee worked example: conceptual domains, transmissivity distribution and GWABS/recharge circles (from the Upper Lee study,)

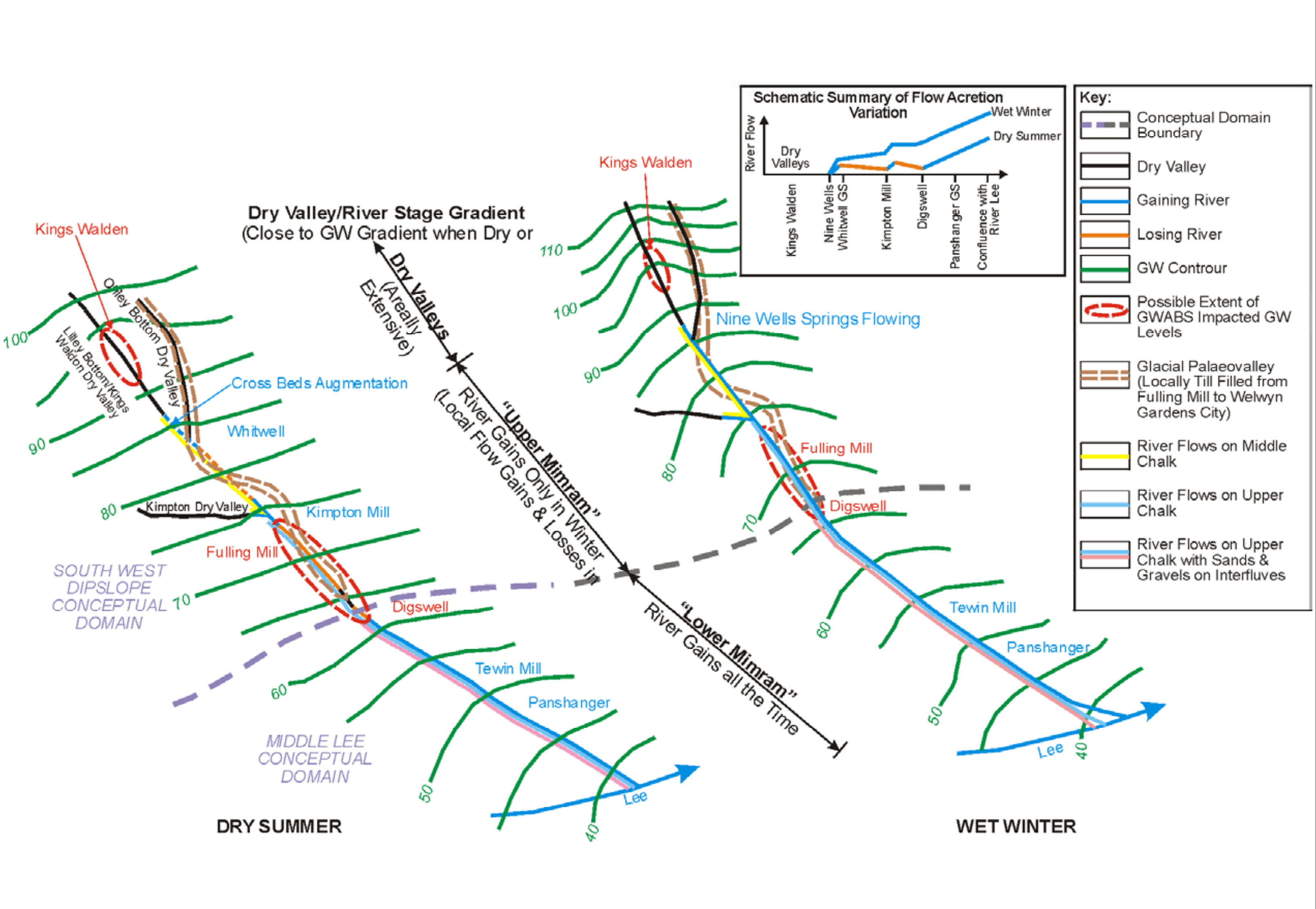


Figure 4.1.6 Example of a rough conceptual sketch illustrating seasonal variations in groundwater - surface water interaction (from the Upper Lee study.)

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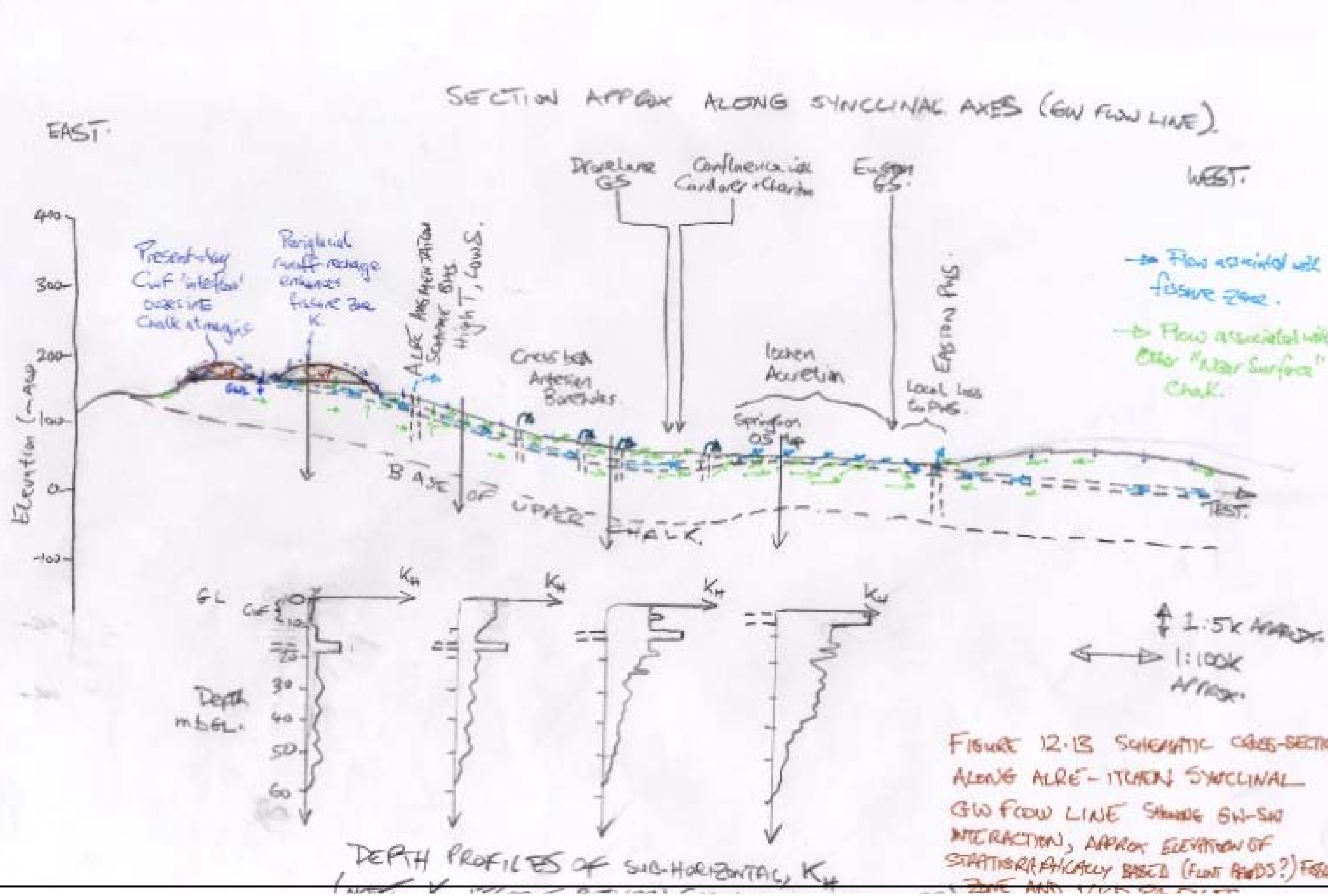


Figure 4.1.7 Rough schematic sketch section along the Rivers Alre and Itchen

4.2 The geological model

The geological model represents a fundamental part of any hydrogeological conceptual model. The amount of time spent in preparing a geological model needs to be appropriate in relation to the purpose of the project:

– There is little point in spending lots of time developing an *over-detailed* geological model if the level of detail does not contribute to the understanding of the flow behaviour of the groundwater system.

– Too little detail will also cause problems and, unfortunately, these are likely to manifest themselves only at a later stage in the project. An example of this was seen in the water resources study of the Fylde aquifer when in some areas of the aquifer the historical simulation did not adequately reproduce the behaviour of the aquifer. This was only improved following a review of existing borehole logs, interpretation of surface geophysical data by the BGS, and drilling of further investigation boreholes, all of which resulted in a major revision of the geological model (See Fylde case study, *Appendix C*).

Particular issues include (see Box 1 for examples/detail):

- structure of the area including folding, faulting, etc;
- identification of layering patterns in Chalk aquifers to represent the primary and secondary permeability distribution. Folding of the Chalk and adjacent strata not only influences the spatial distribution of Chalk properties, but also leads to concentration of flow paths or even diversion of flow;
- distribution and type of superficial deposits.

The understanding of the geological setting should be presented in the form of cross sections, isopach maps and structural contour maps of important units and included in the conceptual model report.

Understanding the geological setting is a pre-requisite to developing a credible conceptual model of a groundwater system.

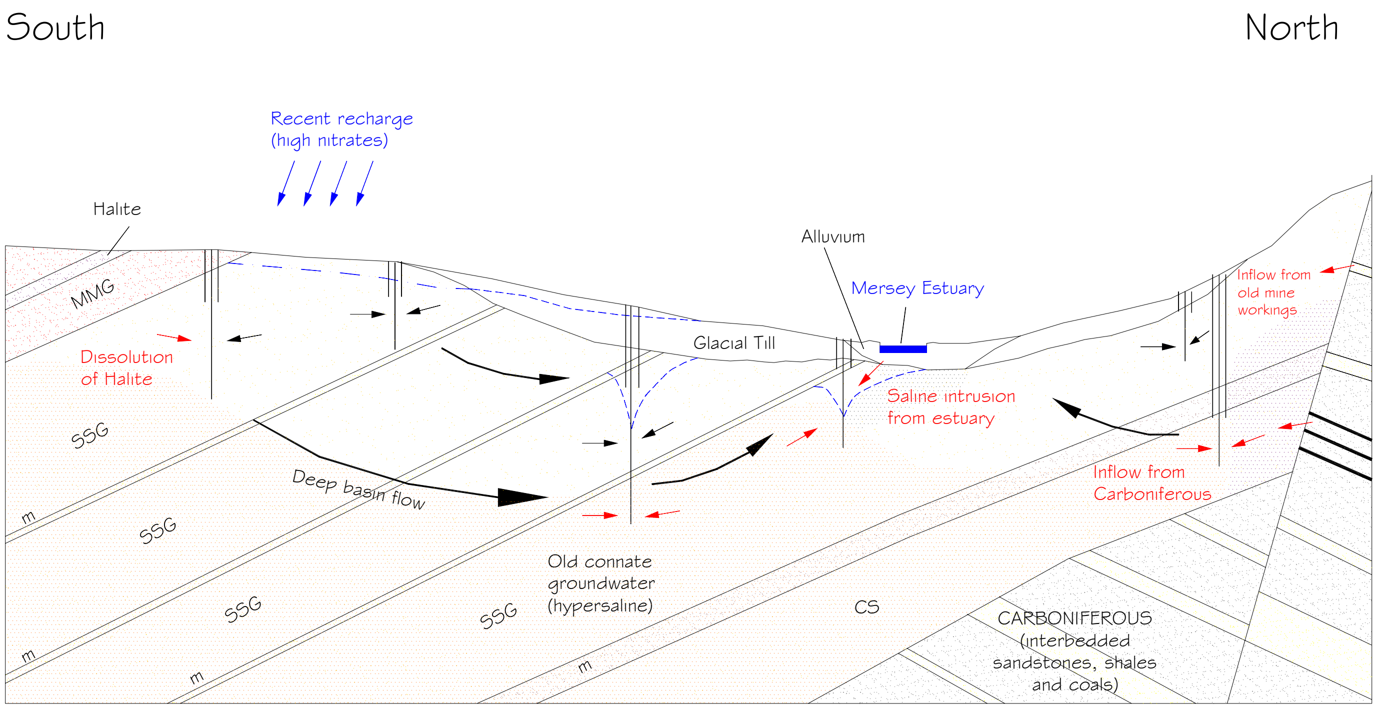
Box 4.2.1. Examples of the influence of the geological framework on groundwater flow

1 Evolution of geological basin	
Sherwood Sandstone: Mersey Basin/ West Cheshire aquifers	Several sources of poor quality (saline) groundwaters: ~ dissolution of halite, ~ old (connate) sea water, ~ recent saline intrusion from Mersey estuary, ~ inflow from Carboniferous strata. Very slow rate of groundwater movement at depth. **See Figure 4.2.1.**
2 Geometry and structure of the aquifer	
Sherwood Sandstone: Fylde aquifer	North-south faults and marl bands divide aquifer into layers/compartments and limit hydraulic connection in an east-west direction. **See Figure 4.2.2.**
Chalk: Chichester Syncline	This deep east-west syncline takes clayey Tertiary deposits to depths of up to 100m below sea level where they act as a barrier to southward, down-dip groundwater flow. They cause groundwater flow to be deflected eastwards to springs at Arundel. The resulting concentration in flow has led to enhanced dissolution and very high permeabilities (karstic conditions). Where the base of the syncline is shallower strong underflows occur associated with high spring discharges on the southern limb of the syncline. **See Figure 4.2.3.**
River Meon	Folding transverse to the River Meon valley has brought the lower permeability Lower Chalk up to river level which has had the effect of “throwing out” higher baseflow discharges to the river along certain reaches. **See Figure 4.2.3.**
3 Boundary conditions	
Sherwood Sandstone: Fylde aquifer	The nature of the contact between the Carboniferous strata and Sherwood Sandstone aquifer (faulted/unconformable) and the lithology of the Carboniferous strata controls the amount of potential cross boundary flow. This needs to be understood for it to be properly represented in the numerical model. **See Figure 4.2.4.**
4 Lithology and distribution of superficial deposits	
Sherwood Sandstone: Wirral & West Cheshire	Quaternary history and deposition of till & sands affects river/aquifer interaction - highly complex and variable drift. **See Figure 4.2.5 (a).**
Fylde aquifer	Low permeability drift cover limits recharge, but some vertical flow from drift induced by pumping from aquifer beneath. **See Figure 4.2.5 (b).** High permeability drift allows good connection with rivers.
Chalk: South Downs Chalk	Low permeability Clay with Flints restricts vertical leakage (direct recharge) and encourages run-off to give enhanced infiltration at the edges of the drift. This acidic run-off enhances chalk dissolution and formation of solution features. **See Figure 4.2.6.** High permeability drift, such as gravels, may provide a path for rapid flow or a high storage zone. In the Chichester area they provide a conduit for Chalk groundwater overspilling the contact with the Tertiary clays. **See Figure 4.2.3.** In areas of exposed Chalk there will be some degree of rapid “direct” recharge which bypasses the soil zone.

Box 4.2.1. Contd.

5 Influence of fluvial processes on groundwater/surface water interaction	
<u>Sherwood Sandstone:</u>	
Fylde	Upland reaches : coarse clean bed sediments, potentially good river/groundwater connection Becoming progressively finer grained (lower permeability) downstream – poorer connection (higher river bed resistance). **See Figure 4.2.5 (c).** Drift underlying stream affects hydraulic connection with aquifer (Glacial till or sand and gravel)
6 History of groundwater development	
<u>Sherwood Sandstone:</u>	
Mersey Basin/ Liverpool/Saline intrusion	A century of changing abstraction patterns has exerted a major influence on groundwater levels and quality; heavy abstraction close to the estuary has caused saline intrusion. Other factors also control the chemistry of abstracted groundwater – see 'Evolution of the geological basin'.
7 Multi-layered aquifer systems	
<u>Sherwood Sandstone:</u>	
Fylde	Quaternary and solid aquifers, in reality very complex (multi-layered, see *Appendix C*); this should be simplified as much as possible in the numerical model.
West Midlands Trias	Several different sandstones with different lithologies; low K zones requiring significant vertical groundwater head differences to move water vertically through low K bands – but a detailed representation of the layers may not be necessary for regional resource estimation.
<u>Chalk:</u>	
South Downs Chalk	The geological subdivision of the chalk in Wessex and Sussex has recently been revised and 10 mappable units are now recognised (Jones & Robbins, 1999). Whilst these new units provide a much finer degree of resolution of the Chalk structures, the identification of effective hydrogeological units is more problematical.
Chalk	Consideration of the Chalk should include hydraulic connection with over- and under-lying formations. Gravels overlying the Chalk may provide a high storage layer with respect to the low storage capacity of the Chalk (e.g. Lincolnshire Chalk)

Figure 4.2.1 Case example - Mersey Basin: influence of geological structure and basin evolution on the origin and distribution of saline groundwaters



Flows of saline groundwaters

MMG = MERCIA MUDSTONE

m = MARL BANDS

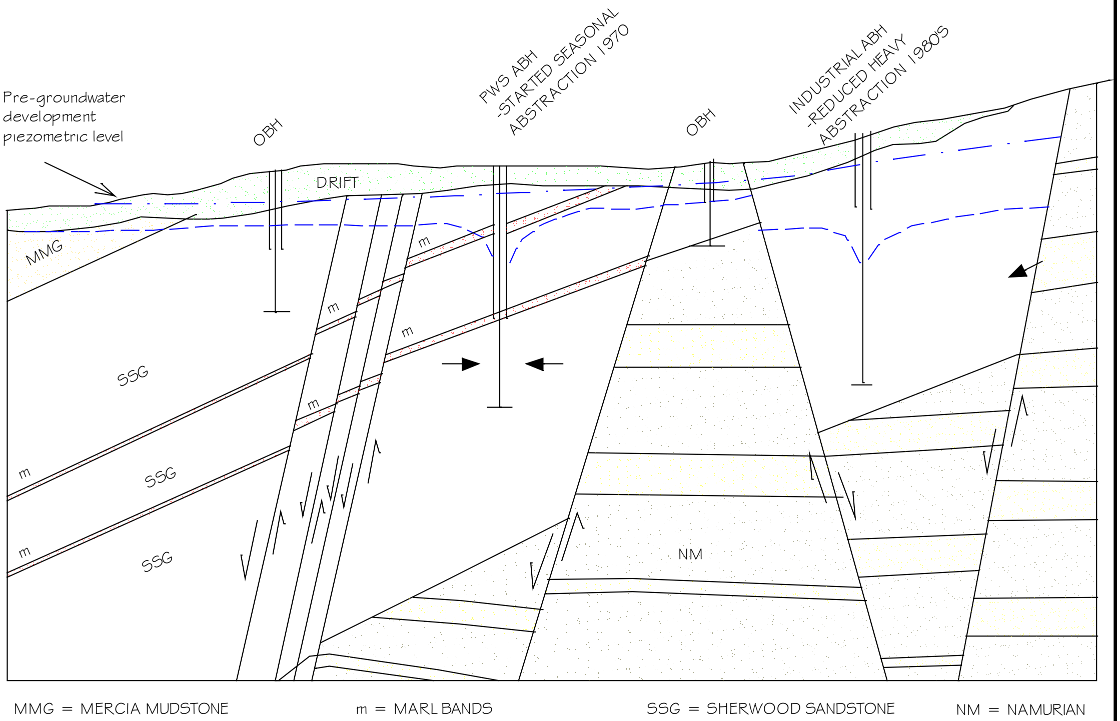
SSG = SHERWOOD SANDSTONE

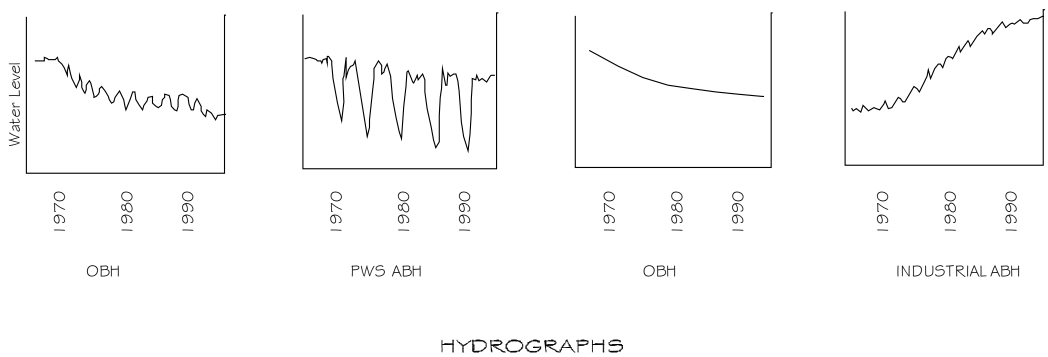
CS = COLLYHURST SANDSTONE

Deep Groundwater flow through the basin is very slow. Depending on the depth and location of abstraction boreholes, different ages and qualities of groundwater will be encountered. These relationships need to be understood and explained in the conceptual model, before they can be represented appropriately* in any numerical model.

*To meet the objectives of the study.

Figure 4.2.2 Case example - Fylde aquifer: influence of geological structure on piezometric response



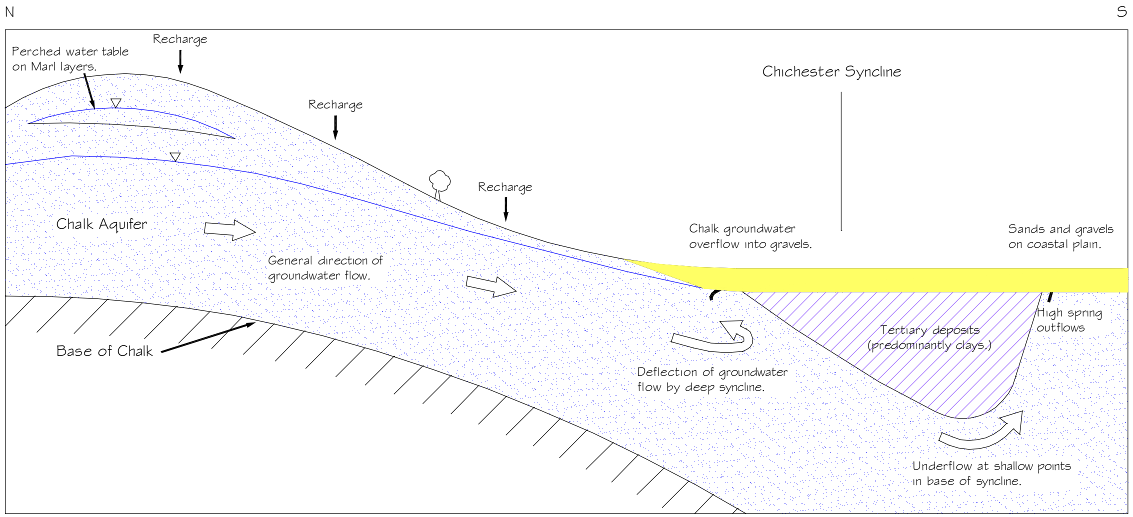


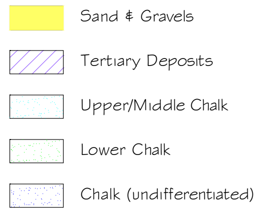
~ 'Horst and Graben' structure (displacement by faults) combined with presence of marl layers within sandstone aquifer result in separate 'compartments'

~ Responses to pumping from different compartments depends on depth and location of observation boreholes in relation to structural features.

~ Enhanced North-South responses, restricted East-West responses.

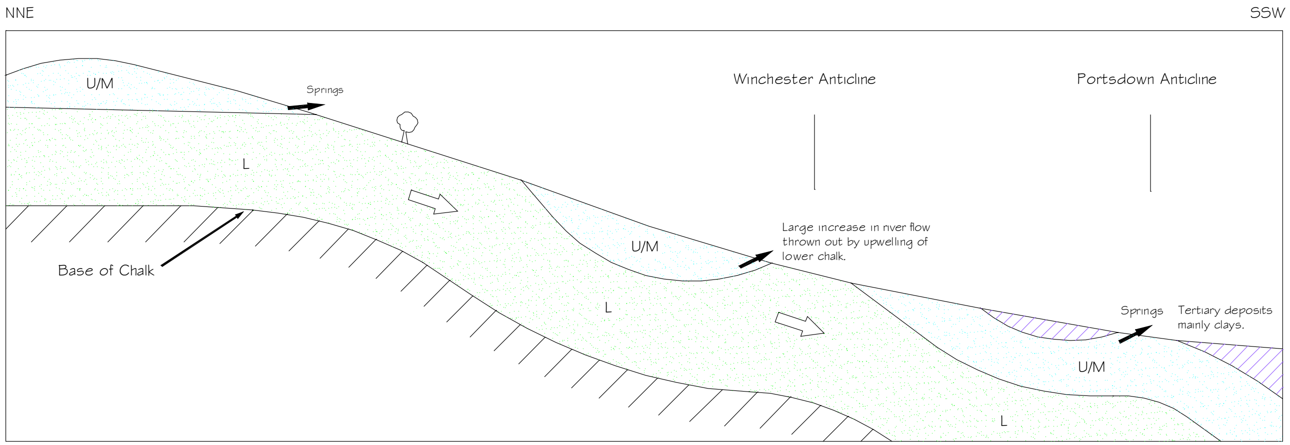
Figure 4.2.3 Influence of structure on groundwater flow patterns and river flow accretion





- Clay-filled Syncline forms partial barrier to down and dip flow.
- Groundwater flows deflected.
- Enhanced dissolution.
- Formation of Karstic features.

Schematic Cross-Section Through Chichester Syncline



- Lower K in Lower Chalk in river bed results in enhanced flows / spring discharges.

Schematic Section Along River Meon, Hampshire.

Figure 4.2.3

Figure 4.2.4 Fylde aquifer - influence of geometry and lithology on cross boundary flows from Caboniferous Strata

contact. (faulted or unconformable) and the lithology of the Carboniferous strata.

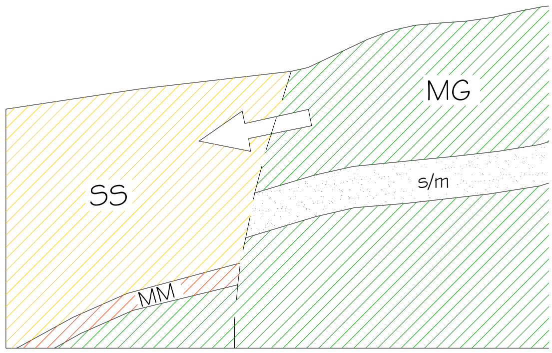
MM — Mercia Mudstone

Carboniferous

MG — Millstone Grit

s/m — shale/mudstone

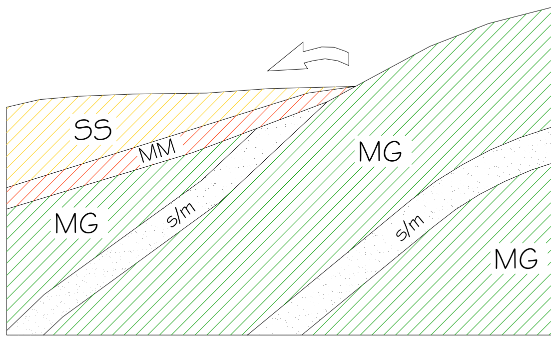
BSG — Bowland Shale Group



Faulted contact

- Thick MG grits (High K)
- Thick SS (High K)

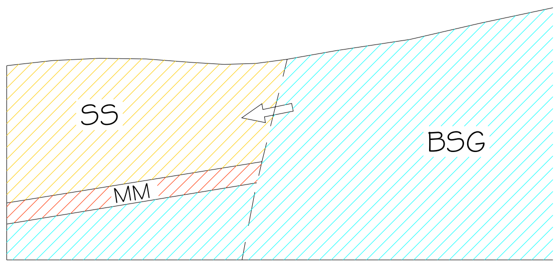
∴ Significant Cross Boundary Flow



Unconformable contact

- Thick MG grits (High K)
- MM = barrier (Low K)
- Thin SS

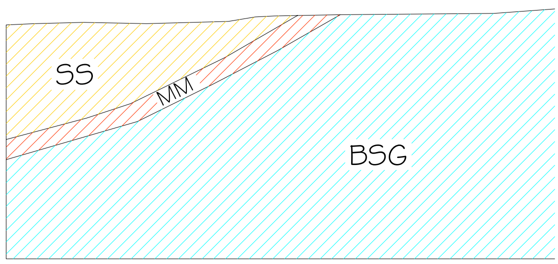
∴ More Limited Cross Boundary Flow



Faulted Contact

- BSG (Low K & S)

∴ Very Limited Cross Boundary Flow

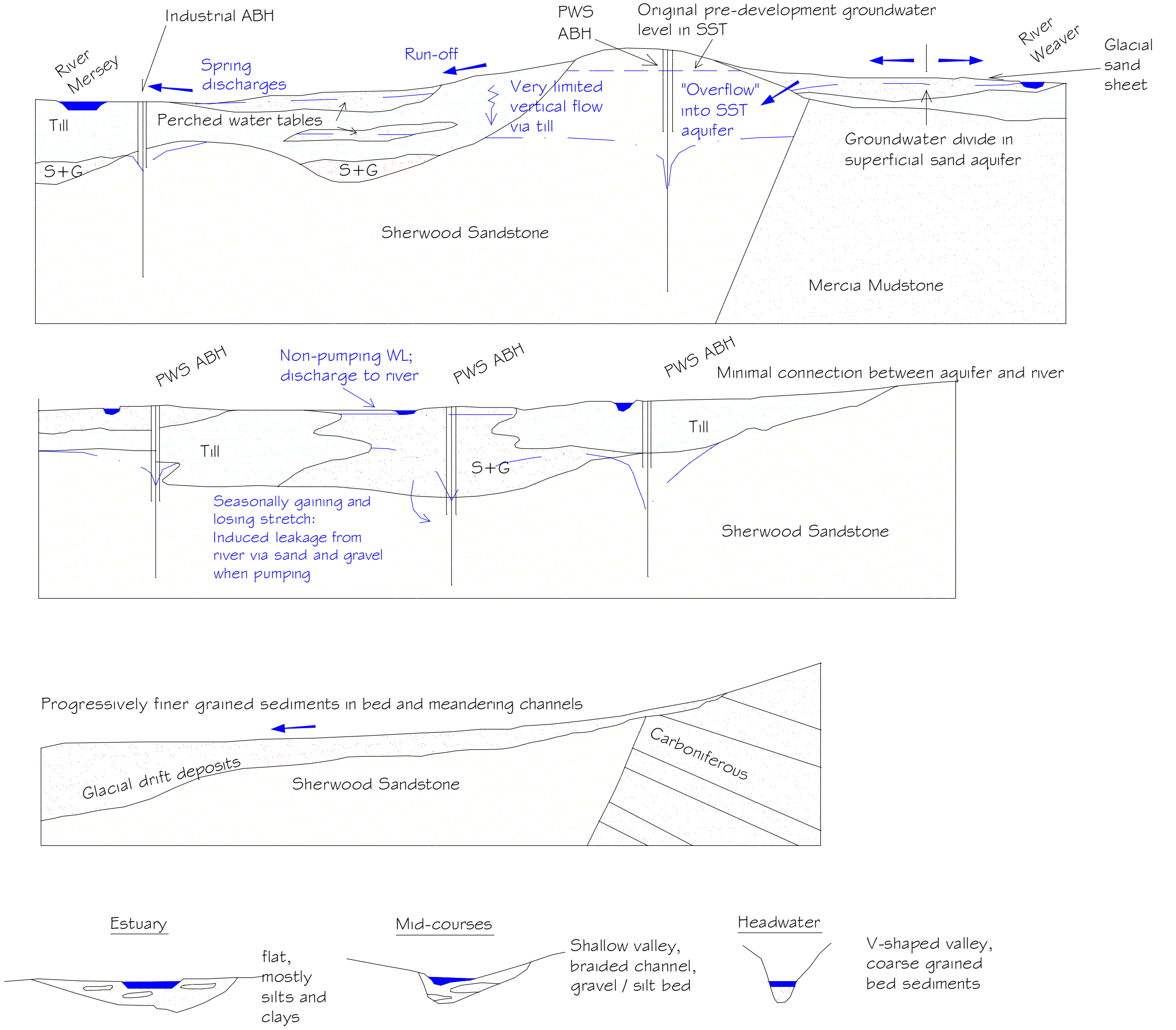


Unconformable contact

- BSG (Low K & S)
- MM (Low K)

∴ Minimal Cross Boundary Flow

(NOTE: Carboniferous boundary represented in model as a fixed gradient boundai varied according to lithology / geometry of the contact.)



(a) Section through West Cheshire aquifer: Influence of drift on recharge

- Variable, complex drift cover dominates recharge to sandstone aquifer.

(b) Section along line of Wyre (Fylde Aquifer): Influence of drift on groundwater/surface water connection.

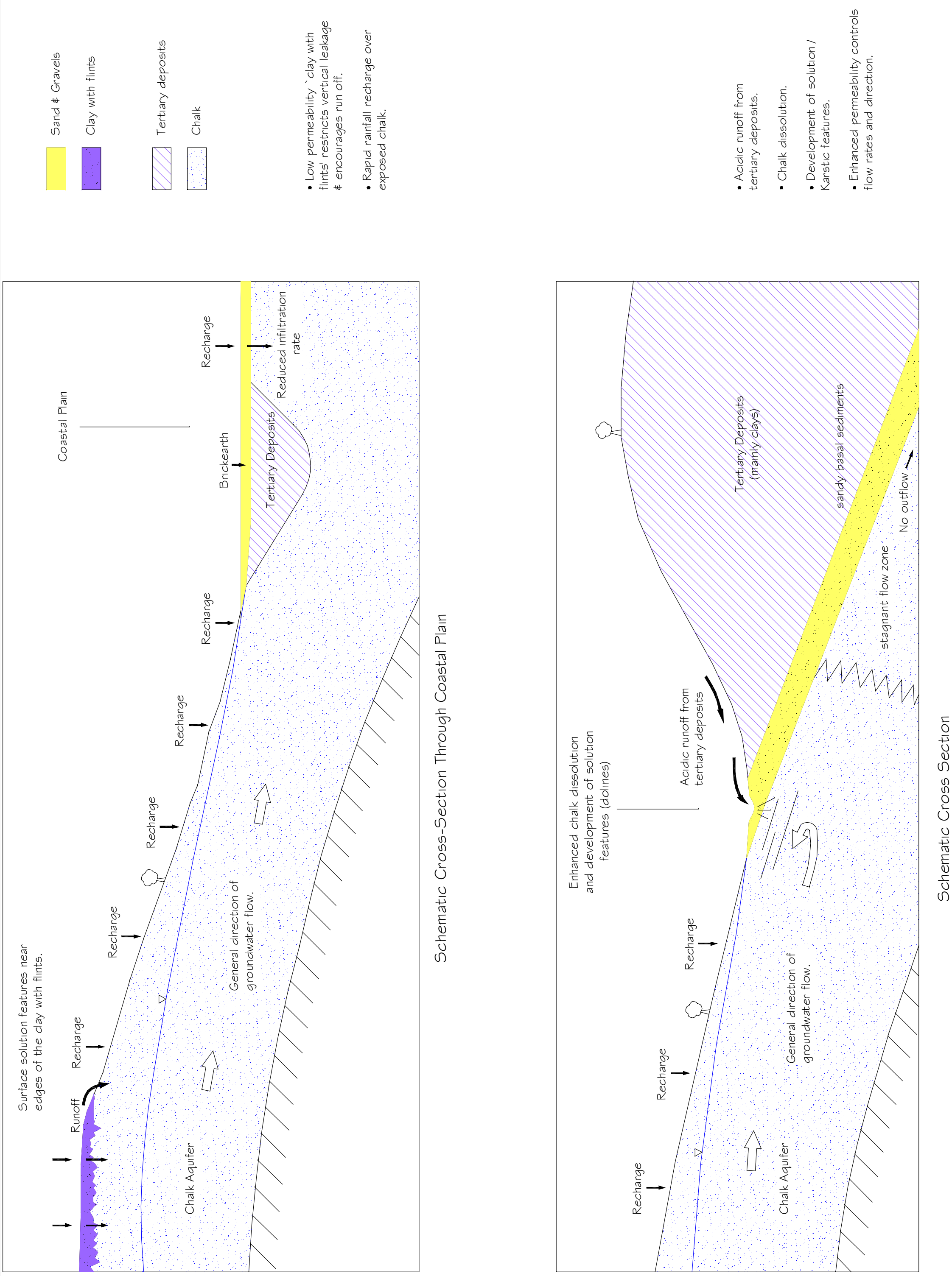
- Good connection where sands extend from river to Sandstone aquifer.
- Poor connection where clay till underlies the river.

(c) Profile along river Wyre (Fylde Aquifer): Influence of fluvial processes on groundwater/surface water connection.

- Lower K sediments increase down the length of the river
- Progressively reduce potential river / groundwater interaction.

Figure 4.2.5 Case examples of influences of drift and fluvial processes on recharge and groundwater/surface water connection

Figure 4.2.6 Effect of drift deposits on infiltration and development of solution features



4.3 Surface Water/Groundwater Interactions

Surface water/groundwater interaction can occur at springs, rivers, lakes or wetlands; the correct physical representation of this interaction is an essential component in the development of conceptual models of the total catchment response.

The importance of careful consideration of this interaction is illustrated by the following situation which can occur in many British aquifers. Before exploitation of the aquifer, most of the water entering the aquifer due to recharge left the aquifer at springs, rivers and lakes; following exploitation of the aquifer, the nature of the surface water/groundwater interaction has changed significantly with springs, streams and lakes drying up. However, if an investigation is required into the improvements in spring and river flows due to significant reductions in abstraction, the historical surface water/groundwater interaction must be identified and quantified so that it can be represented in the predictive model.

There is limited information in the literature about the type of surface water/groundwater interaction which occurs in the UK; relevant literature is listed at the end of this note. Certain of the important considerations in identifying and quantifying surface water/groundwater interaction are summarised below.

4.3.1 Conceptual understanding

The physical reason for the occurrence of springs, rivers or lakes must be identified.

- **Springs** can occur on hillsides where the water table intersects the ground surface, or because of the presence of low permeability strata forcing the water out of the aquifer, or due to enhanced hydraulic conductivity where fissures have developed or for other geological or topographical reasons. Another form of spring is an uncontrolled artesian borehole.
- **Rivers**; if the river gains from the aquifer this will be because the groundwater table is above river level, if the groundwater table is below the river it will lose water to the aquifer provided that there is a sufficient flow in the river. There are often significant seasonal changes in conditions in rivers; a reach which gains water during the winter may lose water in the summer.
- **Lakes** occur naturally where the groundwater table is above a topographical depression, the lake may gain water from a higher groundwater head at one end and lose water at the other end. Man-made lakes formed by constructing a dam may lose water to the underlying aquifer due to the high vertical groundwater head gradient.
- **Wetlands**, when they are influenced by the groundwater table, are similar to lakes since they occur when the groundwater table is close to the ground surface, however the volume of water stored in a wetland is significantly less than that stored in an equivalent sized lake.

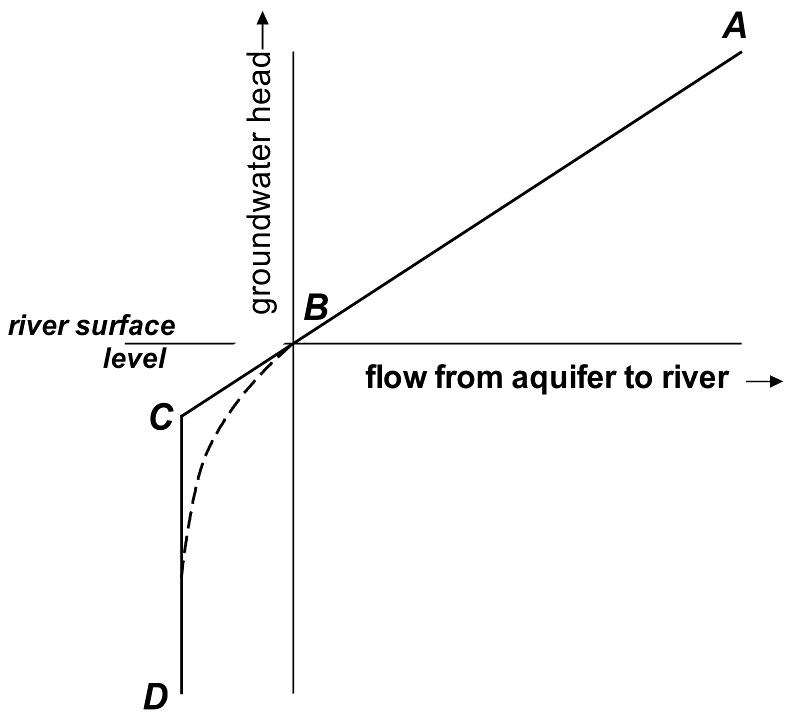


Figure 4.3.1. Diagram illustrating surface water/groundwater interaction

4.3.2 Quantifying the mechanism

Measurements in the field are essential to quantify the relationships between the groundwater outflows or inflows and how they depend on the difference between the groundwater head and the elevation of the spring, river surface, lake or wetland water surface. For **springs** it is usually acceptable to assume that the outflow Q_{spring} is linearly proportional to the difference between the groundwater head and the spring elevation Δh.

$$Q_{spring} = C_{spring}(\Delta h)$$

Although, as indicated by the straight line *AB* of Figure 4.3.1, if the area of the seepages from the spring increases with the groundwater head, it may be appropriate to assume a higher than linear increase in flows. The spring coefficient C_{spring} is defined as the outflow for an excess head of 1.0 m.

When the groundwater head is higher than the elevation of a **river**, the outflow can be estimated in a similar manner to a spring; again it is represented by the line *AB* of Figure 4.3.1. The river coefficient C_{river} may be defined as the outflow from the aquifer to the river per kilometre reach due to an excess head of 1.0 m; this definition is more reliable than attempting to identify the physical properties of a river bed resistance (such as the hydraulic conductivity and thickness of the river bed). When the groundwater head is below river surface level, water (if available) is lost from the river. When the groundwater head is only slightly below river surface level, the loss is proportional to the river coefficient multiplied by the head difference (line *BC* of Figure 4.3.1).

$$Q_{river} = C_{river}(\Delta h) * \text{length in km}$$

However, when the groundwater head is more than about 1.0 m below river surface level, the loss approaches a constant value since the vertical groundwater head gradient is that due to gravity; this is represented by the line *CD* of Figure 4.3.1.

Q_{river} = constant leakage

Since the spring and river flows depend on the difference between the groundwater head and the elevation of the spring outlet or river surface level, accurate field information about these elevations is essential.

Measurements of flows along a river or stream (accretion diagrams) are an essential basis for the estimation of the river coefficients. Despite the practical difficulties encountered in obtaining accurate measurements of flows to prepare accurate accretion profiles, diagrams should be prepared indicating gaining and losing sections of each river and how these conditions change with time. Some rivers dry over part of their course; field records should be obtained showing when the rivers stop and re-start flowing. Figure 4.3.2 illustrates how the information can be gathered and displayed. It is designed to show how the River Bourne in South West Region flows from springs over the chalk aquifer and how flow is lost from the river and restarts in the lower reaches. This diagram is based on monthly visual surveys; not only does it provide a picture of how river-aquifer interaction occurs but it will also be of great value in checking the adequacy of the numerical model which is to be developed.

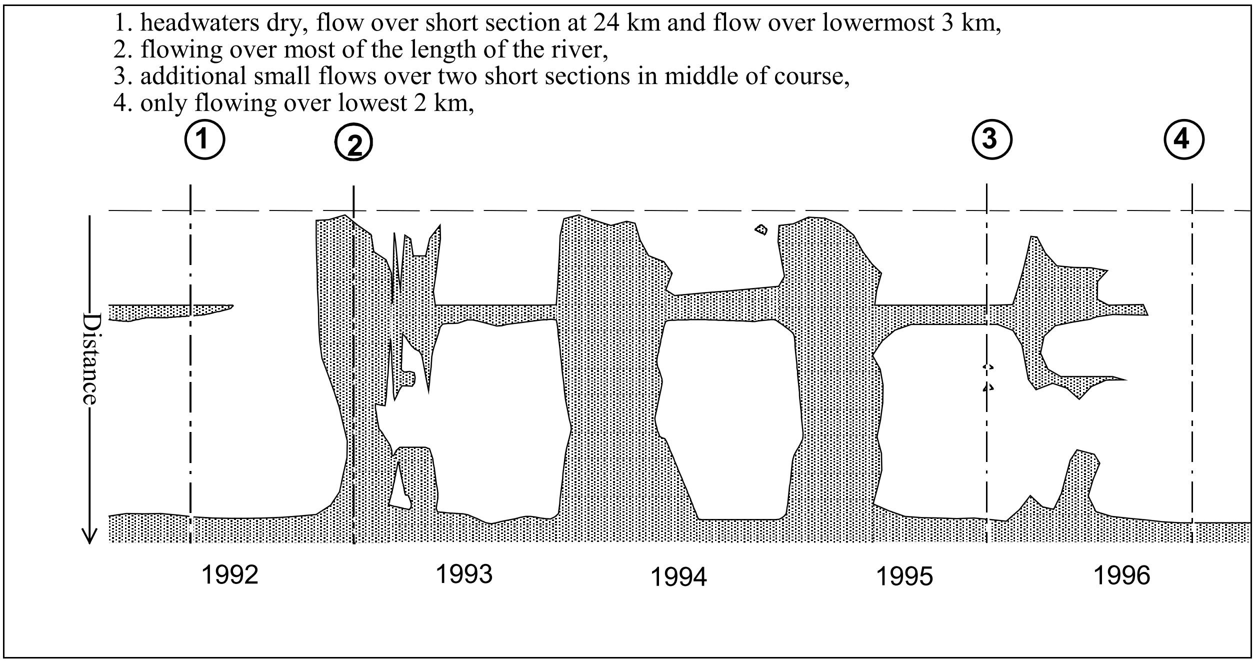


Figure 4.3.2. Winterbourne signature showing where flow occurs in an intermittent river at different times of the year

For **lakes** and **wetlands**, the loss or gain depends on the relative elevations of the groundwater table and the lake or wetland water level. It is difficult to measure gains or losses of water through the bed of a lake. Information on net inflows or outflows can be deduced from a water balance; evaporation from the surface of the lake or wetland is often a significant component of the water balance. Due to the complexity of drift deposits in the vicinity of a lake or wetland it is often difficult to quantify the interaction; a sensitivity analysis during the numerical model refinement is often the best way of identifying suitable parameter values.

4.3.3 Numerical modelling

From the above discussion it is clear that the interaction between the surface and groundwater systems is complex and that different mechanisms apply in different catchments. Certain fully integrated surface water/groundwater packages are available but current experience has shown that these packages are usually insufficiently flexible to represent the extensive interactions which occur in the UK.

Some examples of how surface water/groundwater interactions are represented in MODFLOW are given below. Other codes treat these interactions differently.

Spring and river packages are available for MODFLOW. In the MODFLOW manual, the river conductance term *CRIV*, that produces the same effect as the river coefficient as defined above, is calculated from:

$$CRIV = K_{bed}\, L\, w/b$$

where,

K_{bed} = hydraulic conductivity of river bed

L = length of river cell

w = width of river

b = thickness of river bed

This approach suggests that it is the nature of the river bed, especially its width and vertical hydraulic conductivity, which defines the river-aquifer interaction. In practice there are other important parameters, for example the nature of the aquifer, especially development of fissures, alluvial deposits, etc, which are usually more important than the river bed deposits.

During model refinement, comparisons should be made with all available field information such as that presented in Fig. 4.3.2. The presentation of the model results for river-aquifer interaction is also important. Figure 4.3.3 shows by the colour of the circles how rivers in the West Midlands Sandstone catchment interact with the aquifer according to the numerical model. The colour of the circles show whether the river is gaining from or losing to the aquifer over a 500 m reach. This diagram is compared with all available field information. The sensitivity of the modelled response to the magnitude of the river coefficients should be explored and small adjustments to the spring and river elevations will almost certainly be required to prevent sudden changes in the surface water/groundwater interaction. If springs, streams or rivers occur in an aquifer having a hydraulic conductivity which varies with saturated depth, computational difficulties may occur, especially when achieving suitable initial conditions (Rushton *et al*. 1989). Lakes can be represented in a groundwater model as a layer with very high transmissivity and a specific yield of unity with reduced vertical hydraulic conductivity to represent silt deposits; evaporation must be included since in summer it can be equivalent to 5 Ml/d per km^2 of lake area. Several lake packages have been written for MODFLOW (R.C.Fontaine & D.B.Stone, 1998).

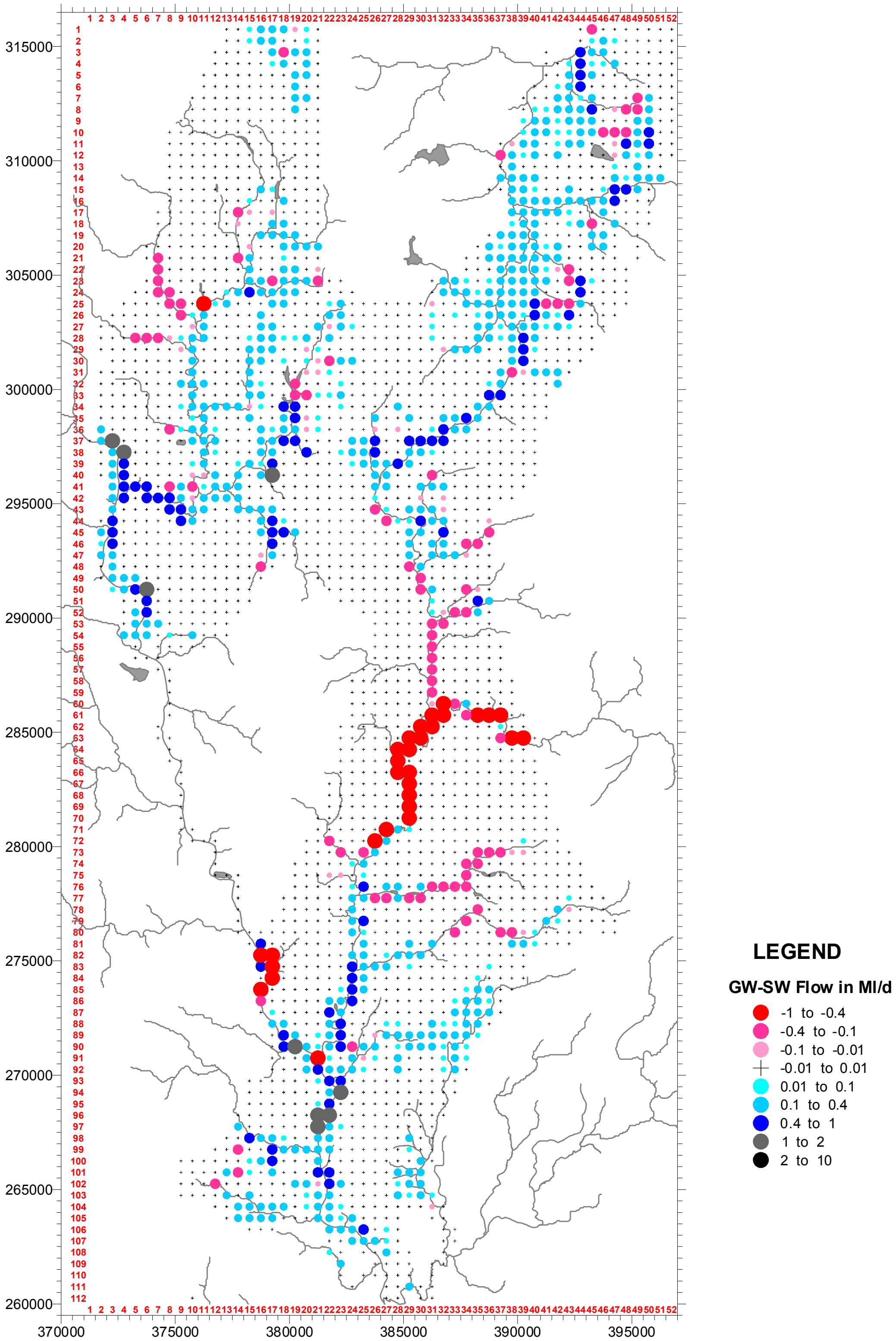


Figure 4.3.3. Diagram illustrating complex river-aquifer interactions for the West Midlands Triassic sandstone aquifer system.

4.3.4 References

Anderson, M.P & Woessner, W.W. 1992. *Applied Groundwater Modeling: Simulation of Flow and Advective Transport.* New York, Academic Press Inc., 381 pp.

Fontaine, R.C. and Stone, D.B., 1998. *Simulating Pit Lake Filling using the LAK2 Package for MODFLOW*. In MODFLOW '98 Proceedings, Volume I. Golden Colorado.

Rushton, K.R., Connorton, B.J., & Tomlinson, L.M., 1989. Estimation of the groundwater resources of the Berkshire Downs supported by mathematical modelling. *Quarterly Journel of Engineering Geology,* **22**, 329-341.

Rushton, K.R and Tomlinson, L.M. 1995. Interaction between rivers and Nottinghamshire Sherwood Sandstone Aquifer System. BHS Occasional Paper **No. 6**. 101-116.

Younger, P.L. (Ed.) 1995. Modelling river-aquifer interaction. BHS Occasional Paper **No. 6**.

4.6 Defining aquifer parameters

4.6.1 Purpose of aquifer parameters

Aquifer parameters describe numerically the hydraulic characteristics of the aquifer. The most important parameters are: hydraulic conductivity *K*, aquifer thickness *b*, and storage parameters *S*. The composite parameter transmissivity ($T_x = \sum K_x \delta z$) is often used. For particle tracking and solute transport modelling porosity *n* and other parameters such as dispersivity need to be defined.

These parameters can be estimated by a number of different methods, as described below, but all of these are subject to a degree of uncertainty and require careful interpretation prior to selecting the appropriate input parameter for a numerical model.

4.6.2 Sources of data

General sources of data for selecting aquifer parameters are covered in Chapter 3. Specific sources include:

- BGS major and minor aquifer property manuals (Allen *et al*., 1997 and Morris *et al*., 2000) are good general reference documents.
- Existing Agency models. The conceptual model documentation may provide a valuable source of data. However, parameters used for the numerical model should be treated with caution until the method used to derive them is understood. It is also risky to assume consistency on a national scale and the parameters used for a model of the Cretaceous Chalk of Kent will not necessarily work for the Cretaceous Chalk of East Yorkshire.
- Pumping test data from Agency or water company records and test results published in technical journals. The use and shortcomings of pumping test results are addressed in the following section
- Packer tests. These can provide useful information on the vertical variation in conductivity. For example, for the Chichester Chalk model they were used to help define the parameters for the VKD function (see Box 1).
- Laboratory test data. May be of limited value to resource models as many of the UK's aquifer units have a significant dependence on secondary fracture porosity and the values obtained by laboratory analysis may be much less than field observation would imply.

4.6.3 Initial Numerical Representation

The geological framework and conceptual model should provide the basis for initial aquifer parameter zone delineation. The conceptual model should include estimates of the plausible range of all aquifer parameters in each hydrogeologically distinct zone.

To incorporate the data collected from the sources described above into the numerical model, for each parameter the aquifer unit is divided into zones over which the value of the parameter is thought to be effectively constant. This applies to hydraulic conductivity, storage, porosity and aquifer thickness (or base of aquifer unit).

Aquifer parameter zoning will be more complex than defining geological units due to the variation of aquifer parameters within formations, and by aquifer heterogeneity and anisotropy, geological structure, etc. However, for an initial numerical representation definition of five or less parameter zones per layer and parameter is usually adequate. The importance of variation of hydraulic conductivity and storage with depth, and the characteristics of this variation, must be considered, and represented numerically if required.

It is important to avoid creating an over complex model at an early stage. It may prove that many identified hydrogeological features have a minor impact on the output and serve only to increase model complexity and unwieldiness. On a local scale, there may be evidence to support the assumption that a particular fault or marl layer may restrict flow, but on a broader scale, the impact of these features may be negligible. If an over-complex initial aquifer parameter distribution is used, then identifying problems during the refinement period and assessing model sensitivities is far more difficult.

Many of the potential problems associated with definition of aquifer parameters are principally the result of issues of scale. On a smaller scale the non-ideal behaviour of the aquifer becomes more significant, for example laminated aquifers, faulting and fractured/karstic aquifers. The scale to which the input data refers should always be considered.

The initial numerical model output should be closely scrutinised. Assessment of the ability of the model to replicate known conditions will enable the decision to be made that a refinement process is all that is required, or possibly that a reassessment of the conceptual model and additional data collection will be needed.

4.6.4 References

Allen, D.J., Brewerton, L.J., Coleby, L.M., Gibbs, B.R., Lewis, M.A., MacDonald, A.M., Wagstaff, S.J., Williams, A.T., 1997. *The physical properties of major aquifers in England and Wales.* British Geological Survey Technical Report WD/97/34. Environment Agency R&D Publication 8.

Environment Agency, 1999. *Representation of the variation of hydraulic conductivity with saturated thickness in MODFLOW. Stages I & II. Code changes and testing against Birmingham University code.* National Groundwater and Contaminated Land Centre Project NC/99/67.

Kruseman, G.P. & de Ridder, N.A. 1994. *Analysis and Evaluation of Pumping Test Data*. 2nd edition. International Institute for Land Reclamation and Improvement. Publication 47.

Morris, B.L., Jones, H.K., Thomas, J.E., Stuart, M.e. & Robinson, V.K., *Eds.,* 2000. *Physical properties of minor aquifers in England and Wales*. British Geological Survey Technical Report WD/00/04. Environment Agency R&D Publication 68.

Box 1. Chalk Permeability

Although the Chalk matrix has a high porosity, because of the exceedingly small pore sizes it has a very low permeability. The aquifer properties of Chalk rely on the presence of fractures. The extent of fracturing will vary depending on lithology and spatially depending on the structural setting. It is the secondary permeability that dominates how the Chalk is to be represented in a numerical model.

In Chalk aquifers, fractures are enlarged in areas where groundwater flow is concentrated, such as river valleys and the zone of water table fluctuation. The result is a pattern of aquifer parameters where transmissivity increases towards river valleys and hydraulic conductivity decreases with depth.

Numerical representation

The secondary permeability profile can be represented in the numerical model using:

1. Multiple layers, e.g. Little Ouse catchment (Allen *et al*, 1997), however, there may be numerical difficulties with drying and re-wetting of model cells. Care must be taken to avoid numerical instabilities at levels of abrupt change in horizontal permeability.
2. Vertical K_h Distribution (VKD) function (Figure 4.6.1. Used successfully in several Chalk catchment models (e.g. The Kennet Valley in Thames Region (see Appendix B) and Chichester in Southern Region).

The application of the variation in horizontal hydraulic conductivity with Depth (VKD) in MODFLOW is described in R&D Project NC/99/67 (Environment Agency, 1999).

Impact on stream flows

An implication of the VKD profiles exhibited by the Chalk is the response of Chalk baseflow in surface water courses to recharge events. Chalk streams are often ephemeral, where the water table falls below the stream bed in summer but the onset of flow is strongly influenced by the location of the water table within the VKD profile. When the water table is within the high transmissivity zone, then very rapid discharge will occur. The definition of the VKD profile in the model will control the form of the resultant baseflow hydrograph and the streamflow accretion profile.

Figure 4.6.1

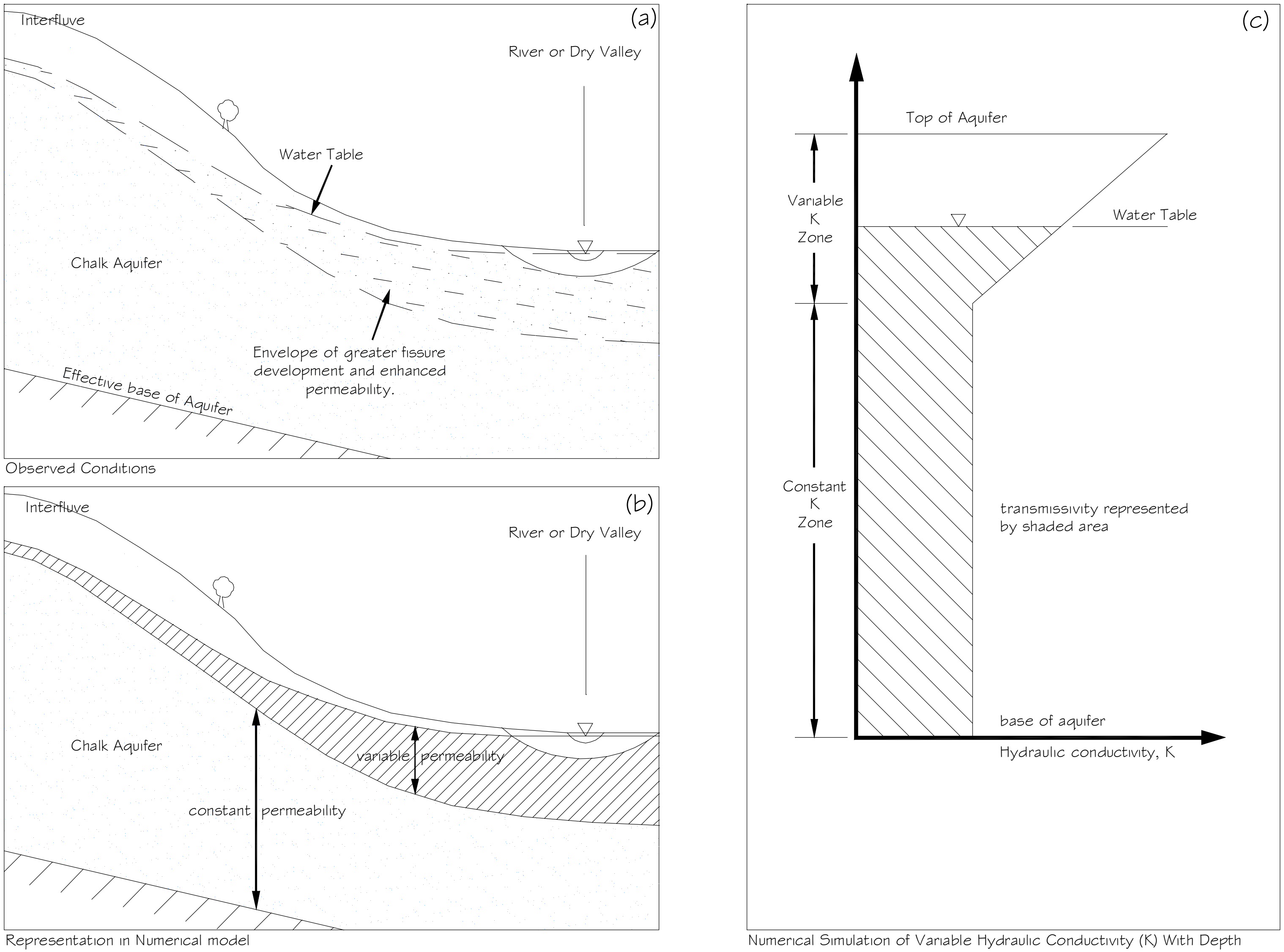


Figure 4.6.1 Representation of vertical permeability profile

4.5 Boundaries

The initial part of this section summarises types of boundaries and how they can be selected. The reader is also referred to chapter 4 of Anderson & Woessner (1992) where these ideas are discussed in more detail.

4.5.1 Introduction

The mathematical equation describing the conservation of mass in a chosen region is expressed in terms of partial derivatives of the hydraulic head in space (i.e. hydraulic gradients) and in time (for transient problems). In order to solve the equation it is necessary to provide both initial conditions and boundary conditions. For transient problems the initial conditions represent the head distribution at the start of the simulated period, whilst for steady-state problems the initial conditions are a first estimate at the solution, and need not be physically realistic. Boundary conditions are mathematical equations that specify groundwater behaviour at a given position. They may be defined at the edges of a model domain (external boundary conditions), or within the model domain (internal boundary conditions). In all models, external boundary conditions are specified for the three spatial dimensions and in every model layer. If not specifically chosen then there is a default, usually no flow. In this sense, recharge applied at the upper boundary of the model is also a boundary condition. For time-variant problems boundary conditions must be defined for each time step.

Mathematically, the main types of boundary conditions that may be applied are (a) specified head and (b) specified head gradient. How these are implemented depends on the modelling software tool. The user must ensure that the boundary conditions available in the selected software tool and the underlying conceptual models are understood. The following options are generally available:

1) Specified head

- fixed head $h = z$ where h is the groundwater head and z the elevation head; this head may be a function of time.

2) Specified flux or volumetric flow rate

- no flow, $\partial h/\partial n = 0$, i.e. the head gradient perpendicular to the boundary is zero,
- known volumetric flow rate at the boundary Q_b (m^3/d); this is equivalent to $Q_b = -K A \; \partial h/\partial n$ where $\partial h/\partial n$ is the gradient normal (perpendicular) to the boundary,
- known Darcy flux q_b (m/d) where $q_b = -K \; \partial h/\partial n$, this type of condition is not available in MODFLOW.

3) Head-dependent flux

- for a head-dependent flux the unknown boundary flow Q_b is calculated from a specified head h_b which may be a river surface elevation or a groundwater head at some distance beyond the boundary, an appropriate conductance[?] KA and the unknown groundwater head on the boundary h.

$$Q_b = -K\,A\;\partial h/\partial n \text{ where } \partial h/\partial n \text{ depends on } h_b \text{ and } h$$

The specified head h_b may vary with time. This type of boundary is often called a 'general head' condition.In practice, within the constraints of the boundary conditions offered by the chosen software tool, the modeller selects the extent of the model region so that appropriate, physically-based boundary conditions can be applied.

There are essentially two types of boundaries that represent a change in conditions:

i. Geological and geographical boundaries– formed by the physical presence of rock or water;

ii Hydraulic boundaries – defined by hydrological conditions.

When neither of these types of boundaries can be specified, it may be necessary to specify arbitrary boundary conditions (Section 4.5.4) to the mathematical model.

4.5.2 Geological and geographical boundaries

Geological and geographical features (e.g. a rock or a large body of water) that have a strong influence on groundwater flow can form boundaries. The conditions at the boundary are defined by the manner in which such features constrain the groundwater flow. See Table 4.5.1 for examples of geological and geographical boundary conditions.

4.5.3 Hydraulic boundaries

Hydraulic boundaries are less easy to determine. They are defined by hydrological conditions and may be inferred using groundwater flow theory. They are not always steady or persistent over time and they may move depending on stresses within the flow domain. See Table 4.5.2 for examples of hydraulic boundary conditions.

4.5.4 Arbitrary boundaries

It is not always feasible to extend the model region to reach physical or hydraulic boundaries. In this case it is necessary to set an arbitrary boundary condition, which might be a specified head or flux-type boundary condition. It is important that any such arbitrarily specified boundary condition does not influence the model results in the region of interest. Fortunately, because of the properties of the partial differential equation, the sensitivity of results at a given point to specification of boundary conditions is related to the relative distance of the point from various internal and external boundary conditions.

The impact of an arbitrary boundary should be tested to determine how sensitive the solution of the model is to the boundary condition. The modelled domain should be expanded (moving arbitrary constraints further away from the region of interest) until the effects of the arbitrary boundary are not significant for the main area of interest in the model.

In a time-variant model, as long as the effects of any newly applied stress do not reach the boundary during the period of the simulation, then the impact of the stress change will be unaffected by any arbitrary condition at that boundary, and so predictions of the response to the stress change will be meaningful.

See Table 4.5.3 for examples of arbitrary boundary conditions.

Table 4.5.1. Geological and geographical boundary conditions

	Geological Feature	Concept	Maths	Example
1	Permeability contrast between different lithologies due to sedimentary/physical characteristics	A low permeability rock base, or a permeability contrast between rock types often provides a basal boundary, where the condition can be defined as no flow (specified flux set to zero). Consider carefully what the permeability contrast is and what head gradients are likely when deciding whether the flow through the low permeability formation can be neglected justifiably. Care should be taken with respect to the water balance, as the basal aquitard may be leaky or may be confining a lower aquifer, such that there may be significant flow downwards or upwards respectively over a large modelled area. If the flux is significant, then the "aquitard" should be simulated, and the model extended downwards until a suitable low leakage basal boundary can be specified. Alternatively, the boundary should be modelled as a specified volumetric flow rate, additional recharge or head dependent boundary condition. Basal bedrock may be weathered for few metres and therefore may be a significant source and pathway for groundwater, therefore the boundary may need to be extended for several meters below the weathered surface. Flows across these boundaries may occur depending on the nature of the contact and the lithologies either side of the contact.	No flow Head dependent flux Specified volumetric flow rate Recharge	Rheidol valley, West Wales – gravel aquifer (K = 1 – 10 m/d) bounded by relatively impermeable basal bedrock, Silurian shales (K = 10^{-3} – 10^{-2} m/d). Carboniferous Coal Measures – has a cyclic nature, comprising shales, sandstones, siltstones, coals etc, all of which have varying permeabilities, thus forming a multilayer aquifer. Often the (semi-) confining layer (eg shales, siltstones) will be significantly leaky, and so cannot be used as an impermeable boundary, but rather as a specified flux boundary (need to know vertical K). Possibly relevant for the Rheidol. Definitely relevant for the Teifi.
2	Permeability contrast between different lithologies by faulted juxtaposition	As above	No flow Head dependent flux	Vale of Clwyd, Triassic Sandstone aquifer in graben. Faults juxtapose Palaeozoics against the sandstone on the east side, Palaeozoics & Carboniferous Limestone on the west side.
3	Rivers - fully or partially penetrating	Rivers can provide an edge boundary, but only if they are able to supply water readily to the saturated thickness of the aquifer. The choice of boundary condition depends on the river and river bed properties. Can be combined with a groundwater divide (see later).	Specified flux Specified head Head dependent flux	Yazor gravels – southern boundary modelled by River Wye is a good example of a constant head boundary.

Table 4.5.1 Cont.

	Geological Feature	Concept	Maths	Example
4	Lakes and seas	Freshwater lakes or seas may provide a good specified head boundary if in hydraulic continuity with and penetrating at least 50% of the aquifer. Tidal fluctuations in seas effectively cancel each other out over one tidal cycle and at sufficient distance from the boundary condition. Therefore for a steady state model or a transient model simulated over a time slice of whole tidal cycles, then the coastal boundary could be modelled as constant head of 0mAOD (water can go in & out, but has to maintain a head of zero). Representing the sea in models may be complex due to the saline-freshwater interface – i.e. a mobile, variable density, diffuse boundary. Often no flow boundary conditions are used at the saline interface.	Specified head No flow	East Kent Chalk in contact with the sea from Folkestone to Deal. Lakes in the form of water-filled gravel pits in the Cotswold gravels, these heads fluctuate.
5	Springs and seepage	If groundwater models take into account the ground surface and limited capacity for infiltration, springs and seepage faces will be simulated automatically. In models such as MODFLOW, the location of potential springs or seepages faces and their elevations must be specified, so that groundwater levels are not allowed to increase above that level at that location. It should be noted that numerical parameters may control the boundary conditions and hence the actual groundwater head simulated.	Head-dependent flux	
6	Water table	Free surface	Specific yield and recharge conditions	Most unconfined aquifers.

Table 4.5.2. Hydraulic boundary conditions

	Hydraulic feature	Concept	Maths	Example
1	Groundwater divide	Often found around topographic highs and lows. When groundwater hydrometrics are not known it is usually assumed to be coincident with the topographic high, or halfway across a partially penetrating river. However, significant flows often occur across the bottom of valleys, therefore they may not be suitable as modelled groundwater divides. Groundwater divides may not be coincident with surface water divides, for example if there is heterogeneity in hydraulic conductivity, if there are solution features, or there is a significant difference in minimum groundwater levels in adjacent valleys. Regional groundwater divides are usually assumed not to move significantly. However, if the model simulation covers a long time period with a range of climatic conditions, this assumption may not hold. Equally, if there are changes in a hydraulic stress (e.g. an abstraction) this can often affect the position of the divide. If a divide is likely to move, it is preferable to extend the model to the next divide even though the representation of conditions in the extension of the study area is less accurate than in the region of interest.	Specified volumetric flow rate (set to zero).	Commonly used in Chalk models (e.g. Chichester model in Southern Region). Boundary set along a partially penetrating river may be used if this is remote from area of interest (Itchen model?) Tower Wood abstraction/Peckforton in North Wales – some evidence for movement of groundwater divide
2	Streamlines	A streamline is an imaginary line that traces the path that a particle of groundwater would follow as it flows through an aquifer. Streamlines can therefore be used as hydraulic boundaries, whereby no flow can cross them by definition. Usually there is insufficient field information to specify streamlines with confidence. In a transient model they will move over time. Different flow systems can also be separated by streamlines i.e. local flow systems within regional flow systems. Streamlines are modelled as specified flow (set to zero) boundary conditions. If a streamline is some distance away from the area of interest and it is not likely to move due to changes in stresses (e.g abstractions) then it could be a suitable boundary to use.	Specified volumetric flow rate (set to zero).	
3	Stable hydraulic gradient Flow in confined area	Flow across boundary under a stable hydraulic gradient may be defined as a specified flow, dependent on permeability and cross-sectional area. This condition becomes difficult to apply when the volumetric flow rate has to be split over more than one model layer. Aquifer flow rates in confined areas may be estimated on the basis of Darcy's Law, and applied as a head-dependent flux or specified volumetric flow rate. Alternatively variations in groundwater levels may be restricted, so that it may be justifiable to specify heads.	Specified volumetric flow rate Head-dependent flux Fixed head	London Basin model is based on an assumption of constant head distribution along the boundary. Flow out of the Mimram model is specified as a flux consistent with flow into the Mimram model.

Table 4.5.3. Arbitrary boundary conditions

	Hydraulic feature	Concept	Maths	Example
1	Distant boundary	When a constant head boundary condition may be appropriately applied at a distance beyond the model region, it is possible to apply a head-dependent flux boundary condition to effectively represent the flow in the portion of the aquifer not modelled, based on application of Darcy's Law. This boundary condition is appropriate for steady-state conditions, but may be more difficult to use in a transient model.	Head-dependent flux	
		In transient simulations a distant boundary may be represented by a no flow boundary at early times before the effects of a new applied stress are propagated as far as the boundary. However, for steady-state models (or for initial conditions due to existing stresses in a transient model) a no flow boundary condition is likely to have significant influence on the model.	No flow	

4.5.5 Setting boundaries

Conceptual Model

The hydrogeological conceptual model is fundamental to the selection of the model domain and the appropriate boundary conditions. The size of the study area (data collection area) and the conceptual model should be larger than the size of the main area of interest, in order that all inflows and outflows that influence the flow conditions in the area of interest are considered. This also allows options for different boundary types to be considered and the probable flow patterns to be estimated.

It is usually best to keep the boundaries as simple as possible and away from the region of interest where detailed results are to be predicted. Geological boundaries should be used wherever possible, as they are easier to identify and define, and are stable. Regional groundwater divides are the next most defensible boundary conditions since, compared to the other hydraulic boundaries, they are least likely to move significantly (note exceptions in Table 4.5.2). If the geological boundaries are too far away from the area of interest in the model to be able to characterise and model cost-effectively, then reliance must be placed on hydraulic or arbitrary boundaries.

Water balance

The boundary conditions are strongly related to the water balance for the model region. From Section 4.5.1 it is seen that for each type of boundary condition either the groundwater head h, or the volumetric flow rate into or out of the cell Q, or both are initially unknown, and are calculated as part of the solution. If there is more than one boundary with unknown Q present in the model, then the balance of water entering/leaving each boundary can be varied by adjusting the model parameters. It is therefore important that there is a good conceptual understanding of the water balance so that physically unrealistic flow rates of water are not modelled. A water balance calculated independently in the development of the conceptual model provides a plausibility check of the modelled water balance. The model should be tested against observed flows as well as groundwater heads. Similarly, for boundary conditions where the head is unknown, the groundwater head of the mathematical solution should be checked for plausibility or against measured heads. Consistency with boundary conditions in neighbouring or overlapping groundwater models should be checked, to ensure that water is not lost or gained.

Convergence of solution

Some hydrogeological situations could be defined using only flux boundaries (including no flow boundaries). This should be avoided for steady-state models as the governing equation for the steady state is in terms of derivatives. If the boundary conditions are also in terms of derivatives of heads, then the solution will be non-unique, i.e. the convergence of the numerical solution will be arbitrary. Steady-state problems need at least one boundary node with a specified head (either constant head or head-dependent flux condition such as rivers) from which to calculate the groundwater head distribution. In transient simulations, the initial conditions provide the reference heads. Convergence is likely to be difficult to achieve if the model contains a few head-dependent flux conditions only.

Range of influence of boundary conditions

In steady state models, the flow pattern is strongly controlled by boundary conditions. In time-variant models, the effect of any new stress propagates outwards with time, and the impact of the boundary conditions may not initially be apparent. For example, consider simulation of an abstraction well. Initially the abstracted water is supplied from storage rather than the boundary condition. With time the radius of influence of the well increases. The steady state represents the maximum influence of the boundary. In a confined aquifer, the abstracted water must be supplied across the boundaries of the model, whereas in an unconfined aquifer it is possible that the influence of model boundaries will not be so significant and recharge may supply all the abstracted water before the capture zone of the well reaches the model boundary.

4.5.6 MODFLOW boundary conditions

The following boundary conditions are available within MODFLOW.

a) Specified head boundary conditions

1. In **constant head cells** the head is specified by the modeller and may vary with time during the simulation. This boundary condition represents a potentially unlimited supply or sink of water, therefore when this condition is applied it is especially important to check the volumes of water flowing into or out of the boundary. Physically unjustified use of constant head cells within a model is particularly discouraged, since the model may then become over-constrained and the solution will simply reflect the perceived ideas underlying the choice of constant heads.

b) Specified volumetric flow rate or flux boundary conditions

1. **No flow boundary conditions.** The default boundary condition in MODFLOW is that there is no flow out of any cell face that does not border onto another active model cell. This boundary condition is applied without the user specifying any data or conditions. Inactive cells lying outside the active model domain may also be defined; no water balance or groundwater head is calculated for these cells.

2. **Specified volumetric flow rates.**
    a. **Well.** A constant volumetric flow rate (e.g. m^3/d) can be specified in a well cell by entering a volumetric flow rate that the model will inject or extract from the cell as long as it remains saturated. This boundary condition may be used to represent a volumetric flow rate in or out of a boundary, however assigning volumetric flow rates to individual cells may be difficult if the boundary is over multiple layers, or there is varying geometry or heterogeneity in hydraulic conductivity. The rate will also be maintained even if model conditions vary beyond the point where physically the flow rate would change (e.g. injection into a confined layer will continue even if the model cannot get water away without generating unrealistic heads).

3. **Specified flux rates.**
    a. **Recharge**. MODFLOW requires a recharge rate (e.g. m/d) to be applied at the water table of an unconfined aquifer. There are options to apply the recharge to the top layer only (i.e. no recharge applied if this is dry), or to the highest active layer. In an unconfined model cell MODFLOW does not take account of the top elevation or groundwater surface: the recharge is added and groundwater heads are allowed to rise, whether there is physically aquifer present or not. This means that springs or seepage faces are not automatically calculated: their location must be specified and modelled using drain cells.

Both recharge and injections lead to volumes of water being added to the cell water balance – there is no difference whether the water is conceptually added to the top, side or centre of the cell.

c) Head-dependent flux boundary conditions

The head-dependent flux boundary conditions may be expressed in terms of a flow rate, but effectively act as specification of a head (not the groundwater head) at the boundary in terms of known quantities. MODFLOW offers several types of boundaries (rivers, drains, streams and the general head boundary) which follow this format. The (unknown) volumetric flow rate out of the boundary Q is expressed as

$$Q = C\,(h-h_b)$$

where h is the unknown groundwater head at the boundary, h_b is a known head or elevation at the boundary. C is the conductance of the porous medium separating the point in the aquifer where h applies with the point at the boundary where h_b applies. The physical interpretation of the porous medium depends on the conceptual model for the boundary, and typically $C = KA/L$ where K is the hydraulic conductivity of the porous features within the boundary, A is the cross-sectional area over which flow occurs and L is the distance over which the head difference $h-h_b$ applies.

a. **Drains**. A drain boundary condition allows water to be removed from the system whenever the groundwater head is above the elevation of the drain h_b. Drains may be applied at the location of springs. When applied over an area they can be used to limit the maximum groundwater head. There is no facility within MODFLOW for routing the flow from drains to surface water features.

b. **Rivers.** A river boundary condition allows transfer of water into or out of a river. The conductance represents river sediments and h_b is the river stage, which must be specified. There is an upper limit to the amount of water leaking into the aquifer once the aquifer head drops below the bottom of the river. The river cell does not check availability of water for infiltration: it is assumed that there is always enough water flowing to supply the calculated infiltration flow rates. Therefore this boundary condition may not be appropriate for models concerned with low flows. In comparing the flows into the river, it should be remembered that the model only simulates the baseflow component of actual measured river discharges. Application of this type of boundary does not necessarily cause a groundwater divide in the model.

c. **Streams**. Stream boundary conditions are more sophisticated versions of the river boundary conditions, in which the actual surface water flow rates are accounted for. The heads in the river can either be calculated as part of the solution (based on the Manning formula) or specified directly. Stream cells have additional data requirements to allow calculation of the river stages and specification of the river network. Stream boundary conditions should therefore generally be avoided unless deemed necessary. However, they are the appropriate choice of boundary condition when actual surface water flows will limit river infiltration to the aquifer. For modelling ephemeral streams the cells should extend high enough up dry valleys to model the source in the maximum groundwater conditions.

d. **General head boundary condition**. The generic form of the head dependent flux boundary condition relates the head in the aquifer to a head at some other location. The conductance represents the properties of the porous medium in between the two. It may be used to apply a constant head boundary condition at a distant location, or alternatively to specify a known hydraulic gradient.

For all these head-dependent boundary conditions both groundwater head and the flow out of the boundary are initially unknown, and determined from the solution of the problem. As conductance increases, the groundwater head approaches head of boundary h_b, however high values of the conductance can cause instability in the solution process.

It is essential that the user understands the relation between the boundary condition type, the simplified mathematical model underlying the boundary condition and the corresponding equations used to represent the boundary condition.

Finally, it is noted that boundary conditions are fundamental to definition of the ‘stress period’, which is a period of time for which all the boundary conditions (external and internal) are constant.

4.4 Estimating recharge

This section on recharge is much longer than most of the others because at the time of writing there is considerable effort being put into developing a consistent approach to the estimation of recharge. This is the result of two important needs within the Agency's implementation of its Catchment Abstraction Management Strategies (CAMS):

1. To provide more accurate recharge estimates for catchment scale water resources assessments and groundwater modelling projects;

2. For the Agency's groundwater modelling programme to develop catchment models which account for the total flow rather than focussing on the groundwater system alone. Hence, flow mechanisms such as vertical flow through drift, runoff recharge, and river–aquifer interaction all need to be included.

The Environment Agency's groundwater models use empirical soil moisture balance models based on the work by Penman and Grindley as summarised by Rushton & Ward (1979). This approach employs critical values of the soil moisture deficit (the constants C & D) to control the actual evapotranspiration. These constants were empirically derived and their validity could not be tested. A review of recharge estimation for British Aquifers (Rushton, 2000) describes some of the approaches employed and lessons learned over the past two or three decades. It also presents initial work on the development of a new soil moisture balance approach for estimating potential recharge which relates the critical values of SMD to actual data on soil water content and crop water requirements. In addition, soil type and evapotranspiration from bare soil is taken into account (Hulme et al, 2001).

This approach is being applied in a preliminary form to current modelling studies (Wirral, Itchen, East Shropshire, Bourne & Nine Mile River) and an Agency R&D project has been commissioned to carry forward further development.

4.4.1 Introduction

The estimation of recharge will be presented as two parts. Part A considers *potential recharge,* which is the water that leaves from the bottom of the soil zone. Provided that the material between the bottom of the soil zone and the permanent water table does not restrict the vertical movement of water, the *actual recharge* at the water table equals the potential recharge. However, in many British aquifers there are deposits of low permeability material between the base of the soil zone and the permanent water table; this restricts the recharge. The term 'Drift' will be used to describe the deposits between the soil zone and the permanent water table. The influence of the Drift on the actual recharge is the subject of the Part B of *Estimating Recharge*.

Potential recharge estimates are based on a soil zone water balance. The key issue is to obtain reasonable estimates of the actual evapotranspiration when the crop is under stress. Previously the Agency has used the Penman-Grindley method based on root constants but now the Agency is moving towards a new approach based on the properties of both the crops and the soil. This topic is covered in far more detail in a report which has been prepared for the Agency.

Recharge is assumed to occur when the soil is at field capacity (the amount of water that a well-drained soil can hold against gravitational forces, or the amount of water remaining when downward drainage has markedly decreased) excess water becomes recharge since the soil is free draining.

Other issues which need to be considered when estimating potential recharge include runoff at times of heavy rainfall, bypass recharge, evaporation from bare soil and the retention of rainfall near the surface for evaporation or evapotranspiration during the following days.

4.4.2 Physical Reality of Potential Recharge and Recharge Influenced by Drift

Potential recharge occurs when water drains through the soil and, if there is no low permeability underlying Drift, moves to the aquifer water table; the actual recharge then equals the potential recharge. For many chalk aquifers a bypass mechanism has been noted in which a proportion of the (effective) rainfall bypasses the soil and enters directly into the aquifer. Potential recharge is considered in Part A.

If there is a substantial permeable unsaturated zone from the base of soil layer to the water table, there can be a delay but the total actual recharge still equals the total potential recharge. If there are low permeability strata between soil and water table, mechanisms apply which reduce the downward movement of water. However, some of the potential recharge can be stored in the Drift and subsequently released to move laterally to seepages and springs to form delayed runoff; this runoff may subsequently enter the aquifer system as it crosses to more permeable parts of the aquifer. This runoff recharge is an important component of the total recharge in many locations.

Much can be learnt about the likely recharge processes from a carefully study of groundwater head hydrographs. Figure 4.4.1 shows how the groundwater heads vary close to the confined boundary of the Southern Lincolnshire Limestone. The first point to note is that groundwater heads rise in late autumn and during the winter, reflecting the occurrence of conventional rainfall recharge. The magnitude of the rise varies from year to year, the largest rises are in excess of 8 m, whereas in the winter of 1972-73 the rise was only 2 m. However, there is an unusual feature of these hydrographs, namely that there is a significant rise during certain of the summers. For example in 1973 there was a rise in the summer of 2 m. This was the result of runoff recharge from less permeable strata entering swallow holes and inliers in the limestone. Runoff recharge is therefore a significant inflow to the Southern Lincolnshire Limestone (Bradbury and Rushton 1998).

Runoff recharge has also been shown to be important for Drift covered Sandstone aquifers and Chalk aquifers covered by Boulder Clay and Clay with Flints. Where the Drift is of a very low permeability, there may be a very small vertical flow which is much less than the potential recharge. Even though this vertical flow may be 0.1 mm/d or less, if it enters the aquifer over a large area, it can be a significant source of water.

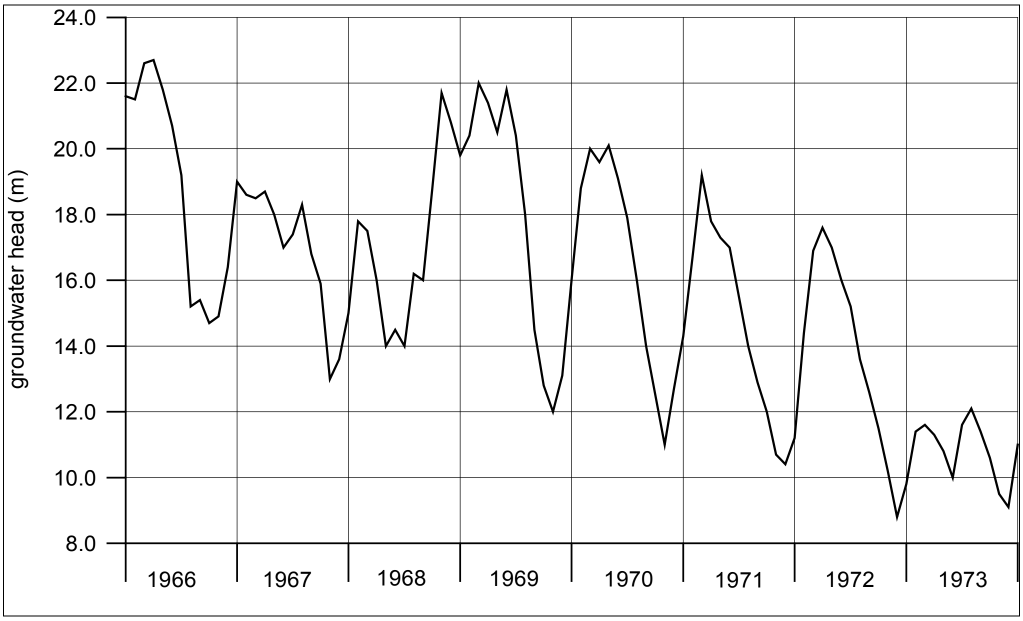


Figure 4.4.1. Example of a groundwater hydrograph for Southern Lincolnshire Limestone

River-aquifer interaction may be an important source of recharge. The loss from the river and, hence, the recharge, may be increased by pumping in the vicinity of the river. It is not only from rivers that water can be drawn into the aquifer. To the east of Doncaster, areas which originally provided outlets for groundwater prior to significant exploitation from the aquifer, now undergo reversed flows especially in summer providing recharge to the aquifer.

In deciding how to appropriately represent runoff-recharge or stream flow losses it is important to consider the relationship between the groundwater level and the river stage elevation, and the time scale over which flow losses occur from the stream to the ground.

Where smaller streams or tributaries flow onto the aquifer from less permeable strata but the water table is always beneath the bed of the stream, flow losses will be dependent on the infiltration capacity of the bed and the amount of water in the stream available to be lost, but independent of the water table elevation. The runoff in such streams is often very ‘flashy’ in relation to rainfall events i.e. flow may only occur for a few days following a storm with the amount of recharge leaking from the bed determined by its infiltration capacity for that short period. This infiltration capacity can be estimated through spot flow surveys of flow loss following a rain storm. Comparisons can also be made between the volume of hydrologically effective rainfall in a single event and the runoff volume flowing over a gauging station a short way from the edge of the aquifer, enabling losses to the aquifer to be calculated in Ml/d/km length of stream. Such recharge mechanisms may also be associated with evidence of rapid groundwater level responses.

At these locations, runoff-recharge is most appropriately estimated at a daily calculation step as part of the runoff and recharge model. Volumes of runoff can be calculated along with volumes of potential recharge according to rainfall intensity, infiltration capacity and evaporative losses (see parts A and B), constrained by the surface water catchment area which, based on digital elevation models, can often be reasonably well defined everywhere. These runoff volumes can optionally be stored, released and routed across the surface to simulate the runoff hydrograph response, with recharge losses from the bed constrained according to daily bed leakage limits.

Further downstream, where the groundwater table is closer to the bed of the river, influent/effluent status may vary seasonally, or in response to groundwater abstraction related drawdown. In such locations it is more appropriate to simulate the head dependent groundwater-surface water interaction as part of the groundwater model. If the stream flow in the groundwater model is intended to simulate total flow (including runoff) as opposed to baseflow only, runoff from the runoff and recharge model should be aggregated over the groundwater model stress period and added to the stream cells, rather than being available for runoff-recharge at the daily time step.

For models where runoff-recharge is an important process (e.g. West Midlands and Upper Lee), it is usually necessary to identify a modelling cross-over point on each stream. Upstream of this point runoff-recharge is calculated daily within the recharge/runoff model. Downstream runoff is added to streams in the groundwater model to allow head dependent groundwater-surface water interaction over a longer stress period.

Part A Potential Recharge

A.1 Conceptual Issues for Estimating Potential Recharge

This section and the following section on Mathematical Representation are concerned with the estimation of **potential recharge** using a **soil moisture balance**. The various concepts which are included in a soil moisture balance are introduced briefly below.

(a) ***potential evapotranspiration of the reference crop (grass)*;** the potential evapotranspiration from a uniform grass well supplied with water can be estimated from meteorological measurements using the Penman-Monteith method (Ward and Robinson 1990).

(b) ***crop evapotranspiration*** varies during the growing season and harvesting of the crop; Fig. 4.4.2 indicates the growth stages of a crop between planting in the spring and harvest in the late summer. Using crop coefficients, K_C, the potential evapotranspiration of the crop, ET_C, can be deduced from the potential evapotranspiration of grass, ET_0. The relevant equation is

$$ET_C = K_C \, ET_0$$

If a study area contains a wide range of crops, the appropriate evapotranspiration of each crop can be estimated.

(c) ***Soil Moisture Deficit (SMD)***: the soil moisture deficit, which reflects the response of a soil to the growth of crops, can be described as follows. Following heavy rainfall (or irrigation) the soil will drain until field capacity is reached. Unless water enters the soil zone (due to rainfall or irrigation), the water content in the soil zone decreases as a result of water uptake by the crop. The deficit (or depletion) below field capacity is called the **soil moisture deficit**. This is an equivalent depth of water since it is the depth of water that has to be supplied to a soil to bring it back to field capacity. It is important to emphasise that the calculations are in terms of an equivalent depth of water; to obtain an estimate of the actual depth of depletion, the soil moisture deficit should be divided by the effective porosity.

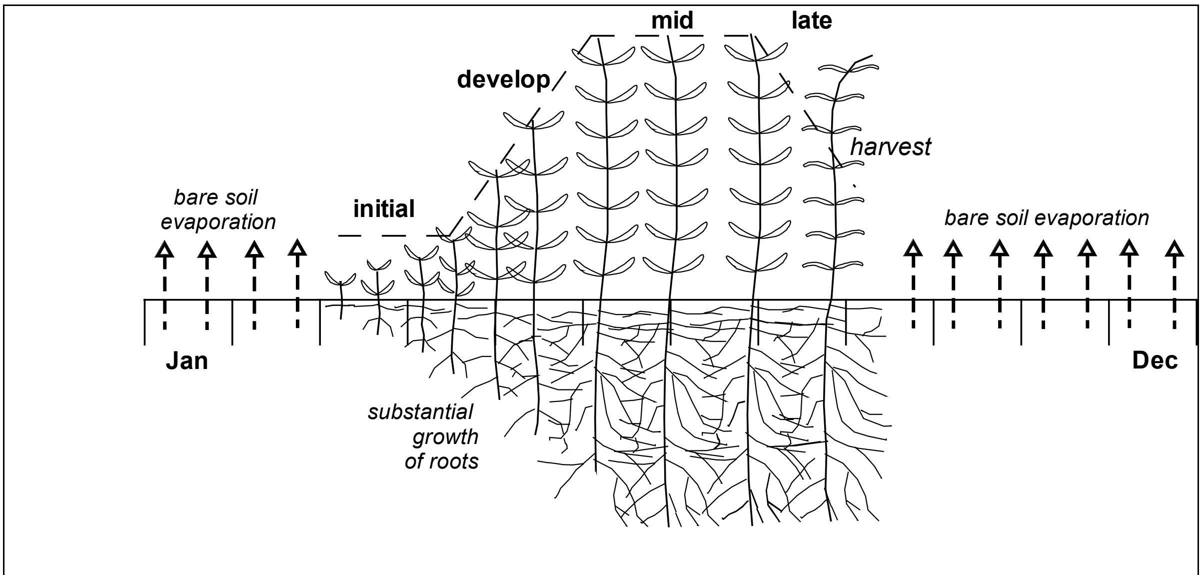


Figure 4.4.2. Growth of crop and roots for a representative spring sown crop; the diagram also shows bare soil evaporation

(d) ***Depth of the roots and the moisture holding properties of the soil***: it is a well known experience of gardeners that plants in clay soils can withstand hot dry periods more easily than plants in sandy soils. The reason is the higher water holding capacity of clays. An important parameter in determining whether roots can transpire at the potential rate is the Total Available Water (*TAW*); this is the product of the root depth, Z_r and the difference between the moisture contents at field capacity, θ_{FC}, and permanent wilting point, θ_{WP},

$$TAW = 1000(\theta_{FC} - \theta_{WP})Z_r \quad (TAW \text{ is in mm})$$

TAW for clay is more than double that for sand. As indicated by the increasing depths of roots with time in Fig. 4.4.2, the *TAW* increases from a small value after planting to a larger value during the main growth.

A second important parameter, the Readily Available Water (*RAW*), is required to represent the condition before the wilting point is reached when the plant can no longer transpire at the potential rate. The limiting soil moisture deficit when the plant transpires at the potential rate is the *RAW*; the *RAW* depends on the nature of the plant and is typically 40% to 60% of the *TAW*. If the soil moisture deficit is greater than the *RAW*, the plant transpires at a reduced rate.

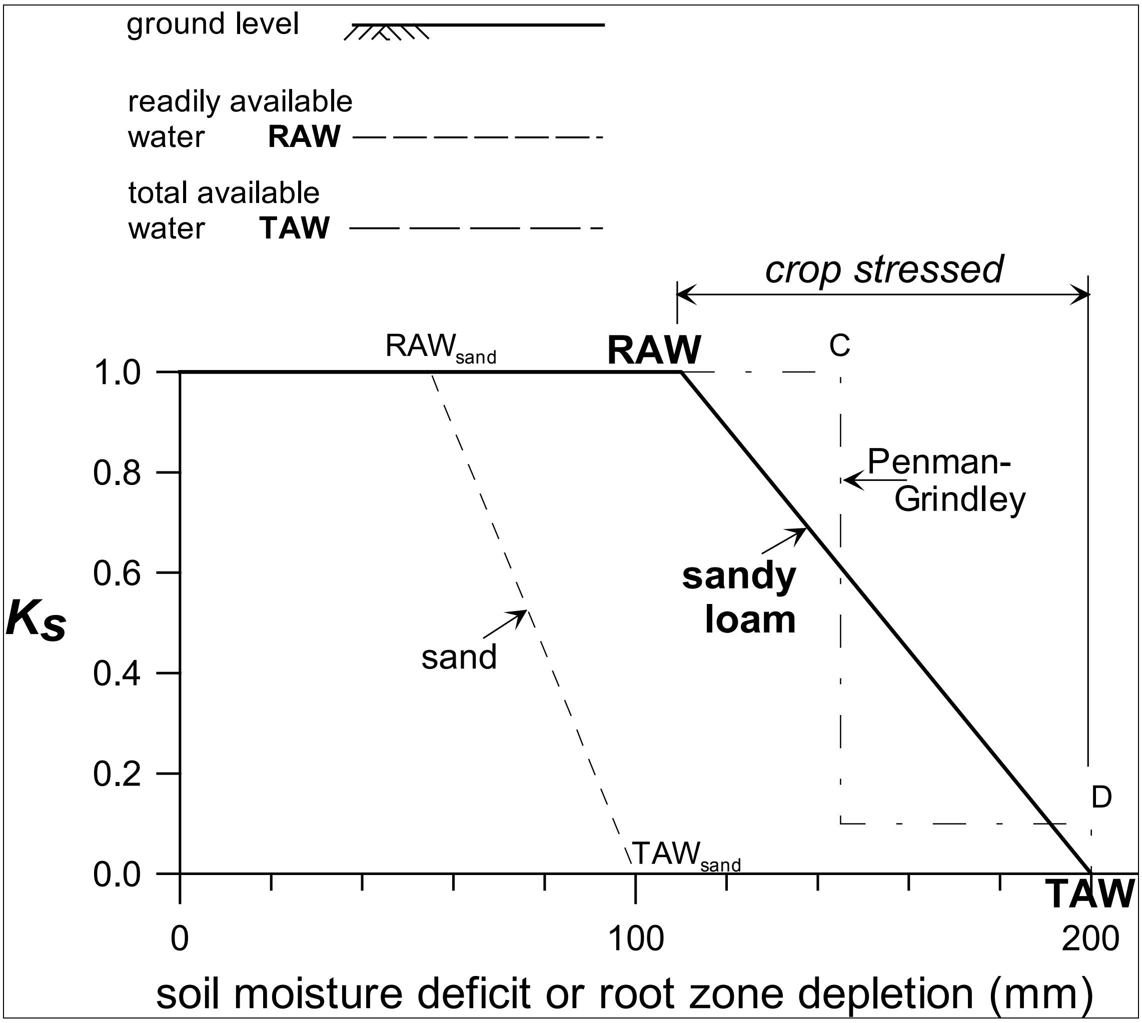


Figure 4.4.3. Diagram showing variation of soil stress coefficient with current soil moisture deficit

(e) ***Crop behaviour under stress***. When the soil moisture deficit is greater than RAW, the plant transpires at a reduced rate. To estimate the actual evapotranspiration, it is necessary to introduce the soil stress coefficient, K_S, such that, *in the absence of any precipitation*, (the calculation when precipitation occurs is considered in Section A.2.1)

$$ET_C = K_S K_C ET_0$$

where K_S is defined by

$$K_S = \frac{TAW - SMD}{TAW - RAW} \quad \text{when } RAW < SMD < TAW$$

Figure 4.4.3 shows that *TAW* and *RAW* for sandy loam are higher than for sand. Therefore the soil stress coefficient remains at 1.0 for soil moisture deficits up to 120 mm for wheat in a sandy loam but only up to 60 mm for wheat growing in a coarse sand. The diagram also shows the Penman-Grindley coefficients which abruptly change from 1.0 to 0.1 at the root constant *C*.

(f) ***Inclusion of runoff***: For most soils, runoff occurs following heavy rainfall, the runoff will depend on the nature of the soil, the slope of the ground and possibly other factors. Runoff must be subtracted from the rainfall to estimate the actual infiltration to the soil moisture store. Estimates of runoff can be made based on the rainfall intensity and the current soil moisture deficit; the estimates must be based on field information for each specific location.

(g) ***Bare soil evaporation***: One of the most important factors in estimating recharge is the bare soil evaporation. Most recharge occurs during winter when, either the soil is bare, or the crop cover is small so that bare soil evaporation is the dominant factor.

The potential bare soil evaporation for a soil, *ES*, can be deduced from the reference crop evapotranspiration using the equation

$$ES = K_e ET_O$$

where K_e is the evaporation coefficient currently taken as 1.10. There is a limit to the depth from which evaporation from soil can occur; there is also a reducing efficiency of evaporation in a similar manner to the limit of evapotranspiration when there is insufficient water available.

Two additional parameters are introduced, Total Evaporable Water (*TEW*) and Readily Evaporable Water (*REW*). The *TEW* is estimated from

$$TEW = 1000((\theta_{FC} - 0.5\ \theta_{WP})\ Z_e$$

where Z_e is the depth of the surface soil layer that is subject to drying by evaporation; it lies within the range 0.10 – 0.15 m. (Also the coefficient 0.5 is introduced before θ_{WP} since evaporation can dry the soil to mid-way between the wilting point and oven dry.)

An alternative soil stress coefficient for actual soil evaporation, K_s' is introduced; it is calculated in a similar manner to K_s but *TEW* and *REW* are used instead of *TAW* and *RAW*, Fig. 4.4.4.

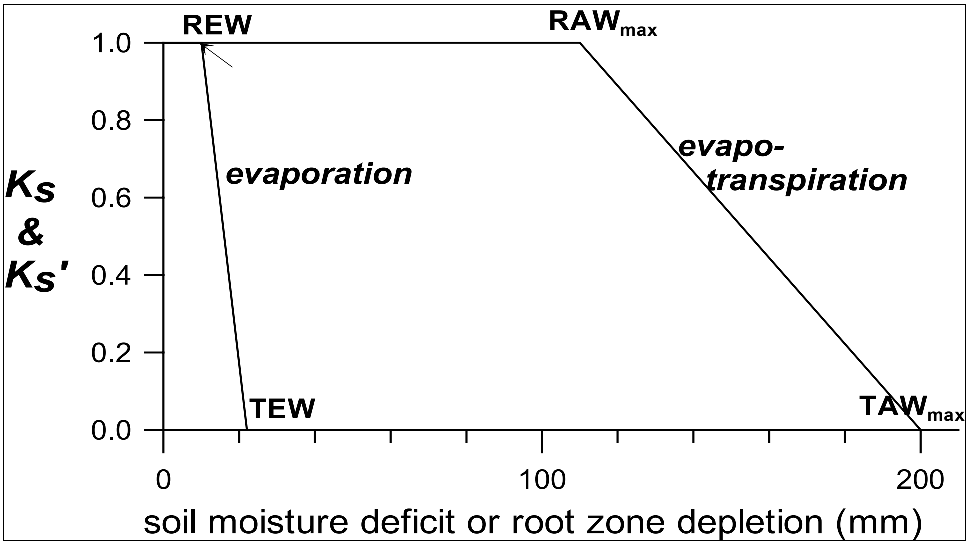


Figure 4.4.4. Soil stress coefficient for evapotranspiration and evaporation for sandy loam soil

(h) ***Bypass Recharge*:** Many workers have observed that there is a recovery in groundwater hydrographs in Chalk aquifers following heavy summer rainfall. A number of physical explanations have been given including a *by-pass mechanism* whereby water travels through some form of preferential pathways to the water table and avoids the soil moisture balance. An alternative explanation is that during heavy rainfall, rapid runoff occurs on the steeply sided hills; the water quickly flows to lower ground and through stream beds into the aquifer. By-pass recharge is estimated as a fraction of the precipitation (or precipitation minus potential evapotranspiration) in excess of a threshold value. The adequacy of the predictions can be assessed by comparisons with the timing of hydrograph responses. If a proportion of the precipitation is included as a by-pass recharge, this must be subtracted from the precipitation available for the soil moisture balance.

(i) ***Water storage at soil surface**:* The reasons for including *near surface soil storage* are as follows. One limitation of the standard assumption of the soil moisture balance technique is that, when heavy rainfall occurs with the soil moisture deficit *SMD* greater than *RAW*/*REW*, the water remaining, after allowance has been made for potential evaporation (or evapotranspiration) and runoff, moves immediately vertically through the soil to reduce the soil moisture deficit. As a result, none of this water is available to evaporate or be transpired during the following days.

This procedure fails to represent actual field conditions. During the autumn or early winter when the crops have been harvested, the *SMD* is greater than the *REW* and possibly greater than the *TEW*. In practice, some of the water from heavy rainfall remains close to the soil surface and evaporation at the potential rate can continue for several days after the rainfall event; this is not permitted in the standard procedure. Therefore in the revised approach, a proportion of the excess water is available for evaporation at the potential rate during succeeding days. This method of *near surface soil storage* ensures that recent rainfall is available for evaporation during the succeeding days; more water is retained for a loamy soil than for a sandy soil.

A.2. Mathematical Representation

A.2.1 Water balance:

The distributed water balance should preferably be carried out for each kilometre square on a daily basis. Data required for the balance include rainfall, weighting functions can be used to estimate the local rainfall from rain-gauge readings. Potential evapotranspiration values are also required, currently MORECS data is used but it is preferable to use the Penman-Monteith equation for the reference crop evapotranspiration of grass. The water balance calculation also requires information about the distribution of crops and soils. Runoff following heavy rainfall can occur, the runoff tends to be higher when the soil moisture deficit is small. From field observations it is possible to develop relationships which will relate the quick runoff to the rainfall intensity and soil moisture deficit (see Part B).

The calculations for actual evapotranspiration or evaporation in Section A.1 are derived for conditions of zero precipitation; modifications to include the effect of precipitation are described below.

Figure 4.4.5 shows a representative unit of soil in which the soil moisture deficit is greater than the readily available water. The following parameters are included in these diagrams.

> *SMD′* and *SMD*, soil moisture deficit at start and end of day,
>
> *Pr*, precipitation and *RO*, runoff,
>
> $In = Pr - RO$ is the infiltration
>
> *PE* and *AE* are the potential and actual evapotranspiration

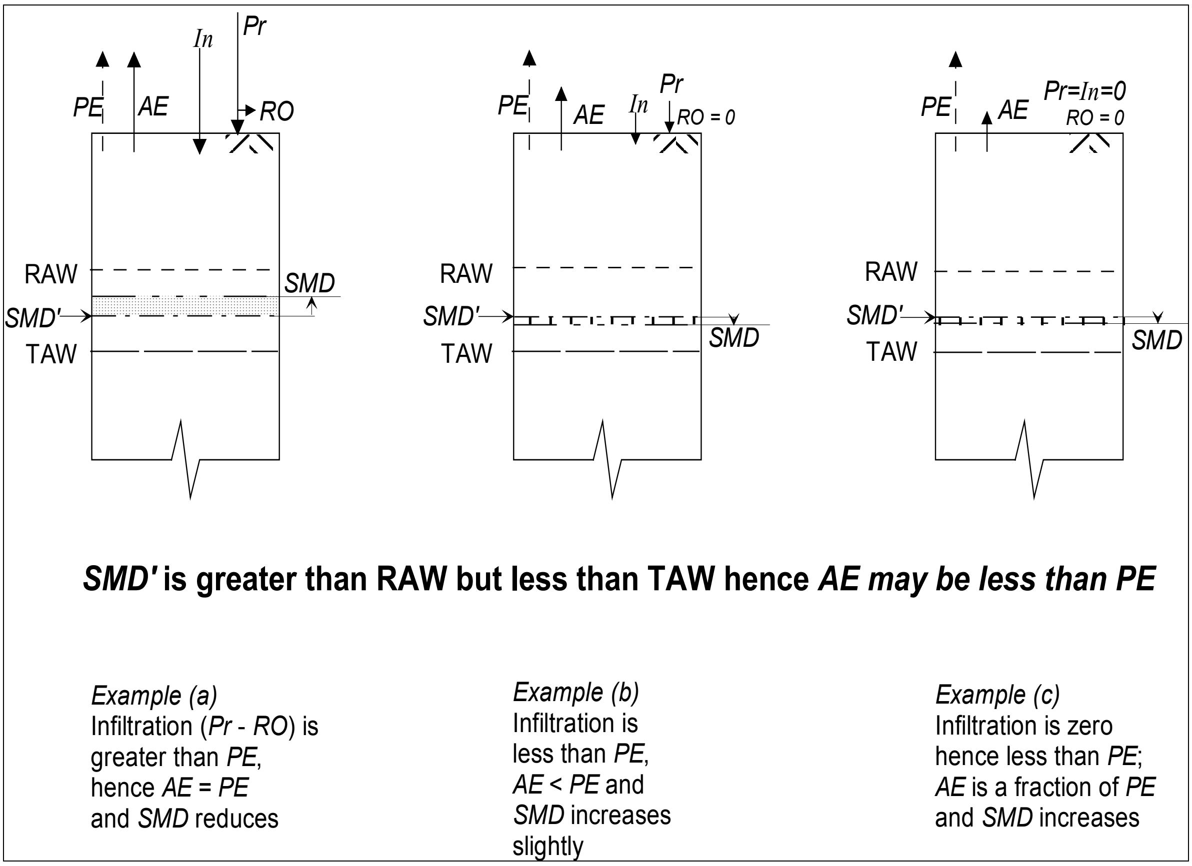


Figure 4.4.5. Typical water balances when the soil moisture deficit is greater than the readily available water so that actual evapotranspiration may be less than the potential

Three examples are considered. When the infiltration is greater than the potential evapotranspiration, example (a), the shallow roots can meet the potential evapotranspiration demand, hence $AE = PE$. However when $PE > In$, example (b), the infiltration is readily transpired but the remaining transpiration demand ($PE - In$) is only met at the reduced rate, the factor being K_S. In example (c), there is no precipitation or infiltration; hence the soil stress factor, K_S, applies (see Fig. 4.4.3) and for this particular example $AE = K_S\, PE$.

Different sets of diagrams are required when the soil moisture deficit is less than the readily available water; the actual evapotranspiration is always at the potential rate. During the autumn and early winter, the soil moisture deficit may be greater than the total evaporable water and a further set of conditions apply.

A.2.2 Algorithms:

All the possible conditions can be represented by the following algorithms;

(i) Estimation of Actual Evapotranspiration

for $SMD' < RAW$ or for $In \geq PE$, then $AE = PE$

for $TAW \geq SMD' \geq RAW$ and $In < PE$, then $AE = In + K_S\,(PE - In)$

where K_S is calculated using the soil moisture deficit for the previous day.

$$K_S = \frac{TAW - SMD'}{TAW - RAW}$$

for $SMD' \geq TAW$ and $In < PE$, then $AE = In$ (this condition can occur after harvest)

Apart from the introduction of the soil stress coefficient, K_S, and the dependence of the potential evapotranspiration on the crop factor, K_C, the calculations are identical to the Penman-Grindley soil moisture balance method. However the coefficients are more soundly based

(ii) Soil moisture balance and calculation of potential recharge

The equation for the daily soil moisture balance is as follows:

$SMD = SMD' - In + AE$

If $SMD < 0.0$, $RECH = - SMD$ and $SMD = 0.0$.

A.2.3 Typical results for potential recharge estimation

Typical results for the estimation of potential recharge during 1970 for a crop of winter wheat in the Southern Lincolnshire limestone are plotted in Fig. 4.4.6; the figure repays careful study, certain important features are highlighted below.

- the upper figure shows the rainfall, the runoff (below the horizontal axis) with the recharge indicated by the black parts of the rainfall histogram.
- the second diagram shows that the crop coefficient is generally above 1.0 (representing the crop and bare soil coefficients) apart from days 180 to 240 when harvest period leads to reduced evapotranspiration.
- the third graph shows the potential evapotranspiration, with the actual evapotranspiration shaded black. When the *SMD* is less than *RAW*/*REW*, the actual evapotranspiration equals the potential evapotranspiration. Actual evapotranspiration also equals the potential evapotranspiration when significant rainfall occurs. Between days 220 and 320 (when $SMD < TAW/TEW$), there are days when the actual evaporation/evapotranspiration is zero.

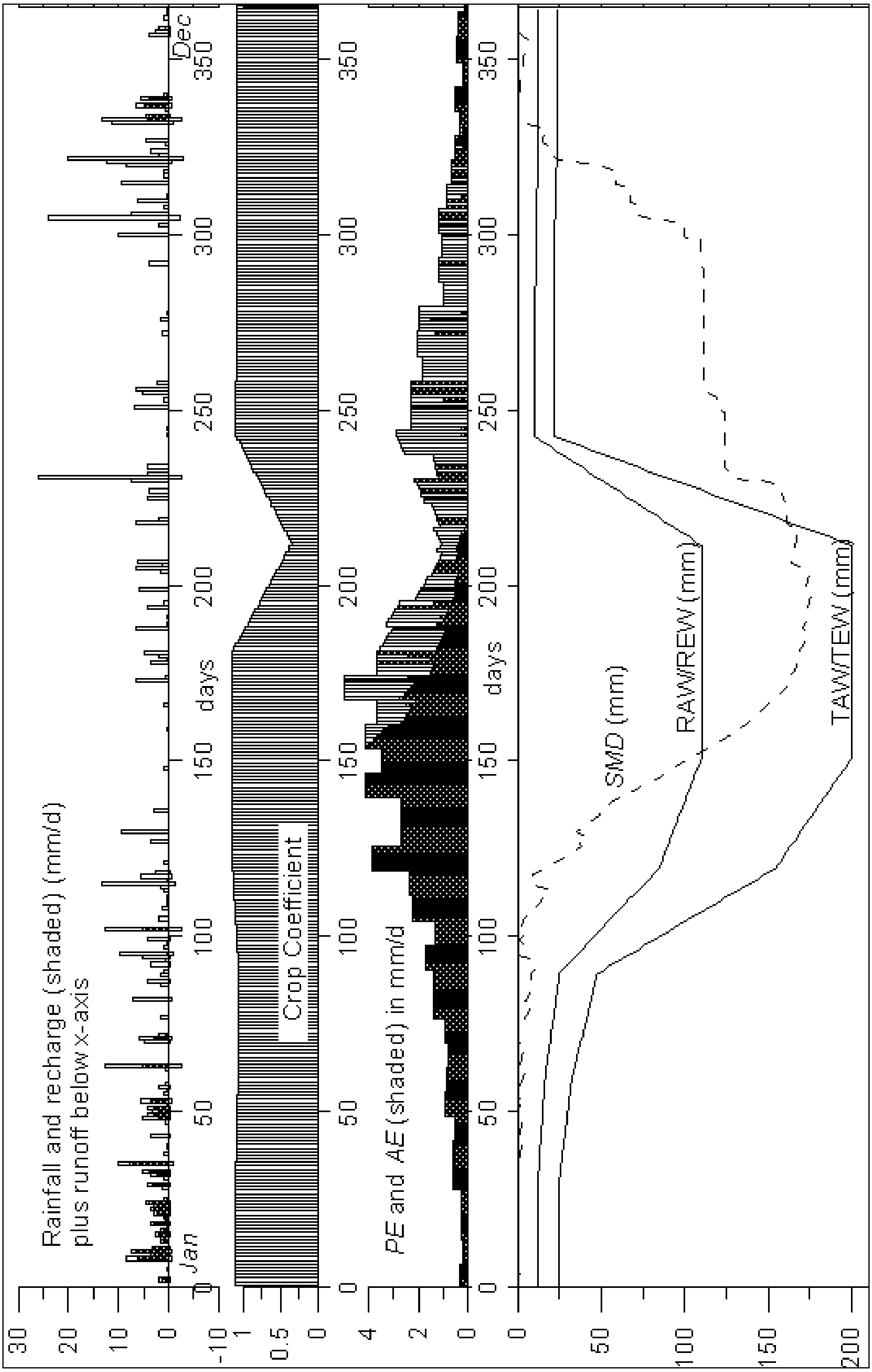


Figure 4.4.6. Typical results of potential recharge estimation for part of Southern Lincolnshire Limestone for year when potential evapotranspiration is slightly less than rainfall

It is the graph showing the relationship between the soil moisture deficit (*SMD*) and *RAW*/*REW* and *TAW*/*TEW* which explains most of the responses. For example, when the *SMD* is zero, recharge can occur. When the *SMD* is between the *RAW* and *TAW*, evapotranspiration is at a reduced rate unless there is significant rainfall.

A.3 Discussion

This first part of the guidance note summarises the current methodology for estimating the potential recharge. Although it has many similarities to the Penman-Grindley method based on root constants, it uses actual information about crops and soils. It also allows a realistic consideration of bare soil conditions in winter and the effect of autumn sown crops.

The estimation of recharge will always involve some uncertainties, hence recharge should be included as a parameter in the sensitivity analysis carried out during a numerical model refinement.

Part B Influence of Drift

B.1. Introduction

The second part of Estimating Recharge considers the effect of Drift on recharge to the permanent water table. Introductory comments can be found on pages 1 and 2. In many British aquifers there are deposits of low permeability material between the base of the soil zone and the permanent water table; this Drift restricts the recharge and the influence of the Drift on the actual recharge is the subject of the Part B of *Estimating Recharge*.

In the following discussion, examples are given of recharge estimates through the Drift. The approach currently recommended is to consider each situation separately, develop conceptual models and estimated suitable factors or parameters. Uncertainties can be explored using sensitivity analyses.

B.2. Alternative Mechanisms for Recharge due to Drift

B.2.1 Runoff due to high rainfall intensity rainfall

At times of heavy rainfall, runoff frequently occurs. Field evidence of actual runoff is provided by the presence of ditches and culverts; a useful impression of the runoff due to heavy rainfall can be gained by visiting the study area during rainfall events. Conditions can differ significantly between summer and winter.

Two alternative ways of estimating the runoff have been used, one is based on the limited infiltration capacity of the soil with the water which cannot infiltrate becoming runoff, the second assumes that the runoff is dependent on the rainfall intensity and the current soil moisture deficit. The second method has proved to be more suitable for groundwater catchments. The runoff from wet ground is certainly higher than for dry ground. When the daily rainfall is high, a greater proportion of the rainfall does runoff; there may be a very small or zero runoff for smaller values of the daily rainfall. For a cell or a nodal area, the recommended approach for estimating the immediate runoff of water (i.e. water which does not enter the soil zone) is to develop relationships which define the percentage of rainfall which becomes direct runoff based on the daily rainfall intensity and the current soil moisture deficit. A typical set of relationship is presented in Table 4.4.1 for a sandstone aquifer; if there is more clay in the soil and slopes are steeper the runoff is likely to be higher than indicated by the coefficients in the table.

Table 4.4.1. Factors for runoff for a sandstone aquifer, P = daily precipitation

			Soil	Moisture	Deficit	(mm)
			0 – 10	10 – 30	30 – 60	60 +
Rainfall	*0 – 10*		0	0	0	0
Intensity	*10 – 20*		0.2*(P-10)	0	0	0
(mm/d)	*20 – 30*		0.15P	0.10P	0.05P	0
	30 +		0.3P	0.2P	0.1P	0.05P

If the low permeability deposits are of limited extent, the runoff can be routed to the edge of the low permeability zone and then enter the aquifer system (this may occur within the same computational cell). Alternatively there may be ditches to remove this excess water; if possible the farmer will route this water to more permeable regions where the water can soak away into the aquifer.

B.2.2 Vertical movement through low permeability strata

It is not possible to measure directly the vertical flow through low permeability strata above the permanent water table. However, indirect field evidence (which could be obtained from walk-over surveys at different times of the year) can be invaluable in quantifying the likely vertical flow. The first consideration is the nature of the soil following heavy rainfall (how many days is it before you can walk on the soil following heavy winter rainfall). If the vertical permeability of the sub-soil is very low, vertical drainage will be very slow. The need to provide tile drains and drainage ditches is another important clue; if the drains run for several days following a period of heavy rainfall, this is a clear indication that there is limited vertical permeability in the Drift. Auger holes, trial pits and trial boreholes are also useful in determining the nature of low permeability strata and the likely effective vertical permeability. One further source of useful information is the response of observation boreholes in the underlying aquifer; a slow muted response is a clear sign of a slow downwards movement.

Three alternative approaches have been used to represent vertical flow through the Drift:

i) The restrictive influence to vertical flow of a low permeability layer within the Drift is illustrated in Fig. 4.4.7. Water perches above the clay layer; it is assumed that the permanent water table is in the lower sand zone or in the underlying aquifer. The flow through the clay can be determined by Darcy's Law and equals 1.2 mm/d.

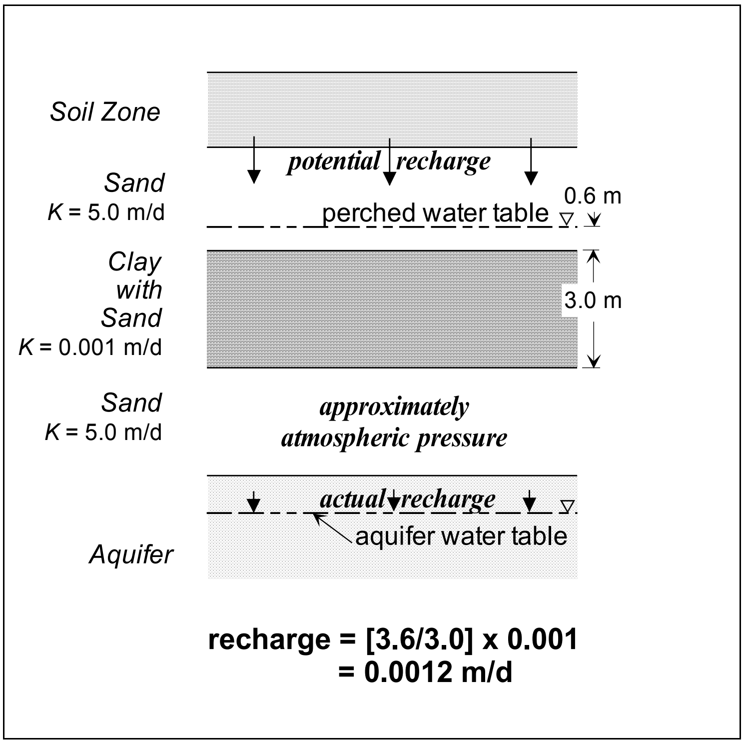


Figure 4.4.7. Movement of water through low permeability layers

The interfluves of the Gipping catchment are a good example of vertical flow which is strongly influenced by the low permeability layers of the Boulder Clay, see the left hand side of Fig. 4.4.8. In this example, the quantity of water actually entering the Chalk in the interfluves is restricted further by the low transmissivity of the Chalk. Estimates of recharge to the Chalk in the interfluve were refined during groundwater model development to reproduce the field groundwater hydrograph (the upper hydrograph of Fig. 4.4.8); from the model studies, the Recharge Component A entering the Chalk on the interfluves is estimated to be 24 mm/yr.

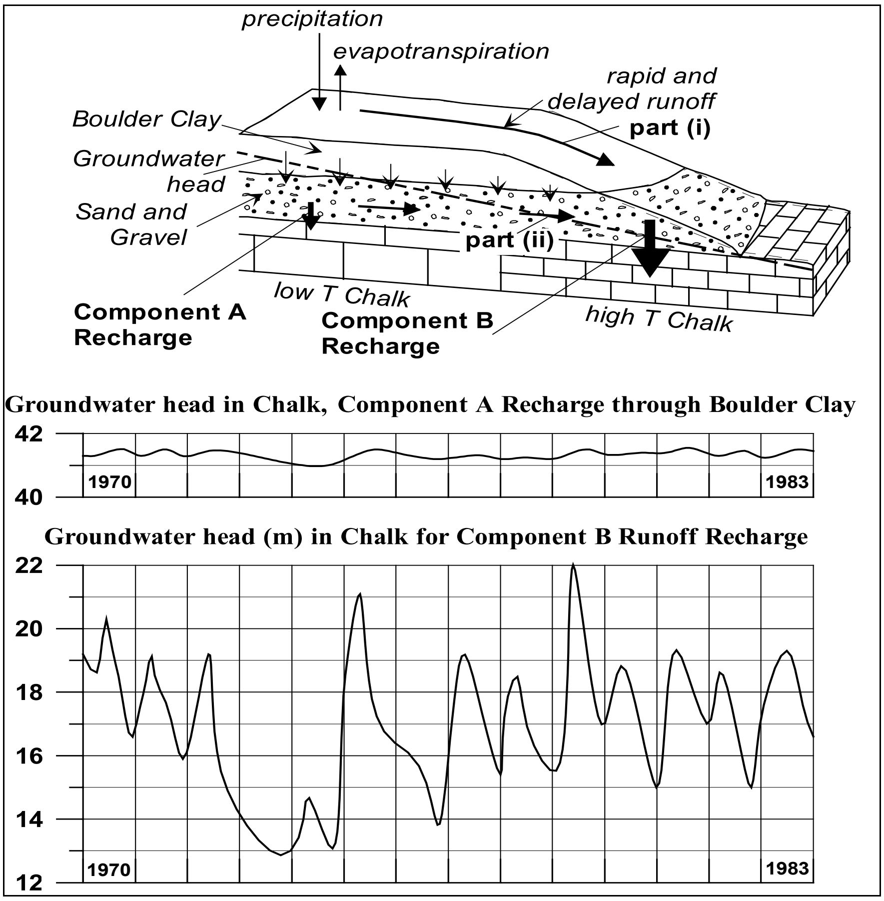


Figure 4.4.8. Conceptual diagram of the Gipping catchment

ii) Another approach to the estimation of actual recharge is to assume that a certain percentage of the potential recharge can move through the unsaturated zone to the aquifer. The percentage is a function of the Drift properties. This percentage approach can be used where there are different types of Drift of different thickness. This is a convenient method when the available information is the proportion of the precipitation which becomes runoff. It was used for the Sandstone of the Lower Mersey Basin; Fig. 4.4.9 (see next page) shows six different categories. They were first determined from site investigation boreholes, subsequently the coefficients were improved during refinement of a groundwater model. As the water table fell, the gradient across the low permeability layers increased; the manner in which this is included is shown in Fig. 4.4.10.

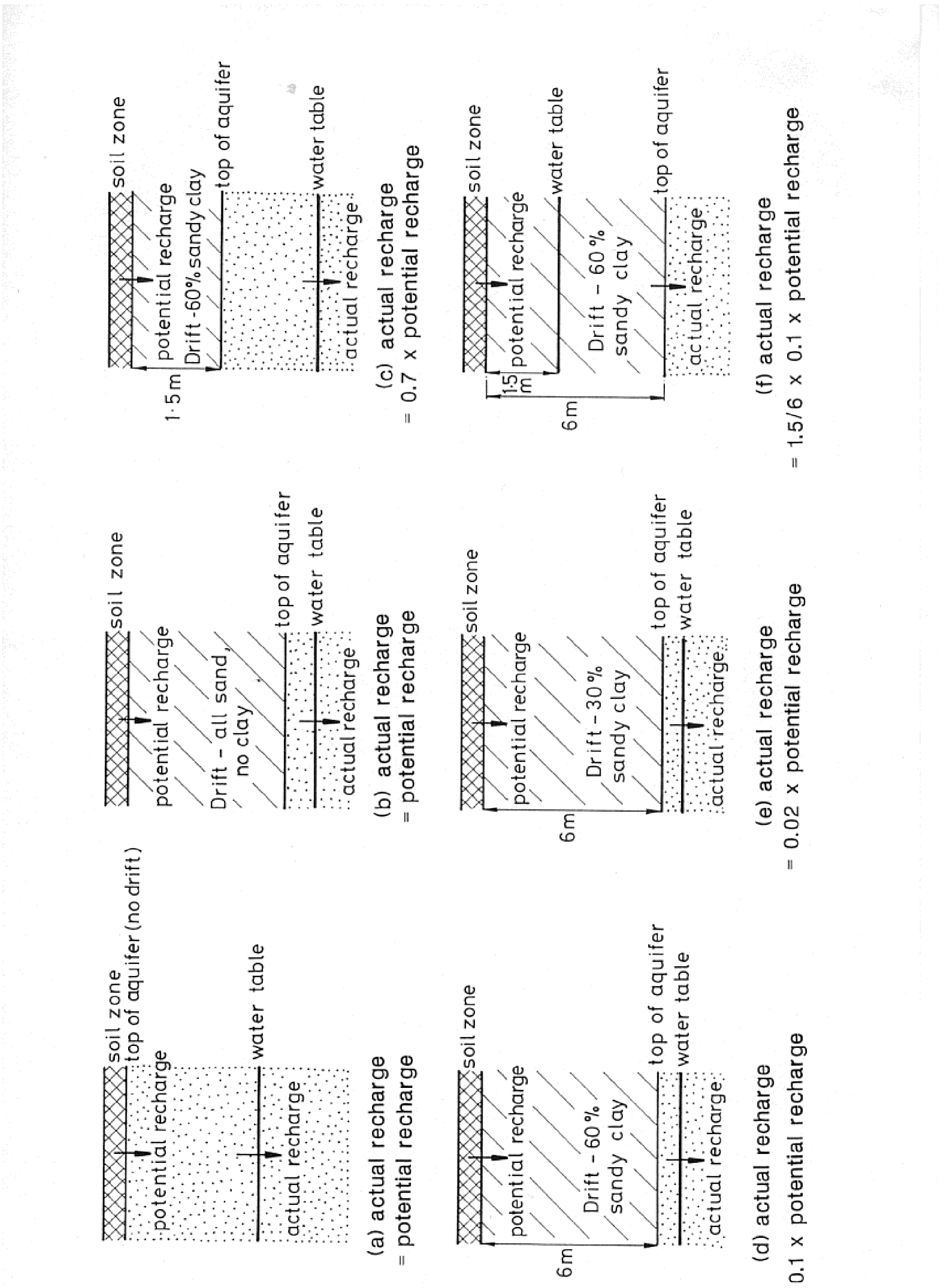


Figure 4.4.9. Estimation of recharge through the Drift of the Lower Mersey aquifer system

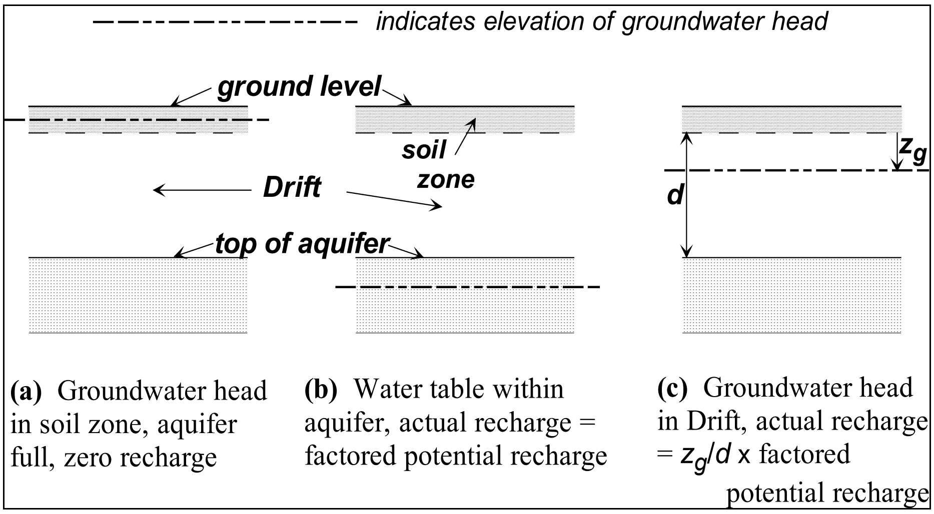


Figure 4.4.10. Effect of elevation of water table on recharge through Drift

It is important to take account of water which does not become vertical recharge but is stored in the Boulder Clay (or other low permeability strata). If the strata contain sand lenses, water can be stored and subsequently leave via springs and seepages. Figure 4.4.11 contains a schematic diagram, the factor of 0.15 means that each day, 15% of the water in the minor aquifer storage leaves as runoff whilst 0.05 mm/d moves vertically to the underlying aquifer. This issue is discussed further in Section B.2.4.

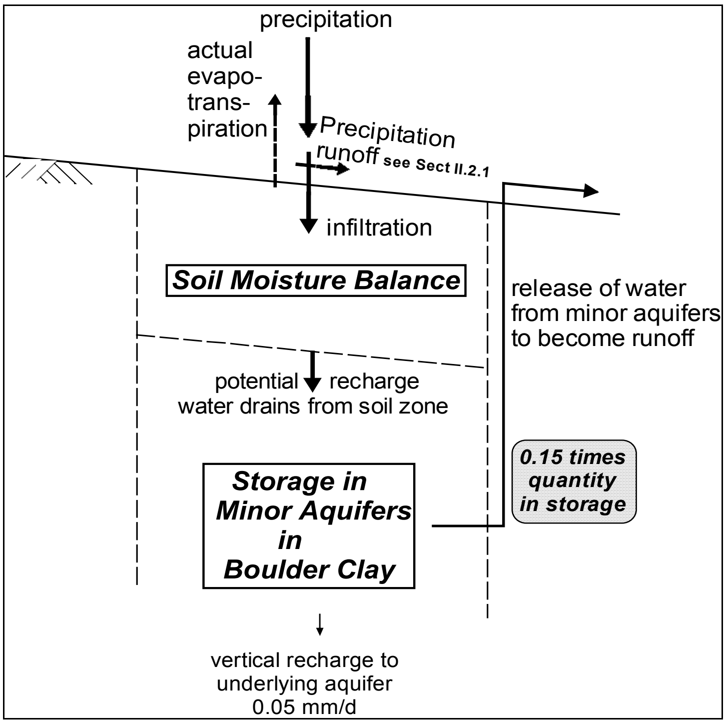


Figure 4.4.11. Schematic diagram of runoff due to release from storage in drift

iii) A third method is to use a classical "leaky" aquifer approach in association with a regional groundwater model. When this approach is used an effective vertical hydraulic conductivity (which will be dominated by the low permeability layers) and the thickness of the Drift must be specified. The flow is then proportional to the difference between the perched water table in the Drift and the groundwater head in the underlying aquifer. An example of the use of the leaky aquifer approach can be found in Fig. 4.4.12; it refers to an area to the east of Doncaster where, historically, water from the underlying Sherwood Sandstone aquifer flowed upwards due to the higher head in the aquifer.

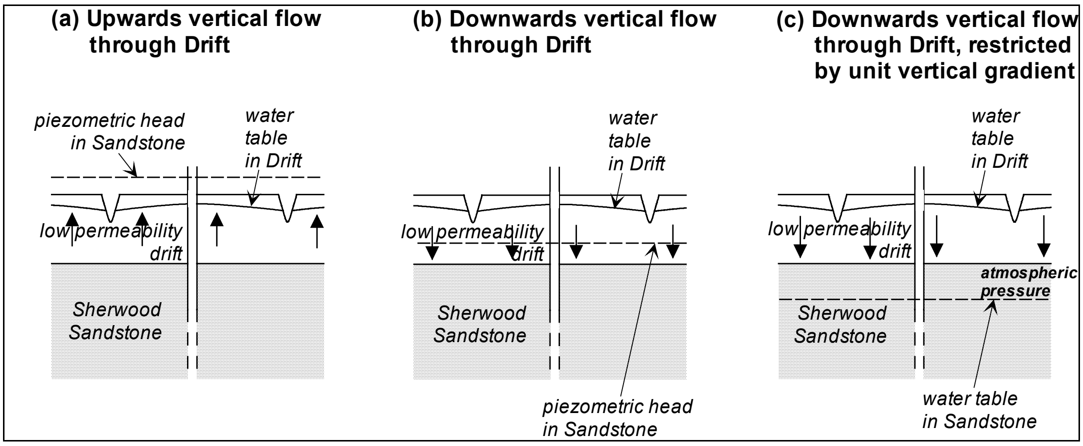


Figure 4.4.12. Conditions in the Doncaster area

To make the land suitable for farming, extensive drainage was constructed with surface pumps to remove the water (diagram (a) of Fig.4.4.12). As abstraction from the Sandstone aquifer increased, head gradients were reversed so that water is now drawn from the drainage channels into the aquifer (diagram (b)). In some locations the water table has been drawn below the bottom of the Drift, Fig. 4.4.12(c); it is then essential that the leaky aquifer response is modified so that the vertical groundwater gradient across the Drift does not exceed unity.

There are a number of *dangers* in using classical leaky aquifer theory to represent vertical flow through Drift as a means of estimating the actual recharge:

- if the water table is below the low permeability layer, Fig. 4.4.12(c), the low permeability layer becomes 'disconnected' and the vertical gradient cannot exceed unity.
- the low permeability Drift is partly unsaturated which leads to reduced values of the vertical hydraulic conductivity,
- the assumed effective vertical permeability may lead to a vertical flow which is not consistent with field evidence of the likely magnitude of the recharge. Whenever possible it is preferable to specify the recharge as described in Figs 4.4.8 to 4.4.11.
- when extensive pumping occurs, it is possible that the use of the leaky aquifer approach results in more water passing vertically through the leaky layer than is available from the potential recharge at the base of the soil zone.

B.2.3 Time lags in recharge reaching water table

There is usually a delay between water passing through the soil zone when the soil moisture deficit becomes zero (which results in free draining conditions in the soil and the occurrence of potential recharge) and water reaching the permanent water table. This delay can be identified from a study of the groundwater head hydrographs (which need to be based on weekly readings or less) and daily recharge estimates. A delay occurs since the Drift is itself an aquifer system with permeabilities and storage coefficients.

A theoretical study supported by field work (Senarath and Rushton 1984) explored the magnitude of the delay which can occur in a relatively permeable leaky aquifer. Assuming a fully saturated overlying layer of vertical thickness of 30 m with a permeability of 0.003 m/d and storage coefficient of 0.0001, with a pulse of recharge entering on day 1, the maximum flow from the base of this layer occurs on day 9. Consequently the flow into the aquifer from the overlying leaky aquifer is like a unit hydrograph reaching a maximum after 9 days but continuing with significant flow into the main aquifer until 50 days. Field comparisons between the onset of recharge and water table responses suggests that delays of one or even two months can occur.

B.2.4 Storage and subsequent delayed runoff in underlying strata

As indicated in the Section B.2.2, the Drift is a complex aquifer system. This is demonstrated by field evidence which shows that streams continue to flow as seepages and springs from Drift aquifer systems; these discharges may continue for several weeks after periods of heavy rainfall. Seepages and spring flows tend to be highest in wet winters, there may be little or no outflow in dry winters. In wet summers there can be significant delayed runoff.

Some strata covering an aquifer are of very low permeability, such as the Gault Clay or the London Clay; they accept and store little water. Nevertheless, there are many occasions when these effectively impermeable strata are overlain by other material such as head, alluvium or sands and gravels which do act as minor aquifers. Elsewhere Boulder Clay (Till) occurs in many locations; the Boulder Clay usually consists of lenses or layers of moderate and low permeability materials. These strata accept some of the potential recharge. They allow a small flow vertically to the underlying aquifer; in addition water is stored within permeable zones (sand lenses or minor aquifers) which is released over a period of time. These flows from the lenses or minor aquifers can be considerable; if they subsequently flow onto an aquifer they become runoff recharge.   A typical example of a computational model for the flow mechanisms in Boulder Clay covering the Southern Lincolnshire Limestone is presented in Fig. 4.4.13.

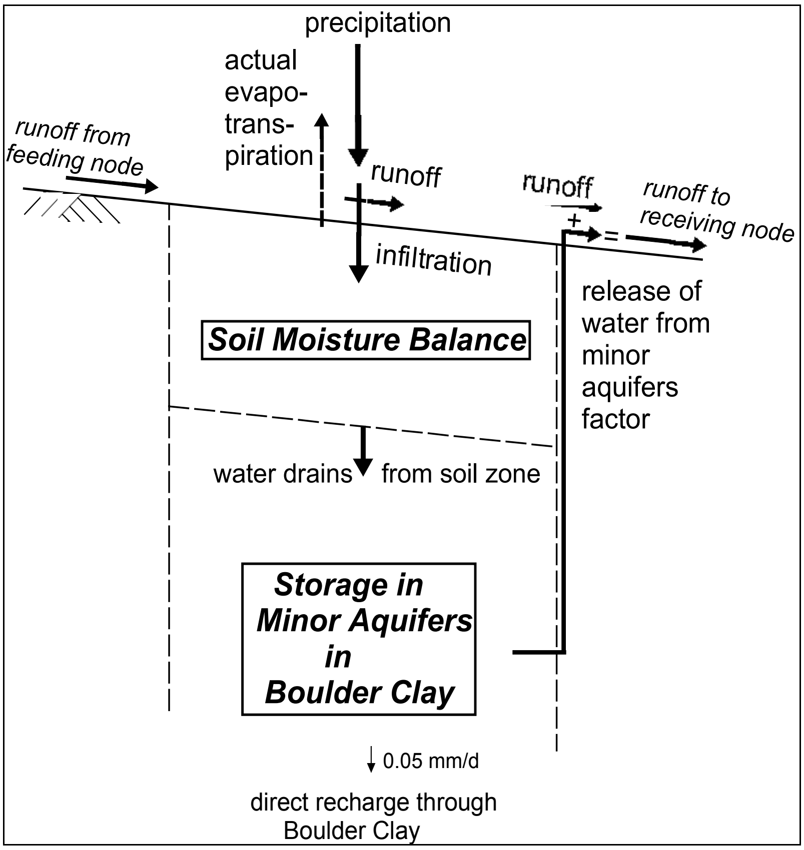


Figure 4.4.13. Computational model of recharge and runoff processes for low permeability strata

The storage properties of the various minor aquifers are represented as a storage reservoir. Potential recharge enters this store. Some water can leave this store by a steady vertical flow to the underlying water table (0.05 mm/d in Fig. 4.4.13). However, most of the water leaves the store to become a delayed form of runoff (or interflow). Figure 4.4.13 is a schematic diagram; the upward arrow, representing *the release of water from minor aquifers to become runoff*, does not mean that the flow is vertically upwards; in practice it is likely to be an approximately horizontal flow to low lying ground where the outlet forms springs or seepages.

Table 4.4.2 Example showing release from store in Drift; the only inflow is on Day 1, the release coefficient is 0.15 day^{-1}.

Day	In Store (mm)	Release (mm/d)		Day	In Store (mm)	Release (mm/d)
1	20.000	3.000		9	5.450	0.817
2	17.000	2.50		10	4.632	0.695
3	14.450	2.168		11	3.973	0.591
4	12.283	1.842		12	3.347	0.502
5	10.440	1.566		13	2.845	0.427
6	9.874	1.331		14	2.418	0.363
7	7.543	1.131		15	2.055	0.308
8	6.412	0.962		16	1.747	0.262

Farmers usually construct drainage ditches to collect this water. The computational technique involves releasing a certain proportion of what is in the subsoil store each day; this is equivalent to a release which decays exponentially. Table 4.4.2 illustrates how water is released according to a delay coefficient of 0.15 day^{-1} (for the Boulder Clay in the Southern Lincolnshire Limestone catchment, the delay coefficient was 0.08 day^{-1}). At Day 15 about 10% of the water is still stored and the release on that day is just over 10% of the release on Day 1.

Similar responses can be observed when areas are drained by tile drains, the delay in releasing water is shorter than in Table 4.4.2.

B.2.5 Transfer of water across low permeability catchment to become runoff recharge
Section B.2.1 indicated that some of the precipitation during days with high rainfall does not directly enter the aquifer due to infiltration capacity limits but becomes runoff. The previous section has

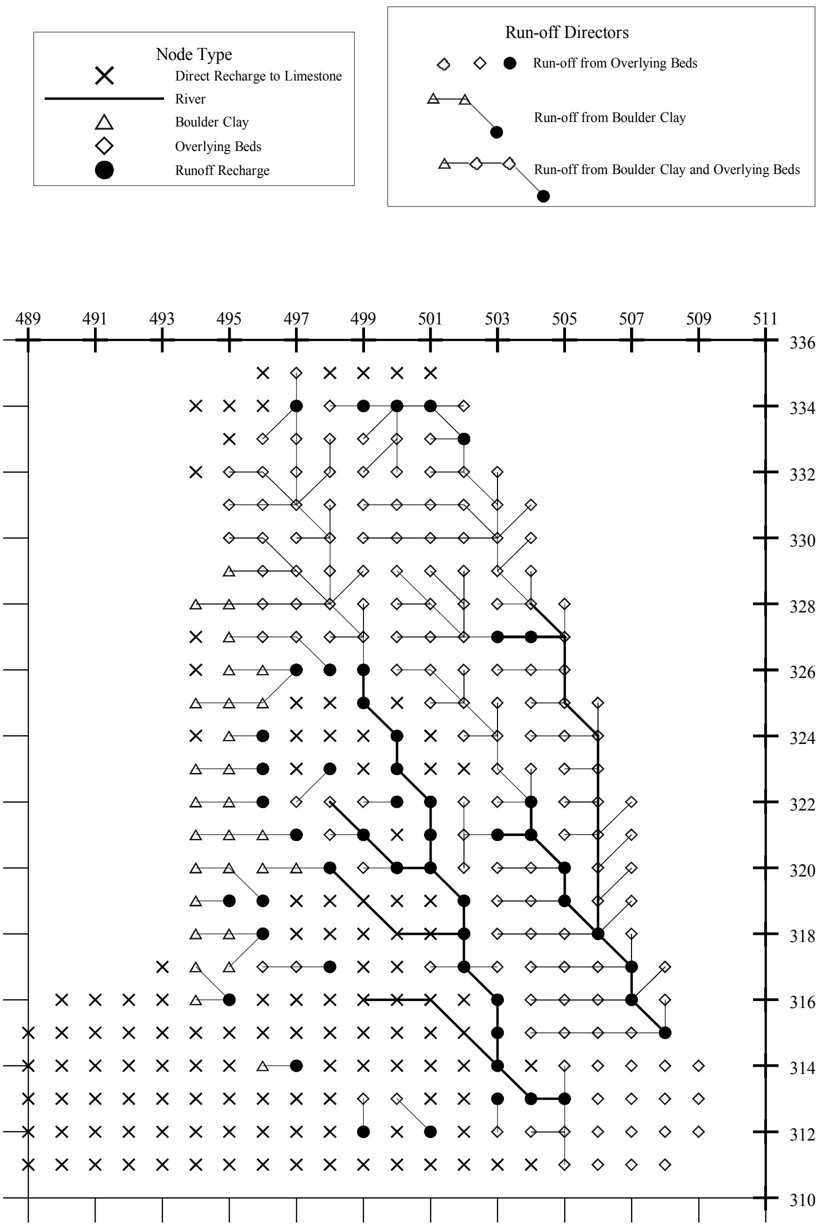


Figure 4.4.14. Director arrays for the Southern Lincolnshire Limestone

shown how water can be released from minor aquifers to become runoff. Both of these sources of water move across the catchment in rivers, streams and water courses. By tracing the movement of these flows, it is possible to see whether this water subsequently enters an aquifer as runoff recharge. The major flows which become runoff recharge can be observed in the field, but there are also smaller flows entering the aquifer system which are more difficult to identify.

Generally rivers, streams and water courses follow the topographical gradients hence their routes can be identified from 1:25,000 maps; however there are instances when water is diverted in artificial channels due to the proximity of more permeable strata. Identification of the paths followed by both rapid and delayed runoff is a critical part of the estimation of runoff recharge. Figure 4.4.14 shows the runoff director arrays for the Southern Lincolnshire Limestone catchment.

Another example of runoff recharge is provided by the Gipping catchment, and is shown on the right hand side of Fig. 4.4.8. The diagram shows how water flows across the Boulder Clay (the flow arrow labelled part (i) on Fig. 4.4.8) and through the underlying sands and gravels (labelled part (ii)), to the Boulder Clay margins where the transmissivity of the Chalk is far higher thereby allowing the runoff and interflow to enter the Chalk aquifer. The occurrence of this runoff recharge, Component B recharge, is shown by the large groundwater head fluctuations in the lower hydrograph of Fig. 4.4.8 compared to those at the interfluves (the upper hydrograph).

B.3. Discussion

This review has illustrated the different mechanisms which can apply when considering recharge through Drift. Several alternative approaches for the estimation of recharge through Drift have been described. Each was developed for a particular situation, hence the methodology selected depends on the specific physical situation, the availability of data and other information and the computing power available at the time when the work was carried out. A number of conceptual models and computational techniques have been presented which have provided adequate representations of the transfer of water through the Drift. These should be used as examples of the possible approaches.

The key to obtaining a satisfactory method appears to be to keep the approach as simple as possible. It is important to be in full ‘control’ of the calculation ensuring that the parameters and coefficients are direct, straightforward and physically meaningful. Only those mechanisms that are significant should be included.

For any new study areas, it is necessary to gather together all available hydrological and hydrogeological information. Field visits are essential at different times of the year. The next stage is to develop conceptual models, transfer into computational techniques and, whenever possible, include the Drift recharge estimates in groundwater models. Improved estimates of the recharge through Drift can be derived during refinement of the model. Alternative values of Drift recharge should be included in sensitivity analyses.

If the “leaky aquifer” approach is used, the movement of water through the Drift into the aquifer system will depend on the current groundwater heads. However, there is a risk that computer codes will take control of the process. For instance, if the vertical flow through the Drift is proportional to the vertical head gradient across the Drift multiplied by the effective vertical hydraulic conductivity, the computer code will determine the magnitude of the recharge even though the calculated value is inconsistent with field evidence. Careful checking of calculated values against all available information is crucial.

4.4.3 References

Bradbury, C.G. and Rushton, K.R. 1998. Estimating runoff-recharge in the Southern Lincolnshire Limestone catchment, UK. *J. Hydrology*. **211**, 86-99.

Cross, G.A., Rushton, K.R. and Tomlinson, L.M. 1995. The East Kent Chalk aquifer during the 1988-92 drought. *Journal of the Institution of Water and Environmental Management,* **9**, 37-48.

FAO, 1998. Crop evapotranspiration; guidelines for computing crop water requirements, <u>*FAO Irrigation and Drainage Paper*</u> **56**, Rome, 301pp.

Hulme PJ, Rushton KR & Fletcher SW (2001) *Estimating recharge in UK catchments*, Impact of Human Activity on Groundwater Dynamics (Proceedings of a symposium held during the Sixth IAHS Scientific Assembly at Maastricht, The Netherlands, July 2001). IAHS Publ. no. 269, 2001.

Jackson, D and Rushton, K.R., 1987. Assessment of recharge components for a chalk aquifer unit. *J. Hydrol*., **92**: 1-15.

Lerner, D N, Issar, A S and Simmers, I. 1990. *Groundwater recharge. A guide to understanding and estimating natural recharge*. International Contributions to Hydrogeology, Verlag Heinz Heise, Vol **8**: 345 pp.

Rushton KR, (Nov 2000) *Recharge Estimation for British Aquifers – A review by Ken Rushton* – Environment Agency internal document (available from the National Groundwater and Contaminated Land Centre).

Rushton, K.R., Fletcher, S.W. and Bishop, T.J. 1995. Surface water and groundwater components of the Nottinghamshire Sherwood Sandstone Aquifer System, *BHS 5th National Hydrology Symposium*, Edinburgh, 2.17-2.24.

Rushton, K.R., Kawecki, M.W. & Brassington, F.C. 1988: Groundwater model of conditions in the Liverpool Sandstone Aquifer. *J. Inst. Wat. & Env. Man.,* **2**; 67-84.

Rushton, K.R. and Tomlinson, L.M. 1995: Interactions between rivers and the Nottinghamshire Sherwood Sandstone aquifer. In: Younger, P L (ed.) *Modelling river-aquifer interactions*, BHS Occasional Paper No 6; 101-116.

Rushton, K R and Ward, C. 1979. The estimation of groundwater recharge. *Journal of Hydrology*, **41**, 345-361.

Senarath, D.C.H and Rushton, K.R. 1984. A Routing Technique for Estimating Ground Water Recharge. *Ground Water*, Vol. **22**, 142-147.

Ward, R.C. and Robinson, M. 1990. *Principles of Hydrology*, 3rd ed. McGraw Hill (UK). 365pp.

4.7 The use of pumping test results in regional modelling studies

Pumping tests have been carried out in most aquifers for which regional models are developed, but the quality of test data and analyses can be variable. Observations of long term exploitation of an aquifer can sometimes be available and can be of great value in identifying aquifer parameter values. How should the aquifer parameter values deduced from these sources be used in developing aquifer parameter arrays for regional models?

4.7.1 Practical difficulties in pumping test analysis

a) *Limitations of actual tests*: there are many practical difficulties encountered in conventional pumping tests. These difficulties range from the failure to maintain constant abstraction rates, the failure to obtain sufficient reliable readings during the pumping and recovery phases, the effect of boundaries, interference due to other pumping boreholes, etc.

b) *Conceptual models for actual tests*: when conceptual diagrams are prepared for the actual test sites, it is usually found that the aquifer is complex with, for example, variations in aquifer thickness, faults or other possible boundaries, significant regional groundwater flows and different strata identified in the lithology of the pumped and observation wells. These conceptual diagrams are often very different to the assumptions of the classical pumping test solutions.

c) *Positive and negative aspects of the use of analytical solutions to analyse pumping tests*: frequently analytical solutions are based on assumptions which are at variance with true field conditions. Consequently, when an attempt is made to match the field data with analytical solutions, a match can only be obtained for part of the data. Furthermore, from the analyses at pumped or observation wells both during pumping and recovery phases, different numerical values of the aquifer parameters are likely to be obtained. It is not acceptable to take an average of these differing values; instead the uncertainties of the aquifer parameters should be recognised. Despite these difficulties, estimates of aquifer parameters can be obtained using analytical methods provided that certain precautions are taken:

- choose the type curve not from the shape of the curve but from the physical situation (Kruseman and de Ridder 1990);
- recognise that in the early stages of a pumping test (approximately the first ten minutes), well storage can provide more of the pumped water than the aquifer itself, (this is illustrated in Fig. 4.7.1);
- during the later stages, boundary or leakage effects are likely to influence the aquifer response;
- take care with automatic fitting which is likely to include times for which data should not be used because of well storage and boundary effects, etc.;
- recovery is often more important than the pumping phase because the recovery reflects primarily the aquifer response whereas the pumping phase is strongly influenced by the pumped borehole characteristics.

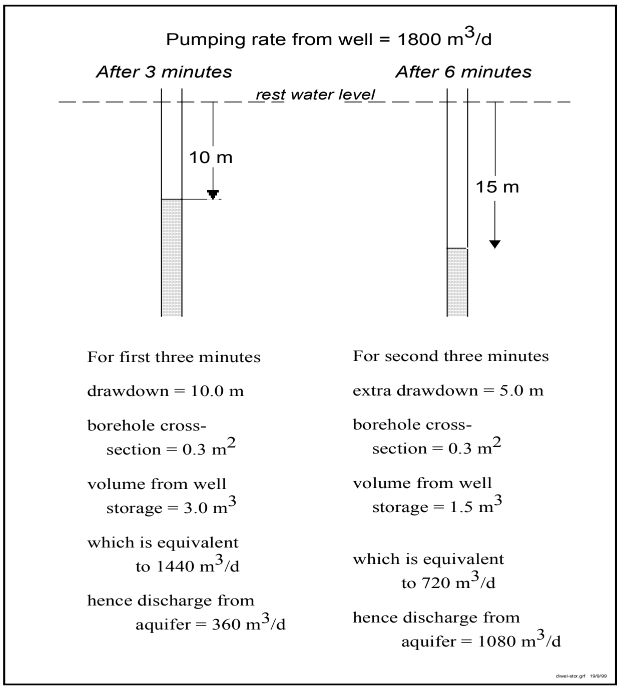


Figure 4.7.1. Significance of well storage in pumping tests

d) *Use of radial flow numerical models to analyse pumping tests*: when numerical models are used to analyse pumping tests, some of the realities identified in the conceptual diagrams can be included, but the numerical models cannot represent regional features. Nevertheless, improved estimates of aquifer parameters and boundary effects (due to faults or changes in transmissivity) can be obtained when numerical model techniques are utilised (Rathod and Rushton, 1984, 1991).

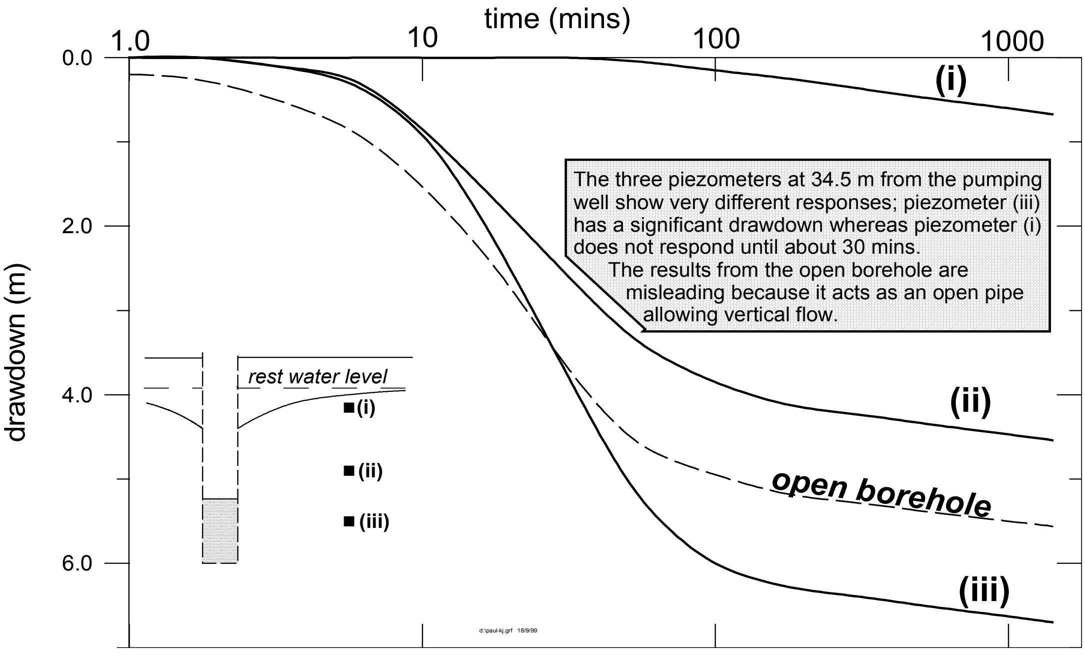


Figure 4.7.2. The response in three piezometers during a pumping test

e) *Vertical flows in aquifers*: significant vertical flows occur in the vicinity of most pumped boreholes; if observation piezometers are constructed at different depths, insights can be gained about vertical properties. The response of three piezometers at different depths in a sandstone aquifer (Fig. 4.7.2) show significant vertical flow components. Numerical models are available which can represent these vertical components of flow (Rushton and Howard 1982).

f) *Averaging of spatial variations in properties*.

- Pumping tests sample different portions of the aquifer at different times;
- Variations in properties are averaged;
- T:S ratio determines the rate at which the influence of the test propagates.

See Barker and Herbert (1982), Butler (1988), Butler and McElwee (1990), Butler and Liu (1993).

4.7.2 The value of pumping tests in developing conceptual models

Although the numerical values of aquifer parameters deduced from pumping tests will be of limited direct use, information gained from pumping tests can provide insights into the aquifer response.

a) *Positive information gained about variations of aquifer properties with depth*: variation of aquifer properties with depth which can be identified by carrying out tests in the same borehole under high and low water tables (especially useful in chalk aquifers).

b) *Regional distribution of parameters*: differing responses to pumping at different locations in the aquifer can provide indications of how the aquifer parameters vary regionally although the precise values obtained from pumping tests should not be used since they are strongly influenced by the particular properties of the pumping and observation boreholes.

c) *Identifying Boundary Effects etc.*: the failure of an aquifer to fully recover following a pumping test can indicated effectively low permeability 'boundaries'; rapid recovery can indicate recharge 'boundaries'.

4.7.3 The value of observations of long term pumping response

As an alternative to special purpose pumping tests, long term pumping from aquifers can be invaluable in developing reliable conceptual and mathematical models; typical examples are quoted below.

a) *Selecting transmissivity and storage coefficients for regional models*: in many regional aquifer studies, a range of aquifer parameters are determined from the analysis of pumping tests, but no clear pattern emerges due to the uncertainties in pumping test analysis. This occurs partly because a conventional pumping test only reflects the properties local to the test borehole. However, information which can be deduced from long term responses includes estimates of the regional transmissivities from the long term yield of boreholes (high yields with moderate drawdown indicate moderate to high transmissivities whilst poor yields suggest low transmissivities). Other insights can be gained from the time it takes for a new equilibrium to be achieved following the commissioning of new abstraction sites; for aquifers with moderate transmissivities and high storage coefficients, it may take decades for a new equilibrium to be reached whereas with high transmissivity but low storage coefficient aquifers, a new equilibrium is achieved in two to three years.

b) *Significant abstraction helps to confirm the magnitude of the recharge*: when records are available of the magnitude of the long term abstraction, the aquifer response will reflect the balance between the abstraction, recharge and other inflows or outflows. This is illustrated in Fig. 4.7.3, which shows the response of two piezometers in the Bromsgrove Sandstone aquifer. The deeper piezometer responds to the pumping; for example there was a significant reduction at a multiple borehole pumping station about 2 km distant during the last three months of 1989. The shallower piezometer responds primarily to the balance between recharge and abstraction; during the winter of 1991-92 there was virtually no recharge (for more information see Rushton 1994). Without significant abstraction it is often difficult to estimate the aquifer resources (especially the actual recharge).

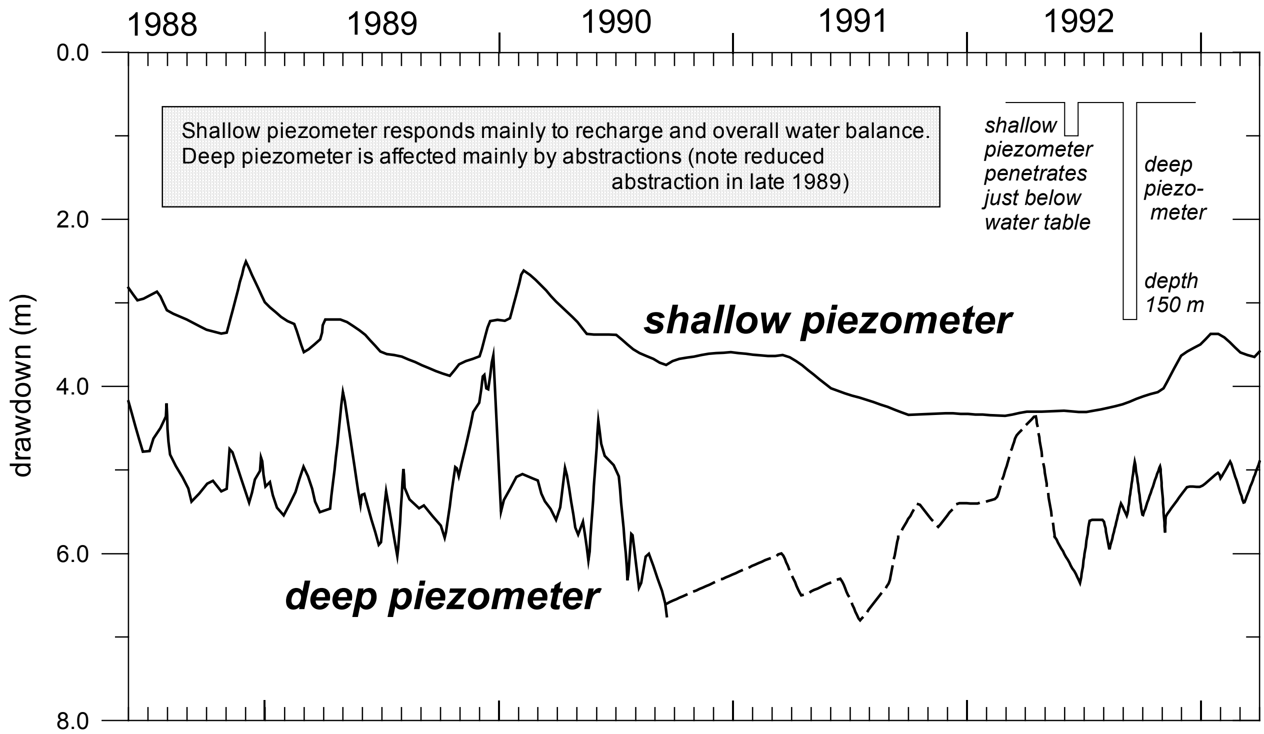


Figure 4.7.3. Differing responses in shallow and deep piezometers

c) *Long term trends are invaluable in refining groundwater models*: a regional groundwater model will only reproduce long term trends if the inflows, outflows and aquifer parameters (especially the specific yield) are realistic.

d) *Significant abstraction may induce further actual recharge*: significant exploitation of an aquifer may induce more of the potential recharge to enter the aquifer system; it may also cause streams to dry up. This 'stressing' of the aquifer is of great value in understanding and quantifying the aquifer response.

4.7.4 References

Barker, J.A. and Herbert, R. 1982. Pumping tests in patchy aquifers. *Ground Water* **20**, 150-155.

Butler, J.J. 1988. Pumping tests in non-uniform aquifers – the radially symmetric case. *J. Hydrol.*. **101**, 15-30.

Butler, J.J. and Liu, W.Z. 1993. Pumping tests in non-uniform aquifers – the radially asymmetric case. *Water. Res. Res.*. **29**, 259-269.

Butler, J.J. and McElwee, C.D. 1990. Variable rate pumping tests for radially symmetric non-uniform aquifers. *Water. Res. Res.*. **26**, 291-306.

Kruseman, G.P. and de Ridder, N.A. 1990. *Analysis and evaluation of pumping test data*. 2nd Ed. Publ. No. 47. International Institute for Land Reclamation and Improvement, Wageningen, The Netherlands. 377pp.

Rathod, K.S and Rushton, K.R. 1984. Numerical Method of Pumping Test Analysis Using Microcomputers, *Ground Water*, Vol.22, No.5, 602-608.

Rathod, K.S. & Rushton, K.R. 1991: Interpretation of pumping from a two-zone layered aquifer using a numerical model. *Ground Water*, **29**; 499-509.

Rushton, K. R. and Howard, K. W. F. 1982 The unreliability of open observation boreholes in unconfined aquifer pumping tests. *Ground Water*, **20**, p. 546-550.

Rushton, K.R., 1984. Assessing Aquifer Exploitation Using Observation Boreholes, *Jnl Inst Water and Env. Man.*, **8**, 156-164.

5.1 Calculation of Preliminary Water Balances

5.1.1 Purpose of Water Balances

Water balances are required to check the identification and estimation of the inflow and outflow components. Flow balances covering different time periods and different areas provide insights into short term and long term aquifer responses and the flow processes in different parts of the aquifer system. Preliminary water balances should be calculated during the development of the conceptual model. Failure to explain any significant lack of balance may indicate that there is insufficient reliable input data to justify proceeding with numerical modelling. Water balances are also a valuable output from numerical modelling in providing an understanding of how the aquifer responds. Examples of water balances for the Nottinghamshire Sherwood Sandstone aquifer are shown in Figure 5.1.1.

5.1.2 Preparing Water Balances

Types of water balance

The aquifer system should be considered in the context of the total surface water catchment; this is especially important where runoff from less permeable parts of the surface water catchment can be a source of runoff-recharge. It is necessary to perform water balances for both the *total catchment* and the *groundwater* systems. The latter includes all strata below the water table where saturated conditions apply.

A more thorough test of the adequacy of water balances can usually be gained using *sub-areas*. These smaller areas may be resource assessment units or surface water sub-catchments, and they may be defined for hydrogeological reasons or might be the area upstream of a continuous flow gauging structure. In devising water balances for sub-areas, additional uncertainties may arise due to cross boundary flows.

Components of water balances

For a *groundwater* balance the components include the recharge (including runoff recharge and urban recharge), vertical leakage through less permeable overlying strata, inflows to or from surface water features, lateral inflows/outflows from adjoining aquifers, abstraction and changes in storage. All of these quantities are based on estimates apart from the abstractions which may be known accurately.

Total catchment water balances contain further components, namely precipitation, evaporation and evapo-transpiration, surface water outflows, groundwater inflows/outflows across the surface water catchment divides, water mains and sewer leakage, outputs of water treatment works, bulk transfers of water, and changes in groundwater and soil storage. In assessing changes in groundwater storage resulting from changes in the water table elevation, the estimate should be based on groundwater head readings from shallow piezometers, not deep piezometers or deep observation wells which are often strongly affected by pumping.

Time periods for water balances

The choice of suitable time periods is essential if the water balances are to test whether there is an adequate understanding of the surface water and aquifer responses. *Sandstone aquifers* are typically slow response systems; water balances for summer/autumn and for winter/spring for an average year, a dry year and a wet year should all be examined. A long term water balance over one or two decades will provide information about long term changes due to the increase or decrease in abstraction. *Chalk and Limestone* catchments show a more rapid response; the aquifer system may refill every two or three years. Water balances for individual winter months and summer months should be examined with particular emphasis on very wet years and drought years. Water into or out of aquifer storage is likely to be an important component of these balances.

5.1.3 Expected Reliability of Preliminary Water Balances

Estimates must be made of *all* the components of the water balances, as illustrated in Figure 5.1.2 which illustrates the water balance developed for the Itchen study area. It is unlikely that the sum of the components of a preliminary water balance will be zero. The temptation to uncritically ascribe the discrepancy in the water balance to a change in storage or cross-boundary flows should be avoided. The uncertainty in each component of the water balance should be estimated.

Sensitivity analyses should be carried out on water balances to identify which, if any, of the components requires further examination leading to improved estimates. If the out-of-balance is more than 20% of the sum of the inflows, this suggests either that the flow components are not known to a sufficient accuracy or perhaps that an important component has been omitted. Without acceptable flow balances, it is not appropriate to commence numerical modelling.

5.1.4 References

The following papers illustrate how water balances are important in developing an understanding of aquifer behaviour.

Rushton, K.R., Kawecki, M.W. & Brassington, F.C. 1988: Groundwater model of conditions in the Liverpool Sandstone Aquifer. *J. Inst. Wat. & Env. Man.,* **2**; 67-84.

Rushton, K.R. and Fawthrop, N.P. 1991. Groundwater Support Of Stream Flows In Cambridge Area, UK. *In Hydrological Basis of Ecologically Sound Management of Soil and Groundwater* IAHS Publication No. 202, 367-376.

Rushton, K.R., Owen, M. and Tomlinson, L.M. 1992. The water resources of the Great Oolite aquifer in the Thames Basin. *Journal of Hydrology,* **132**: 225-248.

Rushton, K.R., Fletcher, S.W. and Bishop, T.J. 1995. Surface water and groundwater components, BHS 5th National Hydrology Symposium, Edinburgh, 2.17-2.24.

Figure 5.1.1. Flow balances for the Nottingham Sandstone aquifer

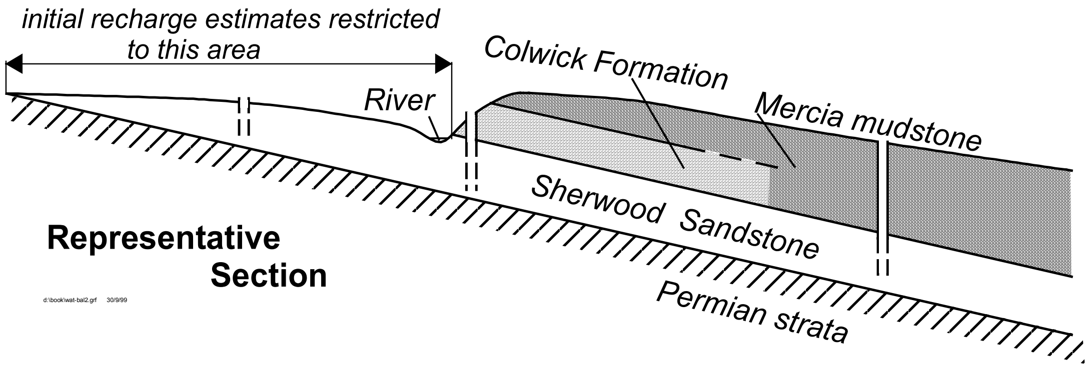


Figure 5.1.1A. Long term balance

An initial water balance included inflows due to precipitation recharge and water from storage (falling water tables) with outflows due to abstraction and flow to rivers; the inflows were about 70 Ml/d less than the outflows. Careful re-examination of field information suggested additional inflows due to recharge from the Colwick formation and from urban areas plus vertical leakage through the Mercia Mudstones and Colwick Formation; there is a small loss across boundaries. The final water balance, derived from a refined model, is shown in the second line of the following table.

Original and Final Water Balances: all quantities Ml/d for Water Years 1974-92

	Recharge			Vertical leakage	Abstraction	Bound. flow	Storage		River flow	Lack of balance
	Precip.	Colwick	Urban							
Initial	230	-	-	-	-285	-	+25	-	-40	+70
Final	232.3	22.9	9.3	40.8	-284.9-4.5	+25.7		-1.6	0	

Figure 5.1.1B. Annual Balances

The following annual balances represent components estimated from physical information (recharge and abstraction) and other components derived from a groundwater model (vertical leakage, change in storage and river flow); river flow is also drawn in the lower diagram to an increased scale. Note that in years of high recharge, water is taken into storage (shaded areas above origin) but in years of low rainfall water is taken into storage to meet the demands of abstraction. Flow from aquifer to river is represented in the lower diagram as being negative since it is a loss from the aquifer; there is a steady fall in the flow from aquifer to river. In the last year included in the diagram, there is a net flow from river to aquifer.

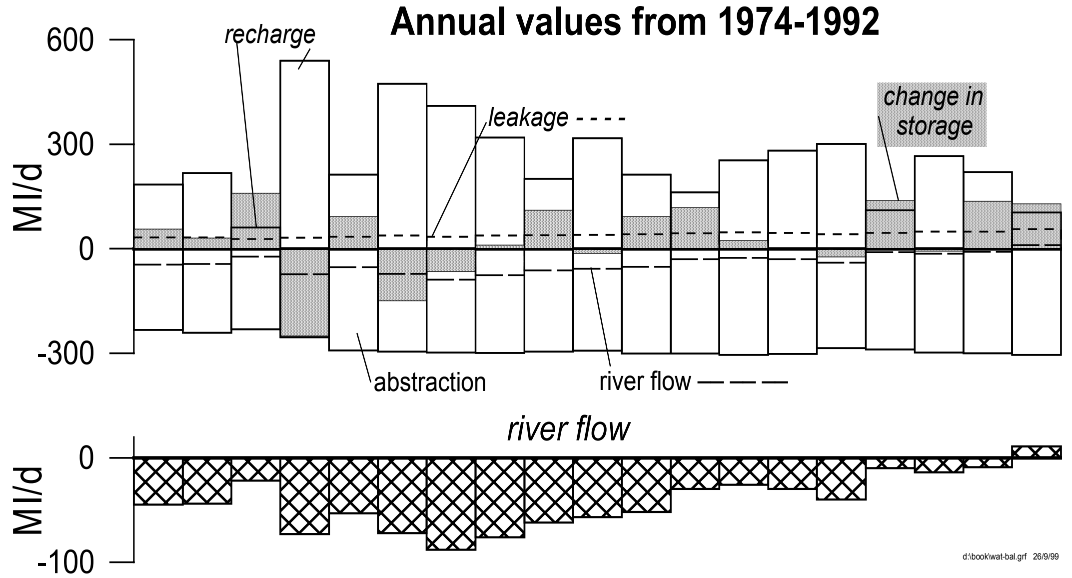
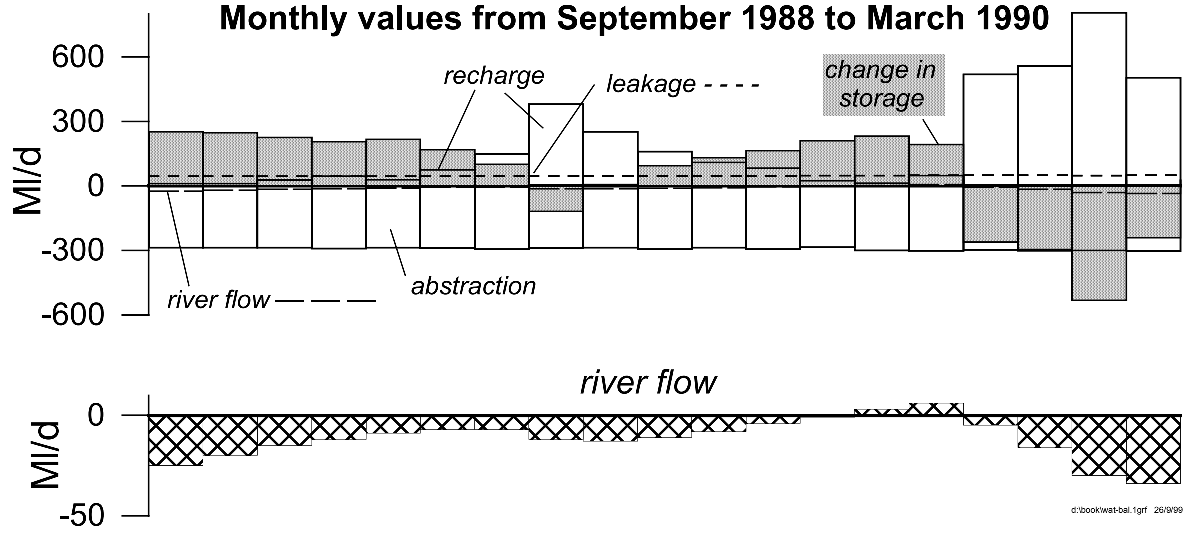


Figure 5.1.1C. Monthly Balance

The period selected to illustrate monthly water balances refers to the winter of 1988-89 when there was a low recharge and the winter of 1989-90 when the recharge was higher. During the first fifteen months, there was only one month when the recharge was sufficiently high not to require water being drawn from storage. However, during the last four months the recharge was high with the result that significant quantities of water were taken into storage. During the first fifteen months, the flow from aquifer to river showed a general decline. However, during the last four months with the high recharge, there was a reversal in this trend although the river flows are slow to respond with the aquifer to river flows increasing for all four months whereas the recharge reached its peak value in the third month.



5.2 The place of analytical solutions

Analytical solutions provide an exact solution to a partial differential equation given the initial condition and a set of boundary conditions. They refer to specific problems which can be analysed by mathematical techniques to give a solution in terms of mathematical equations; these mathematical equations often involve infinite series or Bessel Functions but the results can usually be tabulated or presented graphically. Analytical solutions are based on conceptual models but it is often necessary to idealise the physical problem to match the restrictions of obtaining an exact solution. Analytical solutions can sometimes be used to obtain very approximate solutions to practical problems. They can also be used to check the validity of an approximate method of solution, such as finite difference or finite element.

A wide range of analytical solutions to groundwater flow problems are available including:

- horizontal one-dimensional flow through an aquifer (steady state and time variant),
- Dupuit theory for unconfined flow through a dam,
- steady state and time-variant radial flow towards a pumped well in a confined aquifer (Theim and Theis) with many further developments of these theories,
- use of Ghyben-Hertzberg techniques for fresh water-salt water interface problems,
- dispersion in Cartesian and radial flow.
- Jenkins' analytical solution for impact of groundwater abstraction on river flows (see IGARF software, Environment Agency, 1999).

5.2.1 Positive use of analytical solutions

1. Pumping test analysis using analytical solutions can be a successful methodology for first estimates of aquifer parameters provided that the analytical solution does represent the important features of the physical situation.
2. More complex simulations representing varying abstraction rates or well storage can be included using the addition of a series of solutions (this is called a Kernal Function approach, see for example Rushton & Singh (1987)).
3. One-dimensional flow approximations, which include time-variant recharge, may provide an initial representation for the major flows in regional groundwater flow problems.
4. Analytical solutions can be incorporated within numerical solutions to achieve a better representation of features such as pumped boreholes (Rushton and Senarath 1983)
5. Simple contaminant transport situations can be explored using analytical solutions for one-dimensional Cartesian or radial flow (Al-Niami and Rushton, 1977).

5.2.2 Dangers in the use of analytical solutions

Methods of analysing the effect of pumping are used to illustrate the limitations of analytical solutions.

1. If the physical situation is different from the assumptions of the analytical solution, there is a risk that the results of the analysis will be seriously flawed. This occurs frequently in the use of the Theis theory for analysing pumping tests. For example the aquifer is rarely undisturbed before, during and after the test, and no aquifers have infinite extent; yet these are fundamental assumptions of the Theis theory.
2. Leaky aquifer theory is often used when the physical conditions are inconsistent with the assumption of an overlying aquifer above the aquitard, which can supply an infinite volume of water without any decline in the overlying water table.
3. Analytical methods of estimating stream depletion due to pumping fail to consider many physical realities, such as recharge or the possibility that the stream will become perched (Rushton 1999).

5.2.3 The value of analytical solutions in conceptual modelling

In conclusion, analytical solutions are very useful for initial calculations when developing a conceptual model. However, the assumptions inherent in analytical solutions often mean that they fail to represent adequately the practical field situation. Whenever an analytical solution is used, a check list should be prepared comparing the assumptions of the analytical solution and the actual field conditions.

5.2.4 References

Al-Niami and Rushton, K.R. 1977. Analysis of flow against dispersion in porous media. *J. Hydrology*, **33**, 87-97.

Aravin, V.I. & Numerov, S.N. 1965. *Theory of fluid flow in undeformable porous media*, Israel Program for Scientific Translation, Jerusalem, 511 pp.

Bear, J. 1979. *Hydraulics of Groundwater, McGraw Hill*, New York, 567 pp.

Environment Agency. 2000. *Impact of groundwater abstractions on river flows.* National Groundwater and Contaminated Land Centre Report, NC/06/28.

Freeze, R.A. and Black, W. 1983. *Physical Hydrogeology*, Benchmark Papers in Geology vol.72. Hutchinson Ross Publishing Co. 431 pp.

Harr, M.E. 1962. *Groundwater and Seepage*. McGraw-Hill; 315 pp.

Hunt, B. 1983. *Mathematical analysis of groundwater resources*. Butterworths, 271 pp.

Kruseman, G. P. and de Ridder, N. A. 1990. *Analysis and evaluation of pumping test data*, 2nd Ed., International Institute for Land Reclamation and Improvement, Wageningen, Pub. No. 47, 377 pp.

Polubarinova-Kochina, P.Y. 1962. *Theory of Groundwater Movement*. Princeton University Press, New Jersey. 613 pp.

Rushton, K.R. 1999. discussion on Hunt, B. Unsteady stream depletion from groundwater pumping. *Ground Water*. **37**, 805.

Rushton K.R. and Redshaw S. C. *Seepage and Groundwater Flow*, Wiley, Chichester, 1979, 339 pp.

Rushton, K.R. and Senarath, D.C.H. 1983. A mathematical model study of an aquifer with significant dewatering, *Journal of Hydrology*, **62**, 143-158.

Rushton, K.R. & Singh, V.S. 1987. Pumping tests in large diameter wells with a seepage face by Kernal function techniques. *Ground Water*, **25**, 81-90).

5.3 Exploratory numerical modelling

The Environment Agency has begun to separate its modelling projects into stages, such as the initial conceptual modelling and subsequent numerical modelling stages. This practice is founded on the fact that a good conceptual model is a pre-requisite for an adequate numerical model.

In reality the entire modelling process is iterative. The numerical model is a tool for testing the conceptual model, as well as being a tool for predictive simulation. Therefore the conceptual modelling stage is likely to include some numerical modelling, and the numerical modelling stage will almost always result in modifications to the conceptual model. It should also be recognised that the aims and objectives for the numerical modelling tool will vary at different stages of the project. Exploratory modelling, taking place at the earlier stages of a project, is the subject of this section.

Exploratory numerical models may be useful when new, complex or unusual systems are encountered. They provide a level of detail not obtained from the water balance alone or from using analytical solutions. They allow the modeller to explore ideas and methods to adequately represent the hydraulic processes associated with groundwater and surface water flows in a catchment. Viewed between water balances/analytical solutions and a full numerical model, exploratory modelling offers a useful intermediate step in quantitative testing of conceptual models, in terms of both time and detail. However they need to be focussed on investigating particular issues, e.g. the role of VKD. Otherwise, an undisciplined approach can waste a lot of time.

5.3.1 Uses of exploratory modelling

Investigating the conceptual model

An advantage of an exploratory model developed at an early stage of the project is that it allows investigation at different spatial and temporal resolution to that required for the final model. Typical aims of the exploratory modelling might be to:

- test the hypotheses embodied in the conceptual model, e.g. variation in baseflow is due to VKD;
- relate the consequences of the conceptual model to observed behaviour that is not fully understood, e.g. should the river Mersey be represented by a fixed head?;
- investigate the sensitivity of the model to different sources of uncertainty;
- assess the likely limitations of any numerical model which is built;
- investigate possible numerical representations of the boundaries of the model area;
- investigate interaction between groundwater and surface water;
- investigate interactions between different groundwater bodies in multi-layered aquifer systems (including the number of layers simulated explicitly);
- investigate the incorporation of depth-dependent distributions of hydraulic conductivity and/or storage (VKD/VSD);
- assess recharge to the groundwater system simulated externally to represent unsaturated zone processes;
- assess the effects of the geometry of the boundaries (including base of aquifer).

In exploratory modelling, the model used should be simple so that exploring plausible alternative conceptual models is not hampered by excessively detailed data input and preparation for the specifications of the exploratory model. In general, the sensitivity analysis should be more fundamental than the parameter sensitivity analysis carried out on the full-scale numerical model. It might include alternative model set-ups or representations of processes. However, the model should contain all the essential elements of the water balance in the selected model region.

Refining the design of the numerical model

Exploratory modelling can be used, for example, to investigate the space and time discretisation to be adopted for the full numerical model. The motivation here is to keep the numerical model as simple as possible (following the principle of parsimony embodied in the adage "Keep It Simple Stupid"). Detail and complexity should be justified through physical evidence and required to simulate aspects of the observed behaviour relevant to the aims of the model. Often inclusion of realistic boundaries will introduce the essential features of a flow field: more detail is not always needed. Aspects of model design that might be investigated include:

- required spatial resolution of the grid, horizontally (including areas to refine) and vertically (i.e. number of layers);
- required spatial resolution of parameters, such as whether detailed heterogeneous distributions provide benefits over a broad zonation or a homogeneous (single parameter) description;
- required temporal resolution of, for example, recharge or abstraction.

Refining the model later during a second or third pass, rather than attempting to build a highly complex model at the outset, usually leads to a more effective final model. This is because the model's sensitivity to uncertainty in the conceptual model, as well as the input data, is better understood. It is always easier to understand what is influencing the model's behaviour, and to judge whether that behaviour is reasonable, if things are kept simple and only changed one step at a time.

5.3.2 Options for exploratory modelling

Lumped parameter and analytical modelling

Lumped parameter and analytical modelling can provide a quick and easy way to explore the processes and parameters which may need to be incorporated into any distributed numerical model in order achieve a credible simulation. Such models can usually be constructed using a spreadsheet based on the conceptual understanding and a simplified view of the aquifer geometry, hydraulic parameter distributions, and interaction with surface water features. These models allow alternative concepts and processes to be explored rapidly and can help to determine the simplest representation which may be able to produce an adequate outcome knowing the aim of the study. They can therefore be an important tool in developing and refining conceptual understanding. Although lumped parameter and analytical models may often produce encouraging 'fits' to observed data at an early stage, it can be difficult to transfer the understanding to the distributed model.

Examples of the use of such models include:

- Terry Keating's lumped parameter model of the Candover Chalk (Keating 1982) which explored the influence of variations in transmissivity and specific yield with depth;
- Use of the aquifer response function, partitioning of recharge to different transmissivity and specific yield zones, and variation in soil moisture bypass recharge to explore mechanisms for maintaining low drought flows in Anglian rivers and in the River Itchen;
- Exploration of alternative conceptual models of unsaturated and saturated zone storage and flow processes as part of the River Gade study.

First pass distributed modelling

First pass models are often used when new or unusual systems are encountered and the modeller is trying out some ideas. These might include simple cross-sectional models or models of catchments or sub-units which are small relative to the total extent of a regional model. However, they are complex because they require developing an adequate representation of the hydraulic processes associated with groundwater and surface water flows in a catchment.

It is often useful to carry out some sensitivity runs and some predictive runs with an initial version of the model which includes the crucial processes identified in the conceptual model. By doing this much can be learned about:

- the hypotheses embodied in our conceptual model;
- the aspects of the observed behaviour that we don't understand;
- the likely limitations of any numerical model which we build;
- the data requirements for historical and predictive simulations;
- the possible sensitivity of the model to different sources of uncertainty.

No attempt should be made to refine or add additional complexity to the model at this stage; only ideas are being tested. However, broad-brush sensitivity analysis (parameters, boundary conditions and other aspects of the conceptual model) is valuable.

A good example of such a model is the two layer 'proto-model' of the Alre catchment exploring the need and the practicality of incorporating layering and VKD in order to reproduce flow accretion and the influence of artesian borehole flows from a transmissive fissure zone (Entec).

5.3.3 References

Keating, T. 1982. A Lumped Parameter Model of a Chalk Aquifer-Stream System in Hampshire, United Kingdom. *Groundwater* **20(4)**: 430-436

5.4 Review of options to achieve study objectives

At the end of the conceptual modelling phase, it is vital that a fundamental review of the options to achieve the study objectives is undertaken. This review should concentrate on the following two interlinked questions.

1. **Is the conceptual model adequate in relation to the objectives of the study?**

Inadequate information might mean that fundamental uncertainty exists in relation to key flow mechanisms, with one or more interpretations of the data supporting alternative conceptual models. The plausibility of these alternative conceptual models will need to be tested using appropriate modelling tools or by further data collection.

The conceptual model might not be adequate to support the use of the appropriate tool. For example, to progress to fully distributed numerical modelling a detailed conceptual model is required.

2. **What degree of sophistication is required in any further investigations and assessments to achieve the objectives of the study; and in particular what is an appropriate tool?**

A range of tools, of varying sophistication, are available to test the concptual model and to further any investigation. For example:

- in rare cases the questions framing the objectives of the study will be answered by the *conceptual model* alone. For instance, analysis of groundwater hydrographs, etc, might prove beyond reasonable doubt that a groundwater-fed wetland is effectively hydraulically isolated from an underlying aquifer, and that it is therefore not influenced by groundwater abstractions from the aquifer;

- general questions about the sustainability of groundwater abstractions from a catchment might be answered by reference to *water balance calculations* within the conceptual model;

- the conceptual might prove that the situation or issue in question conforms sufficiently to the defining conditions of an existing *analytical solution*, and that careful application of the analytical solution will yield sufficient information to meet study objectives. Software is also available which combines the results of analytical solutions in space using the principle of super-position;

- exploratory or generic (e.g. lumped parameter, 2D vertical or horizontal) modelling might yield sufficient information to meet study objectives;

- three-dimensional, time-variant, fully distributed modelling represents the most sophisticated tool for progression of the study.

If it is decided that the objectives cannot be met without further data collection, some of the above tools may be used to assess which data has most influence on the results (sensitivity analysis). This will help indicate where data collection would be most effectively focussed.

The future course of the study should be decided in the light of the answers to these questions. It should also consider:

- whether the deadlines for answers to key questions are likely to be met;
- wider stakeholder opinions;
- budget issues.

The decision on how the study should be progressed to achieve the objectives is clearly critical and should be informed, considered and objective. For this reason it is recommended that a formal break in project activities is observed at the end of the conceptual modelling phase, during which the various options can be considered in full. It is also likely that with the time to 'step back', those involved will have new ideas in relation to the conceptual model. Time taken at this stage to arrive at a reasoned and mutually agreed decision can save significant time and resources in the future. With such multi-factored decisions, there is a need for imaginative but pragmatic solutions.

6.1 Code and GUI selection

6.1.1 Code selection

The model code should be selected provisionally at the end of the scoping study and definitely by the end of the conceptual modelling. Table 6.1.1 gives details of codes used by the Agency for groundwater modelling whilst Table 6.1.2 lists the Agency models produced since 1974 and the codes used for each.

Two fundamental areas need to be considered in selecting a model code; *is it appropriate?, is it useable?*

Is it appropriate?

During the scoping study the current ideas about how the aquifer is behaving will be gathered and throughout the conceptual modelling these hypotheses will be challenged and developed. We need to consider the modelling objectives (the questions which the model is being asked to address) and the key flow mechanisms identified during conceptual modelling and ask:

1. Can the code represent the key flow mechanisms? For example, a two dimensional single layer model will be inappropriate if vertical groundwater head gradients are known to be significant.
2. What simplifications are required to represent these key mechanisms? Two examples:
    a. abstraction wells when represented as flow out of the whole cell do not allow for the resistance caused by the converging radial flow
    b. leakage through the drift has been represented using head dependent leakage from an upper layer (see Appendix C, *Fylde model*). However, this assumes that a vertical gradient is immediately developed over the full thickness of the drift layer. This is not correct and results in the drift supplying too much water.
3. Has the code been tested for similar problems to ours?
4. Can the code perform the kind of predictive runs that the modelling objectives will require?
5. Can the model be readily updated as our conceptual understanding grows?

Is it useable?

Since a regional groundwater model represents a significant capital investment and is likely to be used and updated for many years, it will probably be used by several in-house staff in addition to the people who develop it. Therefore, we should also ask:

1. How much effort is required to become familiar with the code?
2. Do we have access to the source code so that the way in which the calculations are performed can be investigated?
3. How good is the user manual? (Does it adequately explain how the code works? Are the input instructions correct? Are there examples data sets?)
4. How good is the user support (speed of response and technical content)?

5. Is there a good and well-tested user interface?
6. How good is the quality control of the code and its user interface?
7. Does the user interface allow digital data to be imported or exported in variety of common formats?

Table 6.1.1. Examples of codes for modelling groundwater flow

Code	Approximation method	GUI	Agency Users	Remarks
AQUA	Finite Element	✓	No current users	
MODFLOW (Modular finite difference Flow Model)	Finite Difference	✓	Midlands North East Thames	Public domain code developed by the USGS (McDonald M.G. & Harbaugh, AW, 1998)
ICMM (Integrated Catchment Management Model)	Integrated Finite Difference	✓	Southern North West Thames	Proprietary code developed by (Mott MacDonald)
SLAY (Single LAYer)	Finite Difference		South West Southern	Developed at Birmingham University
MIKE-SHE	Finite Difference	✓	Thames South West	Developed by the Danish Hydraulic Institute
SHE-TRAN	Finite Difference		No current users	Under development at Newcastle University

Table 6.1.2. Existing agency models

REGION	MODEL	AQUIFER	MODEL CODE	DATE COMPLETED
SOUTHERN	Darent/Cray	L.Greensand & Chalk	ICMM	1993
	Upper Stour	L.Greensand	ICMM	1994
	East Kent	Chalk	BU	1991
	Chichester	Chalk	SLAY	1994
	Meon/Hamble	Chalk	ICMM	1993
	Wallop Brook	Chalk	ICMM	1991
	Bourne Rivulet	Chalk	ICMM	1991
SOUTH-WEST	Otter Valley	Triassic sandstone	Finite Difference	1989
	River Allen	Chalk	ICMM	1992
	River Piddle	Chalk	SLAY	1995
	Hampshire-Avon	Chalk	SLAY	1995
	Malmesbury-Avon	Jurassic limestone	MIKE-SHE	1994
THAMES	London Basin A3	Chalk	Finite Element	1986
	London Basin	Chalk	ICMM	2000
	Kennet Valley	Chalk	Finite Difference	1974
	SW Chilterns	Chalk	MODFLOW	1996
	Cotswolds	Jurassic limestone	MIKE-SHE	1997
MIDLANDS	West Shropshire	Triassic sandstone	MODFLOW	1998
	W Midlands Trias	Triassic sandstone	MODFLOW	2000
	Notts-Doncaster	Triassic sandstone	BU	1993
	Birmingham	Triassic sandstone	MODFLOW	
NORTH EAST	Selby	Triassic sandstone	MODFLOW	1997
	Yorkshire Chalk	Chalk	Modified BU	1995
	Scarborough	Corallian limestone	MODFLOW	1995

Table 6.1.2. Cont.

REGION	MODEL	AQUIFER	MODEL CODE	DATE COMPLETED
NORTH WEST	North Merseyside	Triassic sandstone	BU	1983
	Lower Mersey	Triassic sandstone	BU	1981
	Fylde	Triassic sandstone	ICMM	1997
ANGLIAN	Lincolnshire Chalk	Chalk	BU	1988
	Spilsby Sandstone	Spilsby Sandstone	ICMM	1989
	Central Limestone	Lincolnshire Limestone	BU	1994
	Southern Limestone	Lincolnshire Limestone	BU	1993
	Gipping	Chalk	BU	1984
	Lark	Chalk	BU	1991
	Lodes/Granta	Chalk	BU	1988
	Rhee/Cam	Chalk	Finite Difference	1975
	Pant	Chalk	BU	1981
EA WALES	Yazor Gravels	River gravel deposits	MODFLOW	1997

Notes:
1. BU - Finite Difference code developed at Birmingham University (Rushton & Redshaw, 1979)

6.1.2 Graphical user interface (GUI) selection

A number of the codes noted above have a graphical user interface (GUI) which aids in the creation of input files for the model code to read and for visualising the model output. The AQUA, ICMM and MIKE-SHE codes are supplied with their own proprietary GUIs while for MODFLOW there are a number of different interfaces available, including Processing MODFLOW, Visual MODFLOW and Groundwater Vistas (GV).

Experience shows that although user interfaces are helpful in creating the input files containing the spatial distributions of aquifer geometry and hydraulic parameters, they have limitations, which must be borne in mind. These include a lack of flexibility in creating time variant data (e.g. recharge and abstractions) for which spreadsheets or utilities written in FORTRAN or Visual Basic are often more powerful. In addition, it is not uncommon for a model code to be able to perform functions which the interface does not support. Finally, the rapid development of these user interfaces has too frequently been at the expense of rigorous quality control. Consequently, the necessity for a model user to be familiar with and constantly check the ASCII data input and output files remains as important as ever.

MODFLOW GUIs are generally supplied with a compiled (executable) version of MODFLOW-96 which may contain minor enhancements (e.g. MODFLOWwin32 with Groundwater Vistas GUI)

6.1.3 Best Interim Solution until 2001 - MODFLOW and Groundwater Vistas

In 1998 the Agency selected MODFLOW (model code) and the Groundwater Vistas (GUI) as its preferred groundwater flow modelling software for internal use.

There is no restriction on the codes that an external consultant can use for a modelling project provided they are suitable for the job. However, in practice, the Agency must aim to maintain and update models it has produced, and this will be easier if staff become familiar with only one or two codes and their associated input and output files. There will therefore need to be very good reasons to use an unfamiliar alternative in preference to Best Interim Solution codes. The overheads resulting from the need to familiarise staff with new code will be need to be accounted for in the tendering process.

The modular finite-difference groundwater flow model (MODFLOW) was developed by the U.S. Geological Survey (USGS) and first released in 1988 (McDonald & Harbaugh, 1988). It has evolved continually and is now the most widely used program in the world for representing groundwater flow. It reads ASCII files containing the input data (recharge, abstraction, aquifer parameters, boundary conditions etc.) and performs calculations in order to output heads and flows.

MODFLOW's success as a modelling tool owes much to its original design. It was written in the early 1980s as a modular code to replace the 500 or so pieces of groundwater modelling software which were scattered over the USGS's mainframes. It had to be accurate, easy to understand, easy to enhance and modify and computationally efficient. MODFLOW is well-documented, logically programmed but has never pretended to do everything. As people have wanted to simulate processes of which MODFLOW was incapable, they have written their own modifications.

MODFLOW is continuously under development. Details of the latest version can be downloaded from http://water.usgs.gov/nrp/gwsoftware/modflow.html.

A number of proprietary enhancements of the basic public domain MODFLOW code are available. These are briefly summarised on Table 6.1.3. These codes have been written to make significant changes to the original public domain code. In contrast to the public domain versions, the source code for these proprietary codes is not publicly available.

Groundwater Vistas has been chosen as the Agency's Best Interim Solution GUI for MODFLOW.

6.1.4 The future

The Agency needs to look ahead and consider what functionality it requires from a groundwater modelling code and what approach to follow.

The Agency will support enhancements to the MODFLOW code to take into account mechanisms specific to British aquifers. Examples of this are the variation in hydraulic conductivity and storage coefficient (VKD and VSD) with saturated depth in chalk and limestone aquifers. The initial stage of implementing a package to simulate VKD was completed in early 2000 (Environment Agency, 1999).

The Agency will also monitor research developments on new codes with a view to supporting them if appropriate, on the condition that the code is public domain (see Section 4.4.2 of the Framework for Groundwater Modelling, Environment Agency R&D Technical Report W214).

Table 6.1.3. Proprietary MODFLOW-based codes

Name	GUI Support	Remarks
MODFLOW-VKD (Environment Agency)	None at present (early 2002)[1]	Modified code to include implementation of VKD mechanism to represent the reduction in K with depth in the Chalk aquifer (Environment Agency, 1999).
MODFLOW-SURFACT	VMS interface Groundwater Vistas	Implementation of enhanced transport and flow modules in MODFLOW • Handling of complete desaturation & resaturation of grid blocks • Automatic & correct apportioning of the total flow rate of a multi-layer well to the well nodes • New PCG matrix solution option (PCG4) • Handling of seepage schemes with automatic generation and control of time steps. • Axi-symmetric flow simulation option • Etc.
Stochastic MODFLOW	Groundwater Vistas	Implementation of stochastic simulation using Monte Carlo technique
MODFLOWT	Groundwater Vistas	An Enhanced MODFLOW code designed to simulate 3D advective-dispersive transport. • New packages introduced for simulating transport • Enhancements to existing modules • New solvers • Compatible with previous versions of MODFLOW

Note:
1. GUIs can create input files for MODFLOW-96 and MODFLOW-VKD, but they made need editing prior to running MODFLOW if features are implemented which are not supported by the interface.

6.1.5 References

Environment Agency, 1999**.** *Representation of the variation of hydraulic conductivity with saturated thickness in MODFLOW. Stages I & II. Code changes and testing against Birmingham University code.* National Groundwater and Contaminated Land Centre Project NC/99/67.

McDonald, M.G. & Harbaugh, A.W., 1988. *A modular three-dimensional finite difference groundwater flow model. U.S. Geological Survey, Techniques of Water Resources Investigations.* Book 6, Chapter A1.

6.2 Convergence criteria, water balance errors and solvers

6.2.1 Introduction

In a numerical model, the groundwater flow equations are formulated in terms of the unknown variables, which are usually the heads in the model grid cells. Finite difference formulations, such as that used in MODFLOW, are directly based on a volumetric water balance of flows coming into or going out of each grid cell. As the head in each cell depends on the conditions in the neighbouring cells, all heads must be calculated simultaneously, therefore the groundwater flow equations are assembled as a matrix equation representing the whole system. This section covers issues related to achieving an accurate solution to the groundwater flow equations.

6.2.2 Direct solution vs. iterative solution of the groundwater flow equations

If the system is linear (e.g. for confined flow), it is possible to solve the groundwater flow equations directly in a single step. However, such methods for direct solution of equations are not particularly efficient. There are also situations where the system is nonlinear. For example, for unconfined flows the saturated thickness also depends on the head, so that the flow rate is expressed as a quadratic function of the head. A more general approach is therefore to make successive approximations (i.e. to iterate), until the result is deemed to have converged to the solution. Criteria for convergence include the following:

- The maximum change in head from one iteration to the next.
- The maximum cell water balance error, which is formed by substituting the calculated heads back into the volumetric water balance equations, i.e. a measure of how well the heads satisfy the original equations on a cell by cell basis.

Iterative solvers may offer either one of these convergence criteria, or both in combination. Whilst the maximum head change is a simple indicator, used alone it does not guarantee that the head distribution has reached an acceptable solution to the groundwater flow equations. Thus apparent convergence does necessarily not mean that acceptable accuracy in the volumetric water balance has been achieved.

6.2.3 Solvers: their characteristics and parameters

There are many different numerical solvers available. Each has its own approach to choosing the next approximation to the solution and, consequently, level of smoothness, stability and efficiency in the approach to the converged solution. Common methods are Slice-Successive-Over-Relaxation (SSOR), the Strongly Implicit Procedure (SIP) and Pre-conditioned Conjugate Gradient (PCG) method. SIP and SSOR require fewer input parameters, and therefore appear simpler to use. However, both can be slow to converge and difficult to optimise.

All of the above are available in MODFLOW. However, as implemented in MODFLOW, SIP and SSOR only use the maximum head change in the cell as a convergence criterion, therefore when using either of these methods it is vital that the volumetric water balance error is also checked. As the PCG solver is efficient and incorporates both the maximum head change and maximum volumetric flow error as convergence criteria, it should be the preferred solver for numerical models in MODFLOW. Detailed discussion of the individual methods and parameters is beyond the scope of this section.

Why models can fail to converge

A model may experience difficulty in converging to a solution due to a number of reasons:

- The conceptual model may not be complete; the model may require a flow mechanism to balance the water budget. Boundary conditions such as constant head, general head, river, drain and stream cells perform the role of allowing water into or out of the system dependent on head distribution. Their contribution to the water balance is not specified prior to solving the flow equations, but determined by the final head distribution.
- A convergence criterion (e.g. head change or water balance error) may too stringent. In particular, the criterion should be achievable within the bounds of computer precision.
- The chosen solver may be too inefficient, or the maximum number of iterations too low. Where possible, the parameters of the solver should be adjusted to improve convergence, or another solver used.
- The time steps in time-variant models may be too large. The length of the time steps should then be decreased. It may also help to make the time steps smaller at the start of the stress period. (In MODFLOW this is done by making the time step multiplier greater than 1, so that a value of 1.1 means that the time step is increased by 10% each step.)

6.2.4 Water balances for the whole system

Whilst cell volumetric flow balances show the accuracy in solving the groundwater flow equations for each individual cell, summing up all flows leads to a water balance for the whole system. For transient models, release of water from storage counts as inflow, and water entering into storage appears as outflow. Ideally the volume entering the system should be equal to the volume leaving the system. However, as indicated above, this is rarely achievable in a numerical model. The water balance error is expressed in MODFLOW as the percentage discrepancy between the flow rates (dimensions L^3/T) into and out of the model. Konikow (1978) suggests that the error should be less than 0.1%. In his models, Rushton calculates water balance errors as volumetric flow rate per unit area (dimensions L/T) and recommends an maximum error of 0.01% of the average recharge to a cell.

The significance of the water balance

Apart from checking the convergence of the solution, the water balance should be used to compare the contributions to water budget from different flow mechanisms. Comparison with a preliminary water balance can highlight errors made in entering data, etc. The water balance can also show problems arising from the groundwater flow solution. For example, in MODFLOW when the water level drops below the base of a cell all abstractions from the cell are switched off. A reduction in the abstraction rate can be identified from the water balance, and appropriate action taken e.g. redistribution of the abstraction rate between the lower saturated layers.

What the water balance cannot achieve

The water balance cannot be used to identify contributions from flow components not yet included in the model – the solver attempts to balance the system provided to it. A model which has converged with a good water balance is therefore not necessarily a correct model, in terms of the physical processes included. It should also be noted that, as the water balance is only an indication of the success in solving the actual equations posed, it does not indicate grid convergence, i.e. that the same solution would be achieved on a finer grid. This must be verified by carrying out grid refinement and solving the refined flow equations.

Why a water balance can be or can appear to be poor

The following list gives some reasons why the water balance may not show the desired level of accuracy:

- The convergence criterion/criteria may need to be more stringent. The maximum head change and/or the maximum volumetric water balance error should be decreased.
- Not all components of the water balance may have been recorded and included in the water balance error calculation.
- Heterogeneity of spatial properties included in the model may lead to large water balance errors.
- Irregular grids may lead to poor water balances. It is often cited that, as a general rule, no grid cell should be more than one and a half times the size of its neighbours.
- Unconfined problems can be highly nonlinear; grid refinement is likely to improve convergence performance and water balance errors.

6.2.5 References

Konikow, L.F, 1998. Calibration of ground-water models. *In: Verification of Mathematical and Physical Models in Hydraulic Engineering*. American Society of Civil Engineers, N.Y. pp 87-93.

Rushton, K.R. and Redshaw, S.C., 1979. *Seepage and Groundwater Flow*. Wiley

6.2.6 Bibliography

Anderson, M.P., and Woessner, W.W. 1992. *Applied Groundwater Modeling: Simulation of Flow and Advective Transport*. New York, Academic Press Inc.

Osiensky, J.L., and Williams, R.E. 1997. *Potential inaccuracies in MODFLOW simulations involving the SIP and SSOR methods for matrix solutions*. Ground Water **35(2)**: 229-232.

6.5 Predictive Simulations

6.5.1 Objectives

The principal aim of a predictive simulation is to predict the response of groundwater flow to future events. What those future events may be will largely influence how the prediction simulations are performed and indeed how the model is constructed from the outset. Commonly this will examine the transient changes of groundwater flow in response to the variation of groundwater abstraction and recharge. The predictions should not involve changes to the parameterisation of the model because the physical characteristics of the aquifer are unlikely to change over the time-scales relevant to a water resources study. Indeed, changes made to a parameter to assess the sensitivity of the modelled results are part of the model development.

A groundwater model allows a large degree of flexibility in terms of how predictions are made. Comprehension of the results of a prediction run requires the examination of a large amount of model output, which is a limiting factor on the number of simulations performed. It is therefore very important to have clear objectives that target specific issues, e.g. a local issue such as return of baseflow to a stream or a regional issue such as sustainable yield of an aquifer. It is recommended that a staged approach be adopted for the predictive simulations, because the results of a single simulation may not necessarily have the desired outcome for a particular issue. The first prediction simulations of a predictive study should perhaps be treated as exploratory to gauge how the model responds to the changed stresses as a whole and at the features targeted with each issue.

6.5.2 Baseline Prediction Simulation

It is common practice to perform a Baseline Prediction Simulation (BPS) to aid the assessment of the results of each prediction simulation. The BPS is therefore used as a 'benchmark', and its use is advisable, particularly if more than two or three prediction runs are being performed. The specification of the BPS will depend on the objective of the study. The key inputs that will most likely be considered for a water resource study are abstraction, recharge and length of predictive time-series, all of which are discussed below.

Abstraction

Transient prediction simulations should always use as starting conditions the calculated head distribution of the last time-step of the historical simulation. It is important to recognise therefore that the predictive simulation will inherit the recent flow regime of the historical simulation. The simplest approach to a BPS is to attempt to maintain this recent flow regime throughout the predictive time-series by using an average of recent historic abstractions. In reality maintaining the recent flow regime may not be feasible or desirable, because:

- the historic simulation has not reached a dynamic equilibrium, i.e. there are long-term non-seasonal effects, such as long-term falling heads that indeed may be related to long-term historic over-abstraction;
- there may be licence agreements that are *already in place* that entail future changes to abstractions;
- there may be recent abstraction anomalies due to climatic extremes or operational difficulties at certain sources.

Purely in terms of managing water resources it is probably most desirable to have a BPS with abstraction that represents the expected pattern of abstraction given a future 'licence status quo' and static demand on current licences. This BPS would use a recent average of abstractions, but changes would be made to account for anomalous abstractions and licence changes that are *definitely* programmed to take place. Because such a BPS may involve large changes relative to recent historic abstractions, it may be necessary to quantify the transient effects that are purely related to these baseline abstraction changes.

Length of predictive time-series

The time-scales over which the prediction will be required to gauge the full effect of the predictive scenario (i.e. to reach a dynamic equilibrium) will depend mainly on the overall diffusivity of the aquifer and the magnitude of the perturbation (e.g. change in abstraction) from a natural point of discharge in the aquifer. However, in practice the length of the historic time-series against which the model was validated will determine the length of the predictive simulation. It has been suggested that the length of the predictive time-series should not exceed twice the length of the validation period (Anderson & Woessner 1992). In many cases the model will not reach a dynamic equilibrium at the end of the acceptable predictive time-series. This in itself is very valuable information.

Recharge

It is important that the seasonal variation and indeed annual variations in recharge are incorporated into the BPS. The simplest approach is to repeat the part of the historical recharge sequence that has annual and seasonal variation represented. If a longer time-series is required then this historic recharge sequence can be repeated several times, provided that the length does not greatly exceed the length of the validation period. The value of extending the recharge sequence in this manner is partly limited, because the natural variation of the recharge is not increased concomitantly.

Where the effects of climate change or a sequence of extreme climate conditions are being investigated, then it will be necessary to synthesise all or part of the recharge sequence. However, this may not be strictly appropriate for the BPR, because the application of an unusual recharge sequence, with values outside the modelled historical range, may lead to anomalous results. This could invalidate or lead to the misinterpretation of the results of all prediction simulations based on the BPS.

6.5.3 Design of Predictive Simulation

The prediction simulations should be kept as simple as possible, particularly at the start of a prediction project. If a BPS is used, then the predictive simulation will be a variant on this simulation. The changes made to the BPS for the predictive simulation should be made in light of the issues and associated features that are being examined. It is advisable to address just a single issue with each prediction run, because this minimises confusion with the examination of the modelled responses in groundwater flow. Particular care should be taken if changes of recharge and abstraction are required to examine a particular issue. It may be necessary to assess the responses in separate prediction simulations prior to combining the changes in recharge and abstraction in a single prediction simulation.

6.5.4 Interpretation of Results

The interpretation of results from prediction simulations performed on a numerical groundwater model is a complicated task. The post-processing and design of diagrams should be done so that it is possible to gauge the impact of the predictive scenario on the features identified for each issue, specifically to understand;

- over what time-scales the impacts occur;
- what the impacts are at the end of the predictive time-series taking into account seasonallity;
- check that the model is not producing anomalous results.

The last item is particularly important if the model input values of the predictive scenario is significantly outside the range of values used in the historical time series against which the model was validated. For example, extreme care is needed for an attempt to simulate the impacts of naturalisation of an aquifer with a long history of abstraction, with few or no data on groundwater heads and stream flows for the early abstraction period.

The type of output required will depend on the feature targeted for each prediction run. For most features considered this will include comparing BPS and prediction simulation hydrographs for both heads and surface feature flows and also comparing stream accretion plots. Difference plots with the BPS can be used very effectively to understand the changes in groundwater flow caused by a predictive scenario. In particular, differences in the water balance components convey a large amount of information. An example of water balance difference plot for a predictive study using the Notts-Doncaster groundwater model is given case example below.

6.5.5 Case example - Prediction simulations performed on the Notts-Doncaster groundwater model

Twenty prediction simulations were performed on the Notts-Doncaster groundwater model in 1999. The model had a historical time series of 28 years, from October 1969 to September 1997. A Baseline Prediction Simulation (BPS) was performed of 28 years length that repeated the historical recharge sequence. The abstraction of the BPS was set at a constant rate based on the average of 93-97 abstractions, but with some adjustments made to eliminate anomalous abstractions at certain sources, and to comply with programmed licence agreements already in place. In general terms, the prediction simulations were selected to explore the following issues:

- global reductions in all abstractions, to reduce abstractions to rates below the assessed long-term average recharge;
- re-distribution of pumping, whilst retaining levels of abstraction in line with agreed licence reductions. These include options for focussing abstraction away from the outcrop area into the confined part of the aquifer, and for moving pumping away from rivers and wetlands to areas of lower environmental sensitivity;
- reduction in abstraction at specific sources close to rivers and wetlands, in order to assess the time scales and magnitudes of local recoveries in groundwater levels and baseflows;
- conjunctive use, whereby sources are pumped at peak licence rates for 4 summer months, and then reduced for the remainder of the year in line with group licence totals.

Figures 6.5.1 and 6.5.2 show the results of a prediction run where groundwater abstraction was reduced globally by 18%. Figure 6.5.1 is a water balance difference plot of this prediction run ([prediction run] - [BPS]) for the whole model. This plot effectively summarises how the model responds to the change in abstraction. For this simulation the main conclusion was that only 50% of the reduction in abstraction benefits the surface water features.

It is important to note that a flow difference in a water balance difference plot can mean one of two things. A positive difference in flow means that the aquifer is either taking less water from, or providing more water to, the particular component of the simulated water balance (relative to the BPS). Conversely, a negative difference means that the aquifer is taking more water from, or providing less water to, that component relative to the BPS. It is therefore necessary to use these plots in conjunction with plots of actual heads and flows. For example, from Figure 6.5.2, where head is plotted for the BPS and the prediction simulation, it can be seen that the positive difference in flow for unconfined storage represents flow to unconfined storage rather than a decrease in flow from unconfined storage.

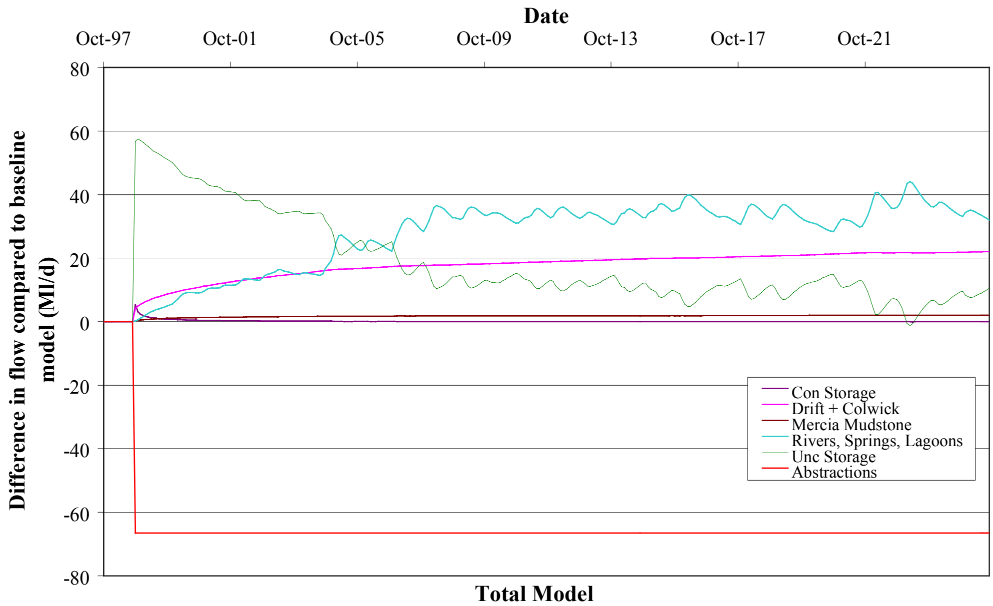


Figure 6.5.1. Water balance difference plot for Notts-Doncaster model prediction run

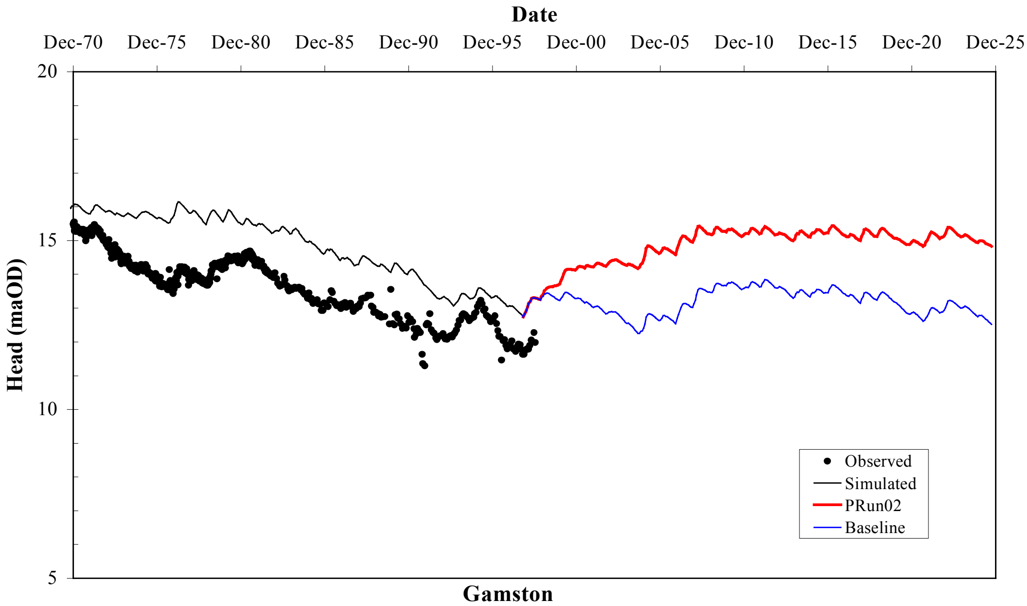


Figure 6.5.2. Comparative plot of groundwater heads (BPS v. prediction) for the Notts-Doncaster model

6.4 Performance expectations and refinement of the historical model

6.4.1 *Calibration* versus *refinement*

Rather than *calibration*, it is preferable to refer to *refinement* of historical simulations since we need to focus on how adequately our model represents the historical behaviour and specifically the key flow mechanisms of the real system and not upon how well a particular numerical model can simply match the observed heads and flows. The former requires hard hydrogeological thought and the discipline to challenge our conceptual models. The latter assumes that both our conceptual model and its current numerical representation are correct, and that our task is therefore to discover the combination of hydraulic conductivity, storage coefficient, recharge, etc, that produces the "best fit". Post-project appraisals (Anderson & Woessner, 1992, p 293) reveal that the flaws which most commonly cause a model to produce the wrong results occur in the conceptual modelling and not in the parameter distributions.

6.4.2 Performance expectations

The numerical model must reproduce the observed behaviour to an appropriate degree before being used for prediction purposes. The performance expectations of the model are often expressed in a number of acceptance criteria. However, these are not rigid criteria which must be achieved before the model is acceptable, but rather targets to aim for. The uncertainty of the groundwater modelling process means that it is impractical to set rigid expectations at an early stage, and it is necessary that they are reviewed and refined throughout the development of the groundwater model. A first exposition of the expectations or acceptance criteria, based on previous experience of similar projects, should be included in the Project Work Plan. Modifications to these will almost certainly be required as project specific information becomes available, for example during the conceptual modelling or during sensitivity analysis of the numerical model.

Performance expectations can be qualitative or quantitative. Some features of model output against which expectations are often set are listed in Table 6.4.1. Some examples, taken from the Itchen study Work Plan, are also included for guidance.

Some more detailed comments on acceptance criteria are included below.

- *Total River Flows.* If an appropriate runoff/recharge model of the model domain is constructed, similar criteria to the above can be set for total surface water flows which may include an adequate simulation of storm runoff at a daily time step, to check that the split of effective rainfall into potential recharge and runoff is credible. Whether seeking to simulate total river flows or the groundwater baseflow component of these, an appreciation of the other artificial influences (surface water abstractions, discharges, etc.) will be essential.

- *Flow accretion:* The model should reproduce baseflow accretion profiles along key reaches. This is one of the more difficult aspects of aquifer behaviour to reproduce but the predicted pattern of the timing and location of the onset and cessation of flows should be similar to the observed and within +/- 30days and +/- 1km of the observed (depending on the timing and nature of the processes being simulated). The simulated flow maxima and minima should be within 10-15% of average observed flows. However, an appreciation of the quality and representativeness of the spot flow gauging data upon which the observed flow accretion is based is essential.

Table 6.4.1. Possible performance expectations (with examples from the Itchen study, 2001-2. (model not built at time of writing))

Feature	**Parameter**	**Additional comments**	**Qual' or Quant'?**	**Example criteria (first iteration from the Itchen Work Plan)**
Groundwater discharge (baseflow and springflow)	Discharge		Quant'	± 10% of observed across full range of flows throughout the simulation period
	Timing	Time of occurrence of maxima and minima in discharge records	Quant'	± 20 days observed occurrence
Groundwater head at key agreed observation points	Mean	Annual mean or long term average	Quant'	± 2 m of observed
	Amplitude	Annual and/or over period of interest?		± 10% of observed
	Timing	Time of occurrence of maxima and minima in discharge records		± 20 days observed occurrence
	System-specific behaviour	e.g. accelerated recession characteristic of water levels in the Chalk when they fall below the zone of enhanced K and S_y	Qual'	Adequate simulation of relevant observed behaviour during the period of the historical model
	Trends	General declines or increases in levels in response to longer-term changes in conditions (recharge or pumping)	Qual' and quant'	Adequate simulation of observed trends decided by visual comparison of hydrographs or comparison of actual water level changes over fixed long-term periods
Groundwater head – spatial distribution	Head distribution (contour maps)	High, medium and low water-table conditions (selected times)	Qual'	Adequate match to observed distribution
	Head gradient	Along selected lines (e.g. recharge to discharge area)	Quant'	± 10% of observed gradient
Surface water flows at key agreed locations	Discharge	If a distributed recharge-runoff model has been constructed, baseflow (g.w. model) + runoff (recharge model) = surface water flow	Quant'	± 10% of observed across full range of flows throughout the simulation period
	Flow accretion	Timing, location and magnitude of influent/efluent flows. Recognised as relatively difficult to simulate.	Quant'	Timing and location of onset/cessation of flows within ± 30 days and ± 1 km respectively of observed. Flow maxima and minima ± 10-15 % of observed.

For example, low flow gauging surveys measure the flow at the time (day and hour), which may be influenced by peak rates of spray irrigation which cannot be represented in a groundwater model with weekly or monthly stress periods.

- *Groundwater head (spatial distribution):* The simulated groundwater head pattern over the whole model area (or primary catchment) should qualitatively match the observed patterns under low, medium and high water table conditions within selected years. Groundwater gradients at selected locations should be within +/- 10% of the observed. That is, the simulation must adequately reproduce the pattern of groundwater flows from recharge to discharge areas under different aquifer conditions. It can be useful to compare the gridded head distributions simulated by the model with those contoured from observations in the conceptual model report as such comparisons may reveal consistent patterns (e.g. heads seem to be generally too low on the interfluves). However, as for other comparisons with interpolated data, caution is required to appreciate the possible errors associated with contouring between the observations. This is particularly true if the observation borehole data are sparse, and no attempt has been made to add other constraints to the contoured grid such as river stage elevations over reaches receiving baseflow.
- *Aquifer response to stresses:* The model should adequately reproduce aquifer behaviour under historical stresses such as large pumping tests or the operation of augmentation schemes. Drawdown groundwater levels and depletion of baseflows should be within +/- 20% of the observed. However, it is important to recognise that the discretisation of a regional model is likely to be too crude to permit adequate simulation of pumped well drawdown.

Consideration should also be given to varying the stringency of the performance expectations, in either time or space, to reflect the need to simulate certain features of observed behaviour more closely since they relate directly to the purpose of the project:

- Key years can be identified during the historical simulation period, e.g. dry year, wet year, average year. For a low-flow investigation it might be appropriate to specify more stringent expectations when the model is simulating observed low-flow conditions.
- It is possible to define spatial regions of varying priority dependent on the aims and objectives of the groundwater model. The priority determines the level of detail and accuracy required in data analysis, representation of features in a model, and simulation of groundwater heads and flows. Figure 6.4.1 illustrates the regions of priority defined for the Upper Colne groundwater model, the primary objective for which is a low flow study of the River Gade. The regions of priority comprise:

  – A - the upper Gade and Bulbourne catchments upstream of Hemel Hempstead: the area of highest priority for the study;

  – B - the lower Gade, which requires some detailed assessment but will not be as critical to the low flow study since surface water discharges help to maintain flows;

  – C - the other main Chalk rivers, which need to be understood to a reasonable degree in order to develop the regional groundwater model;

  – D - the remainder of the study area, which has been included as an area of search for data but which does not require the same level of detailed analysis.

6.4.3 The refinement process

Model refinement needs to be carefully planned but must also allow the flexibility to explore the unexpected as new insight emerges. It includes several stages:

- getting the model to run smoothly and ironing out errors;
- understanding its behaviour and parameter sensitivity and refining within credible bounds to achieve an adequate simulation according to the performance expectations;
- avoiding the temptation to continue tweaking parameters and introducing unjustifiable complexity just to get a better fit; and
- formally exploring the sensitivity of the historical model to parameter and process uncertainty and also checking its behaviour in carrying out predictive simulations which may be sensitive to other factors.

In some cases initial steady state simulations may help to establish credible distributions of average flows. However, time-variant runs should also be tried early on because a poor simulation of the seasonal variations in flows and heads may point to a fundamental flaw in the conceptual model or in its numerical implementation. It is usually possible to shorten the time-variant simulation used routinely for refinement, providing the model is run through enough initial seasonal cycles to adjust to starting conditions. This usually takes between 4 and 10 years of simulation time depending on hydraulic parameters, but this should be subject to investigation(see Initial Conditions in Section 6.3). Much of the characteristic behaviour of the model can be apparent within relatively small periods of time within the historical simulation period so that runs covering the full historical period may be needed less frequently, providing an adequate 'run-in' period has been allowed for the model to settle in to the new parameters being investigated.

Refinement can proceed effectively through a series of controlled variations away from a baseline model, with results recorded and summarised so as to build up an understanding of its sensitivity to different parameters and processes. It is usually worth 'hitting it with a big hammer first', i.e. making significant changes in 'both directions' to recharge timing, transmissivity, storage, stream parameters or other parameters which are within the credible range but can be expected to make a big difference. A new baseline model is then selected and used to explore sensitivity to other parameters, always seeking to achieve a closer simulation of observed data without resorting to processes or parameters which are not credible.

6.4.4 Communication and review of model output

Pictures and tables (see Figures 6.4.2 and 6.4.3 from the Upper Lee/Mimram study) which can summarise a lot of comparative (observed v. modelled) information at a glance are invaluable as they help to maintain an overview of what can be a large volume of data. The format of this regular output should be agreed early on with the whole review team and ways in which results can be shared efficiently by e-mail (e.g. copying summary output into Powerpoint, etc) need to be established so that the process of refinement and the learning which results from it can be a shared experience.

A relatively small technical review group should oversee refinement through monthly meetings and more regular e-mailed results summaries. At each meeting results from previous runs are reviewed and the next runs are planned. The review group and the modellers need to keep an open mind throughout. They should remain closely familiar with the range of credible parameters and processes suggested by the initial conceptual model whilst also being aware of the many uncertainties which should have been identified within it. It will be necessary to challenge poorly constrained features of the model, possibly including recharge processes, transmissivity and specific yield distributions, and stream conductance values, at an early stage.

Some dead ends and re-working are inevitable and a simple run log summary of all runs is essential. This should list the aim of the run (i.e. what is being tried and why), the input and output files, and a summary of the results, particularly noting unexpected or counter-intuitive features. This record is a vital reference for future users of the model and will form the backbone of the report describing its refinement (see Documentation in Chapter 2).

Allowance should probably be made for around 50 to 80 time-variant runs (dependent on approach) to enable a reasonably thorough investigation and refinement of a regional model. With meetings and time for review team involvement and 'buy-in' this will probably take 6 to 9 months or longer. Acceptance criteria should be reviewed regularly based on the need to make pragmatic decisions as to when the process has gone far enough and further refinement is not worthwhile. Before formally stopping however, further valuable insight can be derived by using the model to carry out some of the predictive scenario runs. It may even be worth iterating through the historical and predictive runs several times during refinement as the sensitivity and reliability of these may depend on different factors.

Providing the 'temptation to tweak' can be resisted, time and money should remain for a formal sensitivity analysis to follow model refinement. The credibility of the final simulation should be critically reviewed with respect to the questions which the model has been built to address. An understanding of what constitutes a model which is 'fit for purpose' should be drawn from both the study aims and the performance expectations through discussion with the review team. Areas of the model over which, or time periods during which, the simulation does not adequately meet this standard must be clearly highlighted in the modelling report so that predictive results in these areas/periods are flagged for caution. Careful management of expectations amongst members of the wider project team who have less modelling experience is vital to avoid disappointment and disillusion. Some parts of the model will almost certainly not work adequately and further questions and issues to be investigated will always be generated through modelling. These should also be clearly set out in the report to facilitate future study and ongoing model refinement i.e. there may need to be iteration between numerical modelling and conceptual thinking.

6.4.5 Final thoughts

Experience shows that the historical model rarely 'works' straight away, and that refinement to a satisfactory point will always be a difficult process. In budgeting for the refinement of a model, a reasonable rule of thumb is that it will take around the same time as that required to develop the conceptual model.

Figure 6.4.1. Zones of priority used for the Upper Colne groundwater modelling project

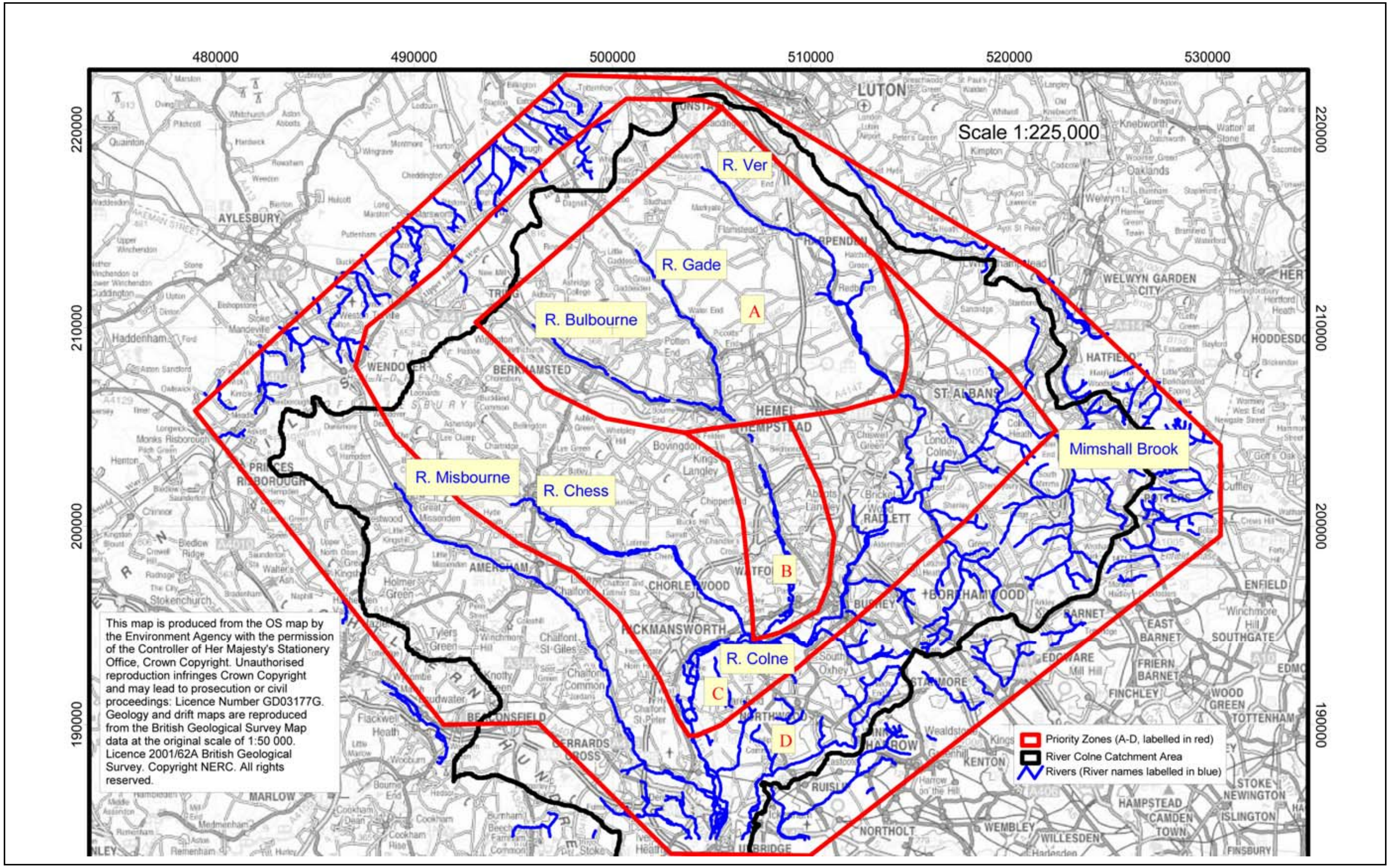


Figure 6.4.2 Stress period average gauged flows and modelled flows for selected gauging stations (average stress period length 10.15 days)

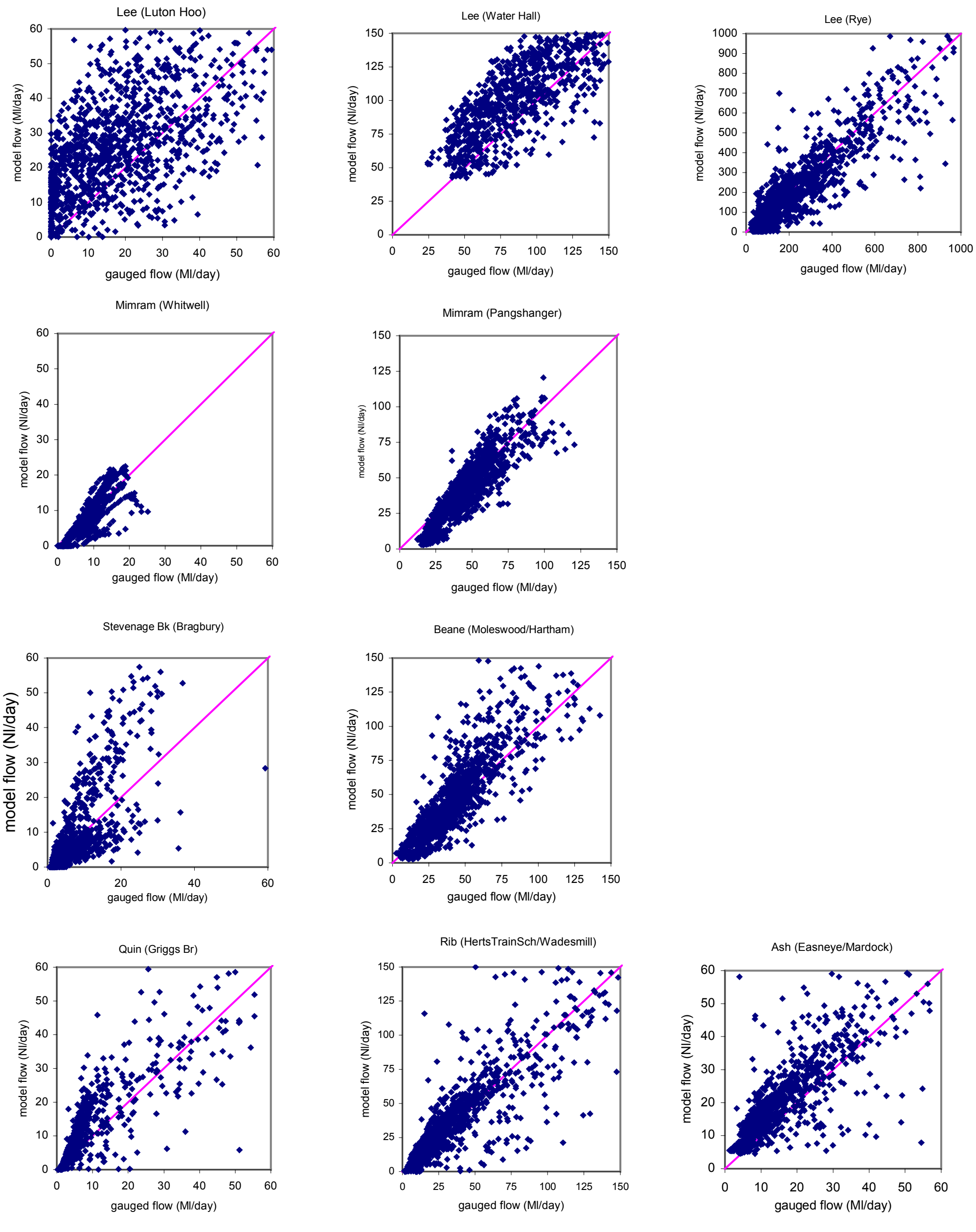
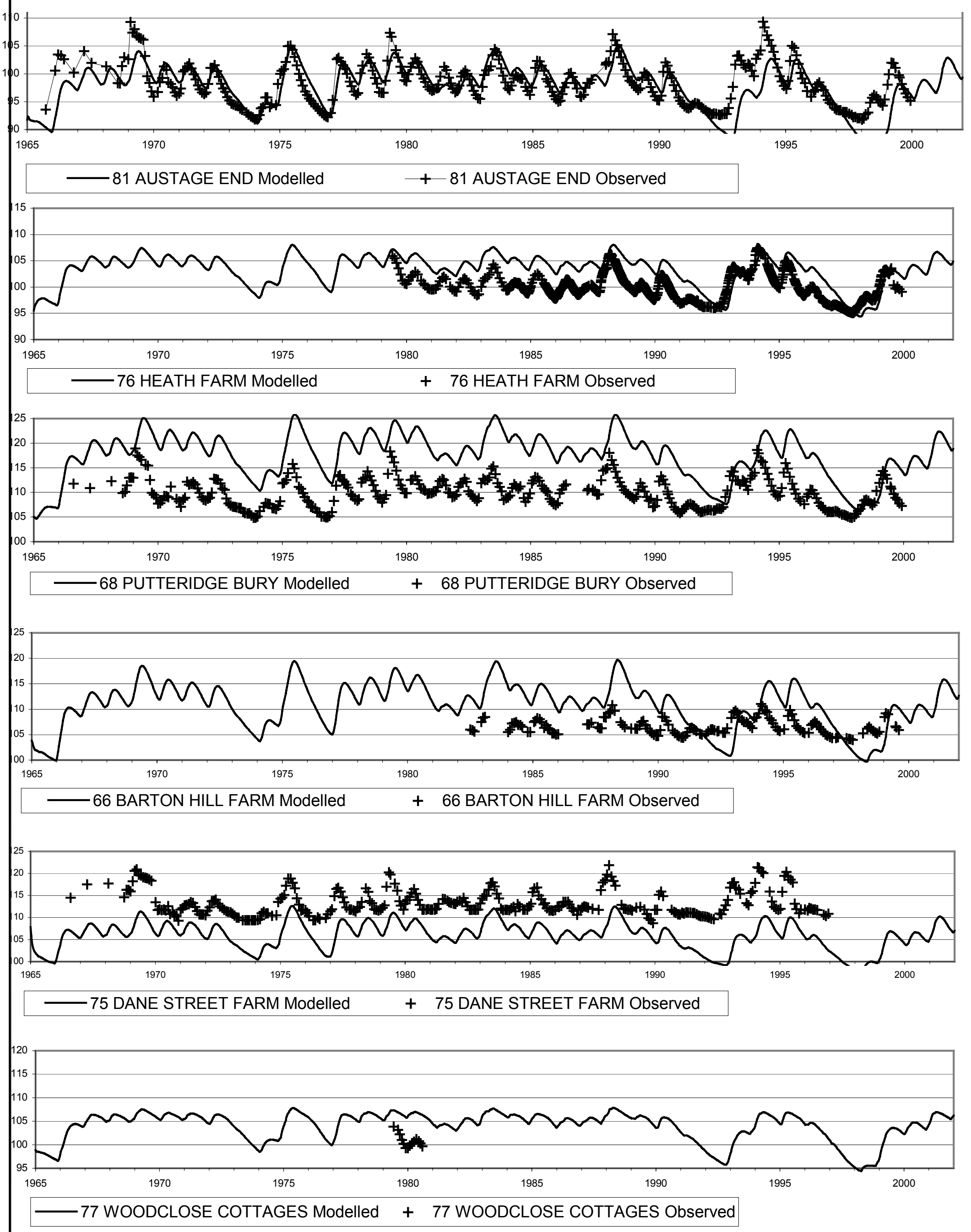


Figure 6.4.3 Observed and modelled groundwater levels (mAOD) for selected boreholes of the Upper Mimram (dry)



6.3 Model construction and the historical model

6.3.1 Model construction

Discretisation of space

The grid (or node) spacing adopted for the model determines the scale of representation of features within the numerical model. Factors which should be considered in deciding the grid spacing include:

- the scale of the processes under consideration;
- the scale of the output required;
- the scale of input data.

Grid spacing has largely been determined to date by computing power which has dictated a maximum number of nodes to achieve reasonable run-times for large regional models. This constraint is now starting to become less important, and in the near future grid spacings will be determined by the scale of key processes. For example, if faults, thin high conductivity layers, wells or fissures are important, small grid spacing may be necessary.

Hence, the key question is: what is the scale of the hydrogeological processes which are key to the purpose of the model?:

- If the work is focused on representing *regional* flow patterns and impacts, then small scale processes can be represented adequately using a large grid scale, e.g. abstraction wells in a regional model. However, it should always be recalled that the representation of local flow processes and detailed output from the model is likely to be unrepresentative.
- If the output required is very *detailed*, e.g. river accretion over a short river reach, then the model grid spacing must be considered in relation to:

– the scale of the processes that dominate the flow patterns in the area of concern?

– the availability of detailed local evidence to parametise and then test the model.

Ideally, the grid scale should be smaller than the process scale, i.e. the process can be represented by one or more model cells/nodes. This means that realistic, rather than effective, parameter values can be chosen. Sensitivity analysis may help in this situation, enabling us to see whether greater definition in input data would make a significant difference to the output with which we are concerned.

It is also crucial to understand the area over which the data is representative as this will help define our confidence in the model output. Failure to do this may lead to a misunderstanding of the processes that are occurring, and therefore to poor quality modelling of the study area. For example, river hydrographs give an integrated measurement of the flow from both the surface water and groundwater catchments to the gauging station. They cannot be used to gain much understanding of the spatial distribution of processes within the catchment. To characterise sub-catchment processes, other, more localised, evidence will be required, e.g. groundwater levels.

If data at the appropriate scale is not available, the model should be treated as an investigative tool, examining the plausibility of different processes and parameter values.

As noted above, the grid spacing should be related to the scale of the processes under consideration. However, there is a practical limit on how small grid spacing can be. Even though very local processes can be identified, e.g. braiding of streams and local solution features, it does not mean that a grid spacing which is small enough to represent these features explicitly should be adopted. Professional judgement is required, and input parameter values can often be adjusted to represent such features implicitly, e.g. adjustments of conductance for stream braiding. The crucial question is whether the increase in grid resolution and hence model complexity and size is outweighed by increase in confidence in answers to the specific study questions and not just in supposed accuracy of model results.

Experience has shown that regular model grids (uniform row/column spacing) have significant practical benefits over irregular grids:

- the finite difference expression for an irregular grid has a larger error than that for a regular grid (Anderson and Woessner, 1992, p. 64-65).
- post-run interpretation of model output is simplified and the models are easier to hand over to the Agency at the end of the project.

It is also preferable for grids to be oriented parallel to the National Grid, facilitating easier transfer of spatial arrays to mapping software and allowing direct comparison of outputs with similarly oriented models of adjacent areas.

Uniform grid spacings have been adopted for all recent and ongoing (2002-) regional groundwater models:

- West Midlands Sandstone, 250 m;
- Mimram, 200 m;
- Itchen, 250 m (proposed, early 2002).

Discretisation of time

Recently produced historical and prediction models have generally adopted a stress period length of one month, reflecting both the time resolution of available data (e.g. abstraction returns, groundwater level monitoring) and the general timescale over which significant changes in groundwater regimes occur. The model of the Chalk aquifer centred on the Mimram catchment (Entec) has 10 day stress periods in order that the time resolution of the surface runoff/recharge model can be used to greatest effect (see Figure 6.3.1).

One problem that is becoming increasingly evident is that the output expected from a modelling study is too detailed with respect to the available input data and evidence. One example of this is the running of models at daily timesteps when the input data for recharge arriving at the water table cannot be estimated or indirectly observed to a greater accuracy than monthly or bi-monthly. We must always consider how well constrained the input data and evidence is in terms of time. Simulations at finer time resolutions should be treated as investigative as they cannot be observed from the available field data.

In most current Agency models, there are three or four timesteps in each stress period. It should be noted however that de Marsily (1986) suggests the rule of thumb that the solution should proceed through five timesteps, during which there are no significant changes in the values of sources, sinks or boundary conditions (i.e. a stress period), before the solution is considered accurate.

Digital file sizes
Table 6.3.1 presents details of digital file sizes for the Upper Lee and River Mimram model. The model is 1 layer, 225 x 250 rows/columns, 3 stress periods per month. Two historical models were developed, a short exploratory model covering 8 years (288 stress periods) and a full historical period model covering 37 years (1332 stress periods).

Table 6.3.1. Digital file sizes for the Upper Lee and River Mimram model

	Short Exploratory Run	**Full Period Run**	
	Size (Mb)	Size (Mb)	**Comments**
MODFLOW(VKD) Model Input Files			
Basic Package (*.bas)	1.5	1.5	
Block Centred Flow (*.bcf)	5.4	5.4	
Well Package (*.wel)	5.7	5.7	
Output Control (*.oc)	0.5	0.5	Output requested at the end of each Stress Period, rather than at each timestep, to limit file size. Separate run required to save all data for the purposes of performing full zone budget options.
PCG Solver (*.pcg)	<0.01	<0.01	
Recharge Package (*.rch)	190	880	Large size due to spatial and temporal variation in calculated recharge
Stream Package (*.str)	148	683	Large size due to inclusion of calculated runoff.
Total	**352**	**1577**	
MODFLOW(VKD) Model Output Files			
Head Output file (Binary *.hds)	63	293	
Cell by Cell flow file (Binary *.cs1)	253	1170	
Output Progress and Details file (*.out)	4	19	Recharge and Stream information not automatically written to Output Record file to minimise disk space required.
Total	**320**	**1482**	
Estimated Total Disk Space required for full run and processing	**0.8 GB**	**3.5GB**	

6.3.2 Historical models

If the historical model can adequately reproduce observed behaviour, it is assumed that the model is a good basis for predicting system responses to future conditions. It should be noted, however, that uncertainty in predictions will increase as future conditions deviate from those represented in the historical model.

What period of historical time do we need to simulate? The first considerations are the timescale of the processes at work and the initial conditions. The processes timescale will vary significantly according to the speed of the system. In general, high transmissivity/low storage systems react quickly whilst low transmissivity/high storage systems react slowly. This clearly means that to investigate and simulate impacts in fast systems, e.g. Chalk, we can consider shorter simulation periods. In slower systems, e.g. Sherwood sandstone, similar impacts will develop over far longer periods in the field and will require correspondingly longer simulation periods. However, we also need to consider the time boundary conditions, or initial conditions. In a similar way to the physical boundaries of the system, the time boundary is important. If the initial conditions are incorrect, model results will be unsafe.

Simulation periods

The value of the model refinement will be increased if the historical simulation period:

- includes important changes in the catchment such as increased (or decreased) abstraction;
- covers a range of climatic conditions (due to the very wet and very dry periods since the mid 1980s, it may not be necessary to include the 1970s for studies in chalk and limestone aquifers);
- is sufficiently long for any inconsistencies in the starting conditions to become insignificant;
- extends back to the time after which regular and reliable time series data are available.

The longest possible historical simulation period extends from just before the first abstractions from the aquifer (pre-anthropogenic conditions) to the present day. In practice, the considerations outlined above mean that a historical *period of interest* is identified on which model refinement is concentrated. For most recent modelling projects this period of interest has been from the 1970s to present. A case can be made for a shorter period of interest for chalk and limestone aquifers (e.g. from the 1980s to present) because of their rapid reaction to changes in conditions and the increased variability of climate over this period.

For systems which react more slowly to prolonged abstraction (i.e. sandstone aquifers), it is often necessary for the historical simulation period to start from pre-anthropogenic conditions. For example, the historical models for the Lower Mersey aquifer system (Fig. 6.3.2), the Bromsgrove aquifer (Rushton and Salmon 1993) and the West Midlands Trias cover historical periods of 100 years or more. For the Bromsgrove aquifer model the starting conditions represent the situation one hundred years ago when there was little groundwater abstraction and groundwater fed streams were able to support a number of water mills.

Simulations of periods before the period of interest usually have limited value in terms of model refinement as relatively few observations of groundwater conditions are usually available. Their function is mainly to provide a lead-in so that the starting conditions for the period of interest are sufficiently accurate.

It may be convenient to use longer stress periods for simulating conditions before the period of interest. For the Lower Mersey Sandstone aquifer model (Figure 6.3.2), during the period 1847-1947 the stress periods were increased by a factor of ten, whereas for the period 1947-1980 (the period of interest) monthly stress periods were used. The steady decrease in the representative groundwater heads of Fig. 6.3.2 between 1847 and 1947 demonstrates the necessity of including the earlier period in the historical simulation.

Initial conditions

The initial conditions of a time variant simulation are the initial heads, the aquifer properties and the flows at the beginning of the run. These must adequately represent the real system's behaviour. However, the real system is always dynamic, whereas the model must move from static initial conditions to dynamic conditions.

Heads, flows and aquifer properties in groundwater models are not independent variables. They are related by Darcy's Law. Specifying any two automatically sets the value of the third. For example, if we have specified *arbitrary flat starting heads*, then the flow between nodes during the first time step will be calculated as zero regardless of any recharge applied.

If *field-derived heads* are used, they are also likely to be inconsistent with the other initial conditions (aquifer properties and flows) and produce a lack of equilibrium with effects that may be felt for many years (Rushton & Wedderburn, 1973). Consequently their use is discouraged.

Starting heads which are consistent with the other initial conditions can be obtained by using the model. It can generate:

- long-term average steady state heads;
- time instant steady state heads;
- heads which are in dynamic balance.

An aquifer system is at steady state when it is in equilibrium, i.e. the flows, heads and the volume in storage do not change with time. *Long-term average steady state heads* are derived by running the model with zero or very low storage and using long-term average inflows and outflows.

Deriving starting heads in this way is quick. However, if the real system is not at equilibrium the heads are unlikely ever to represent the real heads. For example, a time variant run beginning in August which uses long-term average steady state heads as initial heads will not reflect that this is a summer month when heads are low and water is being drawn from storage. The time-variant model may have to be run for many years before the influence of this discrepancy is no longer significant.

A time instant solution produces *time instant steady state heads.* It is simple and quick because it is undertaken using a steady state simulation. Rather than using long-term average flows, it uses the flows (recharge and abstraction) from the spring or autumn when groundwater levels have started to recess or just started increasing and changes in storage are low. In addition, the estimated change in storage is added to the actual recharge and abstraction for each node. This combination is termed the “equivalent recharge”. The heads so derived can then be used to begin a time variant simulation in the spring or autumn as appropriate. This will mean that dynamic balance is achieved more rapidly which is important for chalk or limestone.

If a model is run as a time variant simulation using, for example, monthly stress periods with monthly average inputs (recharge, abstractions etc.) over a cycle of several years, the resulting heads also follow a cyclical pattern and eventually repeat themselves. Although storage changes month by month, the net change over an annual cycle is zero, and the model is said to be in *dynamic balance* (or to produce *cyclic dynamic* heads [Anderson and Woessner, 1992]). The heads from this type of model more realistically represent a system in a dynamic, rather than static, equilibrium.

The historical time variant simulation can be started at any time of the year by selecting the corresponding heads from the dynamic balance run. Rushton and Wedderburn (1973) state that the time taken (*t*) to achieve dynamic balance starting from long-term average steady state conditions is a function of both the aquifer parameters (transmissivity, *T,* and storage, *S*) and the length of a typical flow path (*L*) from recharge to discharge:

$$t = 1.5\frac{L^2 S}{T}$$

Times are typically measured in single years for confined aquifers and tens or hundreds for unconfined aquifers (Rushton & Redshaw, 1979, p 155).

Final thoughts

Experience has shown that it is more efficient to develop the structure of the model in a stepwise fashion, gradually increasing the level of complexity. The model should be run after each construction step to confirm that it will converge within accepted criteria. The alternative is to spend a large amount of time constructing a very complex model, only to find that it does not converge, and then having to spend further extensive periods of time finding the cause of the lack of convergence and making major modifications to the input files.

Key outputs from the model, relating to the project objectives and the acceptance criteria as defined before numerical modelling commenced, should be identified and act as the focus for model development. Time invested in creating efficient methods for extraction and display of model outputs pays dividends over a prolonged refinement period. For example, it is often useful to create external utilities using FORTRAN, Visual Basic, etc, to extract data from the model output files and spreadsheets to display time-variant data. Methods for verification of input data (i.e. digital QA) outside the immediate working environment of the GUI should be investigated.

6.3.3 References

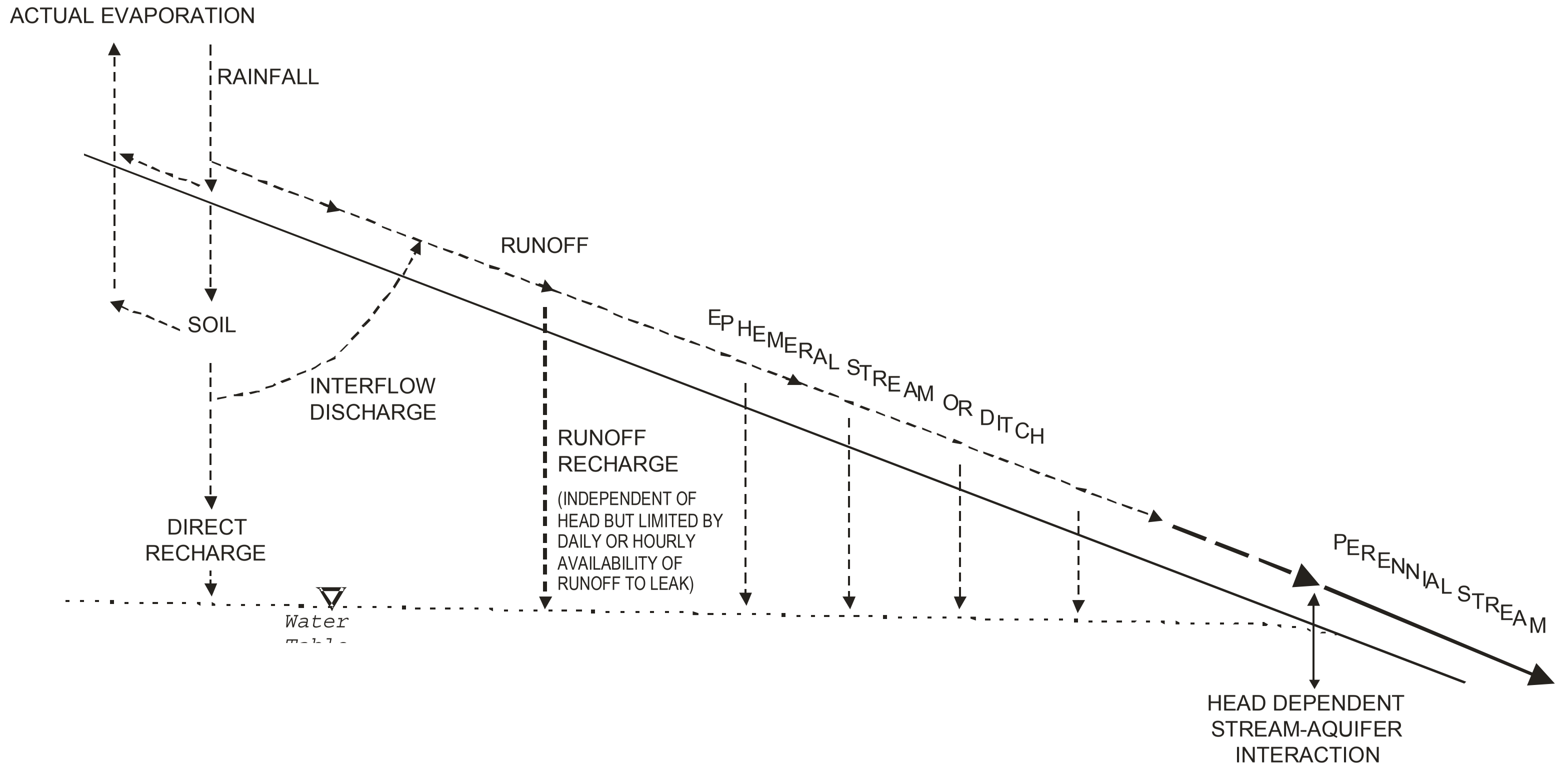
Anderson & Woessner, 1992. *Applied groundwater modelling.* Academic Press Inc., US.

de Marsily, 1986. *Quantitative hydrogeology*. Academic Press Inc., US.

Rushton, K. R. and Salmon, S. 1993 Significance of vertical flow through low-conductivity zones in Bromsgrove Sandstone Aquifer, *J. Hydrol*. **152,** 131-152.

Rushton & Wedderburn, 1973. Starting conditions for aquifer simulations. *Groundwater* Vol. **11**, No. 1.

Rushton K.R. and Redshaw S. C. *Seepage and groundwater flow*, Wiley, Chichester, 1979, 339 pp (out of print).



Conceptual Model Notes:

- Rapid Runoff and Interflow dominate on Carboniferous, Mercia Mudstone or Till;
- Evapotranspirative losses are losses assumed to be determined by a Penman-Grindley type soil moisture balance model depending on crop type and season;
- Recharge processes dominate on Sandstones;
- Runoff-recharge will be most significant where streams or ditches flow from Till, Mercia Mudstone or Carboniferous on to the Sandstones and may be enhanced by existence of old mill ponds;
- Interflow may be considered as the exponential release of water from minor near surface aquifers;
- Recharge to the sandstone water table lags behind rainfall according to the unsaturated thickness and the existence of Till cover;

Figure 6.3.1. Conceptual Model of Natural Runoff, Evapotranspiration and Recharge Processes for the West Midlands Sandstone Aquifer. Illustrates the Importance of Considering Runoff Recharge Processes as Part of Daily Recharge Calculations, in Contrast with Head Dependent Stream - Aquifer Interaction which is more appropriately Calculated by the Groundwater Model Over a Longer Stress Period (from the West Midlands Study, Entec 2001).

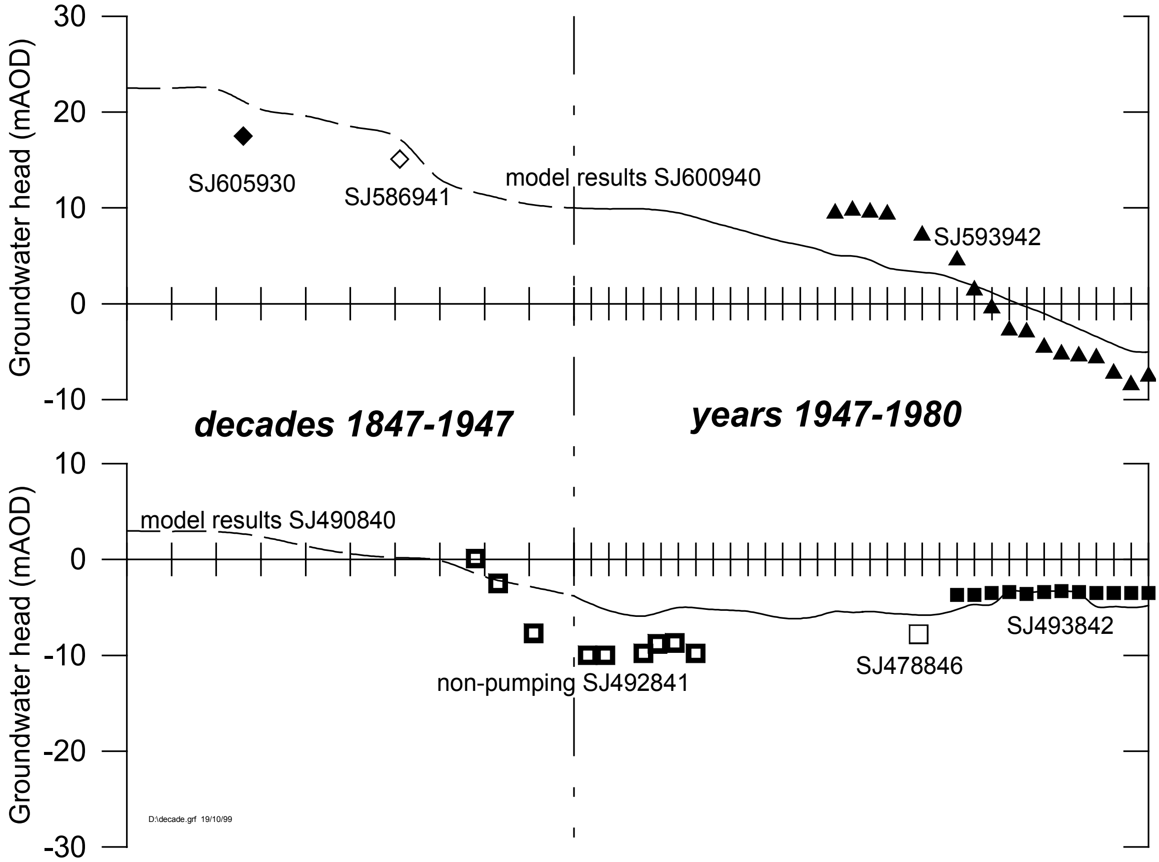


Figure 6.3.2. Time periods for Lower Mersey Sandstone aquifer; from 1847 to 1947; data inputs were for decades, for 1947 to 1980 monthly data were provided for inflows and outflows. In the diagrams, comparisons are made with observation well field data within one mesh interval of the model node.

6.6 Assessment of Uncertainty in Modelling

6.6.1 Sources of Error

A model is a simplification of reality hence there are errors inherent in its development which give rise to uncertainty. A summary is given here of the five main sources of error:

- *Field data.* Inherent uncertainty in field data, scale of measurement (i.e. point measurement vs. measurement averaged over a large area), measurement error.
- *Conceptual model.* The most serious cause of error in modelling results arises from deficiencies in the formulation of the conceptual model. Alternative conceptual models can be formulated which are equally plausible so that both require testing. For example, the maintenance of summer baseflows may be due to aquifer storage or delayed runoff recharge or both but applying the correct mechanism in the model will influence the predictive results.
- *Model input data.* There are errors introduced due to the uncertainty in the model input parameters (parameter uncertainty). For example transmissivity values derived from pumping tests at one location are frequently a factor of 3 higher or lower than those from a nearby pumping test which would be in the same model cell. Model parameters are applied to cells or zones across which the properties are averaged thus not representing the real heterogeneity of the system. This is very scale dependent so greater accuracy requires much greater detail and for which the data may not exist or may not be practically obtainable.
- *Mathematical representation.* There will be inherent errors associated with the mathematical representation of the physical processes (e.g. the governing equations and boundary conditions are simplified mathematical descriptions of the conceptual model). In addition the numerical approximations used to solve these equations and the associated spatial and temporal resolution introduce further errors.
- *Predictive uncertainty.* There will be errors in the model predictions because, for example, future abstractions and recharge patterns are estimated but will in reality be different.

The latter two are the simplest categories to address. Uncertainty in the conceptual model is likely to have far reaching effect. Gorelick (1997) stated, ‘Going from limited observation of the true system to the conceptual model is the most crucial step in simulation model development. This is the stage where we either capture the essence of system behaviour or introduce the greatest uncertainty’.

6.6.2 Sensitivity Analysis

Sensitivity analysis identifies which mechanisms (including different conceptual models) and input parameters have the most influence on the model outputs, and particularly the outputs that are crucial to addressing the project objectives. These may be the effect at particular locations, such as the water levels in sensitive areas or the effect over a distance such as the flow accretion along a sensitive reach of river.

Sensitivity analysis tests the effects of perturbing the values of one or more parameters from a base case and within plausible limits. This means, rerunning the model with, say, the hydraulic conductivity or storage doubled (or halved).

Sensitivity analysis should be carried out at different stages of the model development:

- At the model development stage sensitivity analysis provides a vital role in testing out the conceptual model and developing an understanding of the responses of the model to processes and parameters.
- After the historical model has been developed and tested, a systematic sensitivity analysis should be carried out to quantify the effects of uncertainty in all of the key parameters.

The sensitivity approach can be used to:

- provide understanding of the interactions between the parameters of the model;
- provide insight into parameter combinations which produce extreme results (e.g. worst case scenarios);
- highlight problems in the numerical model (e.g. undue influence of boundary conditions);
- identify which uncertain parameters have significant effects on the results;
- identify which type of additional field data would be the most valuable in terms of reducing model uncertainty;
- quantify the range of results possible from plausible input parameters.

Brown (1996) points out the need to conduct sensitivity analysis of the historical model and the predictive model in parallel in order to assess the real influence of input uncertainty on the final results and the management decisions based on them. For example, a historical model with little abstraction in a particular catchment may not be sensitive to whether a stream in that catchment is hydraulically connected to the aquifer or not as represented by the river coefficient. However, for a predictive model with increased abstraction, this uncertainty may make a significant difference to the impact on the river.

A current Agency project is looking at systematic statistically based sensitivity analysis in order to help identify non-unique solutions and alternative conceptual models.

6.6.3 Stochastic Modelling

Stochastic modelling attempts to quantify the consequences of uncertainty in terms of average results, and the nature of the possible variation in the results. Unlike sensitivity analysis, therefore, stochastic modelling assesses the likelihood of a particular result occurring.

At first sight this is attractive but in effect it is only practical to assess the uncertainty due to parameter inaccuracies which are often not the largest source of error. In addition, Voss (1998) warns “Assigning likelihood to a given scenario is an even less certain procedure than making predictions with groundwater models” – stochastic modelling should not lead to a false sense that uncertainty has been quantified.

By far the most often applied stochastic technique for quantifying the effects of uncertainty is the Monte Carlo method, which is based on multiple predictive simulations (‘realisations’) of a numerical model. The use of the Monte Carlo method is impractical for time-variant regional models. The number of simulations necessary to define the statistics of the results cannot be predicted in advance but is usually thousands and since typical run-times for time-variant regional models are 4-8 hours (2002), you would be waiting a year or two for the results.

6.6.4 References

Voss, C.I. 1998. Groundwater Modelling: Simply Powerful. *Hydrogeology Journal*, **6 (4)**: A4-A6

Gorelick, S.M. 1997. *Incorporating uncertainty into aquifer management models. In: Subsurface flow and transport: A stochastic approach*. Ed. G. Dagan and S.P. Neuman, Cambridge University Press, Cambridge.

Brown DM. 1996. Reducing modelling uncertainty using ASTM Groundwater Modelling Standards, Subsurface Fluid-Flow (Groundwater and Vadose Zone) Modelling, ASTM STP 1288, Joseph D Richey and James O Rumbaugh, Eds., American Society for Testing and Materials, 1996.

6.6.5 Bibliography

Anderson M.P. and Woessner, W.W. 1992. *Applied Groundwater Modeling: Simulation of Flow and Advective Transport.* New York, Academic Press Inc. 381 pp.

Zheng, C. and Bennett, G.D 1995. *Applied Contaminant Transport Modeling: Theory and Practice.* Van Nostrand Rheinhold, 440 pp. (Chapter 11).

EPA 1997. *Guiding Principles for Monte Carlo Analysis*. EPA/630/R-97/001

Template of a Project Brief for inclusion in the Tender Document for a Contract to Develop Conceptual and Numerical Models for a Groundwater Resource Study of [X] Catchment(s) Issue 1 [DATE]

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Appendix 1
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1 INTRODUCTION

Preamble

1.1 [Brief description of history of the aquifer, major users and any particular problemS]

Purpose of the Study

1.2 ***[LIST THE GENERAL PURPOSE OF THE STUDY INCLUDING DATA COLLATION, DEVELOPMENT OF CONCEPTUAL MODEL, CONSTRUCTION AND REFINEMENT OF NUMERICAL MODEL, USE OF MODEL FOR PREDICTIVE PURPOSES]***

1.3 At the end of the Study, the model will be used to investigate the following problems: -

[PREPARE A LIST OF THE SPECIFIC QUESTIONS WHICH THE STUDY IS BEING DEVELOPED TO ADDRESS]

1.x The appointed Consultant will be expected to undertake the tasks as outlined in Chapter 2 to enable the Agency to answer these questions. To ensure that the work is completed to a sufficiently high standard it is proposed that the Study is monitored by a Project Review Panel, staffed by senior personnel from the Environment Agency ***[REGION]***, Water Undertakings and an independent modelling expert.

Study Area

1.x ***[BRIEF DESCRIPTION OF AREA BOUNDARIES AND MAJOR SURFACE DRAINAGE]***

Available Information

1.10 The Agency has various sources of data and information available, which could be useful in developing an understanding of the aquifer system as well as the type of model required. The information is attached as follows: -

Appendix 1 - Brief description of the ***[CATCHMENT NAME]*** catchment

Appendix 2 - List of known references

Appendix 3 - Known issues for conceptualisation

Appendix 4 - Data available within the Agency

Appendix 5 - Functional objectives for the models

Figure 1 Study Area

2 PROJECT STRUCTURE

Introduction

2.1 The Agency envisage that the Study will comprise the following five Phases of work:

Phase I: Part A Data Collation. Analysis and Presentation,

Part B Formulation of Conceptual Model;

Phase II: Development and Refinement of the Historical Model;

Phase III: Modelling of Resource Options;

Phase IV: Final Report; and

Phase V: Training and User Support.

Note that in some projects, the first contract may be restricted to Phase I; this will require adjustments to a number of the tasks..

Each of these Phases is described in more detail below.

Phase I: Data Collation and Formulation of Conceptual Model

Phase I will comprise the following twelve tasks:

Task 1: Study Inaugural Meeting and Area Visit

The Study will be launched at a one-day Inaugural Meeting, to be held at the Agency offices in ***[OFFICE LOCATION]*** and attended by two senior representatives of the Consultants project team (the Project Manager and Senior Modeller) and the Project Review Panel (including the independent modelling expert). On the following day a member of the Agency will travel with the senior consulting staff on a one-day visit to the Study Area. As part of its proposal the Consultant will be expected to indicate what it considers to be the key items to discuss and to examine during the meeting and site visit.

PART A DATA COLLATION, ANALYSIS AND PRESENTATION

Task 2: Data Collation

Purpose:
The study area is defined in Figure 1 and the main study period will be from ***[19?? to 200?]***. It is proposed that the numerical model(s) should be capable of adequately representing historical aquifer and river-flow conditions for the period ***[HISTORICAL PERIOD]*** inclusive. Data collection and collation should concentrate on the study area and the time period [***HISTORICAL PERIOD]*** although it may be necessary to obtain some information for a larger area and cover a longer time period.

Approach:

The collation of geological, hydrological and hydrogeological information available and relevant to the ***[STUDY AREA NAME]*** and study period will primarily be the responsibility of the Consultant, though Agency and ***[WATER COMPANY]*** staff will assist with the collation of in-house data where the task does not impinge on their other work commitments.

Where data is available from the Agency, then this would be provided at no additional cost to the Consultant. However, where data is to be provided by a source external to the Agency and the Consultant, then this will be purchased by the Consultant. ***[this approach may change]*** The Consultant shall make provisions within their tender proposal for the acquisition of data. In any event, the Consultant is reminded that any data obtained as part of this Task shall remain the exclusive property of the Agency.

In its proposal the Consultant is expected to demonstrate an awareness of the various issues that are likely to arise during this extensive data search. Any possible additional sources of data should also be mentioned (but not costed) in the proposal. Where appropriate the Consultant will enter or import the raw data into Excel compatible spreadsheets to enable later presentation of the data or further analysis. These spreadsheets should be passed over to the Agency at the end of the project.

Outputs:
As an absolute minimum the Consultant will be expected to have acquired, inspected and quality assured the following data covering the above stated study period:

1) The most recent topographic (1:25,000 and 1:50,000), geology (1:10,000 and 1:50,000) and soils maps, mineral assessment reports and memoirs for the ***[STUDY AREA]*** (available from British Geological Survey in Keyworth).

2) Lithological logs for the Solid and Superficial deposits within the ***[STUDY AREA]*** (hard-copy records are available from the Agency (incomplete) and/or British Geological Survey in Keyworth and Wallingford);

3) Daily rainfall for a number of Meteorological Office rainfall stations, the number and choice to be agreed with the Agency (data generally available as ASCII files from the Agency);

4) Potential and actual evapo-transpiration (monthly/weekly figures distributed on a daily basis) should be available for two or more Meteorological Office climate stations;

5) Parish Crop Returns for a number of sample parishes, the number and choice to be agreed with the Agency (data available as hard copy from either the Public Record Office or MAFF - Statistics Section) (Satellite data for crop types are available for ***[AREA]***);

6) Daily river-flow records and 15-minute river level data (where available) for permanent current and disused gauging sites. For the rivers in the study area approximately ***[No.]*** station years of data are available as chart records and ASCII files from the Agency;

7) Occasional current-meter gauging surveys along low-flow sections of the river network during summer conditions (hard copy summary records are available from the Agency);

8) Licensed abstraction quantities (annual, daily and peak daily and hourly) and actual monthly groundwater abstractions for all public water abstraction sites (***[No.]*** station years of data) are available from Agency or Water Companies in various forms but generally in hard copy. Details of other groundwater and surface water abstractions are available in hard copy from The Agency;

9) Groundwater levels for approximately ***[No.]*** observation boreholes in the ***[AQUIFER NAME]*** and Superficial Deposits for ***[STATION YEARS]***;

10) Interpretations of the results of earlier pumping tests and borehole geophysical and/or fluid logging in the area (hard-copy records from the Agency). The Consultant is expected to confirm the results of pumping tests or undertake its own analysis of pumping test data;

11) Additional information on aquifer properties may be available from British Geological Survey's Aquifer Properties Manual; and

12) Groundwater quality data for abstraction/observation boreholes within the study area (available from Agency Groundwater Quality Archive in text file format - approximately ***[No.]*** sites with variable range of analyses and frequencies of sampling).

Task 3: Literature Review

Purpose:

Information about the study area is available in reports and other forms of literature associated with the study area. The literature review is to provide a comprehensive summary of the contents of all the relevant literature. Not only is the review important for the current project but it will also provide a valuable long term resource for the Agency.

Approach:

A list of known References is given in Appendix 2. This list is not meant to be all-inclusive, and the Consultant will be expected to examine other reports and papers as appropriate. Sources of reference material include, papers in published Journals, Geological Memoirs, Water Company and Agency reports (and those of the previous organisations), University theses and reports, reports of contractors, maps (geological, hydrogeological, topographical, soils, mineral assessments, etc.), computer programs,

The main tasks in a literature review include:

(a) Providing a list of all the available literature,

(b) Preparing a brief summary of the contents of each item;

(c) For references which have a particular relevance to the current study; the important information or insights should be presented in the main text of the Phase I report (Task 12).

(e) Critical yet constructive comments should be provided about the important contributions.

Outputs:

A brief summary of each key reference will be presented by the Consultant as an Appendix to the Phase I report (see Task 12).

Task 4: Interpretation of Lithological Logs

Purpose:

The Consultant shall utilise the lithological logs together with various geological and topographical maps, memoirs and mineral reports to develop an understanding of the geology and to define the hydrogeological units.

Approach:

The borehole records acquired by the Consultant during Task 2 should be entered into a database to enable visualisation of the Solid and Superficial deposits in aerial plan and cross-section. (This work is considered to be of high priority and will form the main basis for assigning the various layers in the later numerical model.)

The Consultant should use MS Access 97 for this or any database work undertaken in this study. The Agency should be consulted as to the database format required to ensure compatibility with any existing database. The resulting data set must be made available to the Agency at the end of the project.

The Consultant will be required to explain in their proposal how the issue of limited or conflicting evidence will be resolved.

Outputs:

During this Activity the Consultant shall produce the following:-

1) Contours of the base of the ***[AQUIFER NAME]*** aquifer(s);
2) Contours of the top of the ***[AQUIFER NAME]*** aquifer(s);
3) Contours of the thickness of the ***[AQUIFER NAME]*** aquifer(s);
4) Contours of the thickness of separate drift deposits - where possible (e.g. boulder clay, fluvial sands/gravels);
5) Solid and drift geology maps for the study area;
6) A sufficient number of geological cross-sections to adequately understand the aquifer system.

The Consultant shall produce 1:50,000 scale maps with Ordnance Survey background information as well as cross-sections with a horizontal scale of 1:50,000 to show the above lithological log interpretations. All map overlay images will be maintained in .DXF format for later use by the Agency. Both the maps and cross-sections shall show the same current BGS classification for colouring, ornamentation and stratigraphy. The maps shall post the lithological log sites and the corresponding depth/height value used in the interpretation, while the cross-sections shall show all lithological logs with either full or annotated descriptions. The Consultant shall produce a 1:50,000 scaled map showing the location of all cross-sections, clearly indicating which lithological logs were used in each cross-section. The scale of the maps will be reviewed to ensure that the information illustrated is visible and of a high quality.

Task 5: Interpretation of Hydrochemistry

Purpose:

Insights into the flow processes can be gained from a study of the hydrochemistry. Furthermore the occurrence or risk of contamination of the aquifer system also needs to be examined.

Approach:

The Consultant shall use the groundwater quality data obtained from current and disused sampling points to assess the type, age and origin of groundwater within the study area and whether there has been any change with time. The Consultant shall use the hydrochemistry data available from all water quality monitoring sites to interpret any natural and anthropogenic trends in the aquifer system (including direct abstraction, changes in land use and industry).

Outputs:

The Consultant shall produce time-series and analysis plots to highlight the summary and conclusions of this Activity. In addition, the Consultant shall produce 1:50,000 scale maps with Ordnance Survey background information to show:-

1) isochrones of key determinands (including total hardness, chloride, nitrate), and;
2) regional changes in key determinands.

All maps shall show each sampling point and the corresponding determinand value used in the isochrone interpretation. If in the Consultants opinion the scale of 1:50,000 needs to be reviewed, then this should be discussed with the Project Manager.

PART B PREPARATION OF CONCEPTUAL MODEL

Task 6: Groundwater level analysis

Purpose:

Insights into the long term and short term response of the aquifer to inflows and outflows of the aquifer system can be gained from an examination of the groundwater head hydrographs. Information can also be gained about the horizontal and vertical flow components. The purpose of this task is to examine all the groundwater head information to assist in the development of the conceptual model and to provide a data base against which the adequacy of the groundwater model can be assessed. In examining the groundwater head hydrographs it must be recognised that the response can be influenced by the construction of the borehole (e.g. the length of the open section), the geological structure in the vicinity and the effect of nearby water bodies, pumped boreholes etc.

Approach:

All Groundwater head hydrographs shall be inspected and a full understanding of the hydrograph will be presented. Each description should indicate the quality of record as well as identify and explain influences and significant variations to the hydrograph, especially in terms of seasonal and climatic changes in rainfall, abstraction as well as aquifer properties (e.g. transmissivity, storage). The hydrograph shall be quality checked and any anomalies shall be corrected or removed following agreement with the Agency Project Manager.

Each hydrograph shall be compared to adjacent hydrographs to identify any anomalies or inconsistencies. This will be done by the comparison of hydrographs and not by inspection of contouring. The description for each hydrograph shall also detail a summary of this grouped comparison. In assessing the significance of the hydrographs, a description should be presented of horizontal and vertical flow patterns and hydraulic gradients

If the Consultant proposes to undertake contouring via a computer package then the Consultant will be expected to produce at least one hand drawn contour for each of the contouring periods identified. The computer generated contouring method will be adjusted and the generated contours compared to the corresponding hand drawn contours until a good fit is realised with the same parameters. All required contours may be generated using the best-fit parameters. Each contour shall be inspected and any anomalies, inconsistencies and trends shall be documented.

Whichever technique is selected for contouring, the Consultant shall take into account the effect of ground features on water levels (including ground surface, confining areas, rivers, springs etc.); data points should be presented on all contour diagrams.

Outputs:

Plots of all groundwater head hydrographs using at the most three vertical scales. Any lines drawn through field data should be discontinuous where data are missing.

Contours for various times throughout the refinement period shall be prepared. At a minimum all contours for the following periods shall be included and supplied as 1:50,000 maps and DFX files.:-

1) contours for the climatic wettest year;
2) contours for the climatic driest year;
3) contours for an average year; and,
4) contours for the first and last year of the study period.

The Consultant shall provide an audit of any changes made to the data together with reasons for the changes. The audit shall document all Agency Project Manager approvals relating to the correction or removal of data.

The Consultant shall draw on the lines of maximum, minimum and average water tables or piezometric heads for each of the cross-sections produced in Task 4.

Introductory Comments on Tasks 7 to 9

Tasks 7 to 9, Calculation of Effective Rainfall and Estimation of Actual Recharge, River Flow Analysis and Preparation of Preliminary Water Balances, are all part of the understanding and quantifying the flow processes within the aquifer system. There will be uncertainties when carrying out these tasks, especially when interaction between groundwater and surface water is involved. Nevertheless, it is essential to attempt to quantify the processes (acknowledging the uncertainties) so that a decision can be made as to whether there is sufficient information and understanding to proceed with modelling.

Task 7: Calculation of Effective Rainfall

Purpose:

An important part of the study is to understand and quantify the runoff and recharge processes so that the total catchment response (both surface water and groundwater) is represented. Therefore the first step is to identify the nature of the flow processes close to the ground surface and soil zone and also from the bottom of the soil zone to the permanent water table. The approach should consider both rural and urban areas. Conceptual models should be developed for the different types of conditions that can occur. All possible conditions should be considered such as near surface drainage, the possibility of runoff subsequently recharging the aquifer, the ability of the aquifer to accept the water, leakage through drift, etc.

Approach:

The calculation of effective rainfall and potential recharge is an important 'first-step' in the estimation of both rainfall recharge and runoff. The Consultant should describe in its proposal how it intends to use the rainfall, potential evapo-transpiration, soils and land-use data collected earlier to calculate effective rainfall (potential recharge) on a daily (not monthly) basis for various rainfall stations over the previously defined study period.

The Agency is developing a standard methodology for estimating precipitation recharge based on a Distributed Precipitation Recharge Model. The method will allow modifying (monthly) factors to be applied to the effective rainfall to allow future modelling of the effects of climate change. Any computer programs (source code and executable) used by the Consultant to undertake this calculation should be available to the Agency at the completion of the project.

Outputs:

The Consultant shall produce 1:50,000 scaled maps with OS background information showing all rainfall and climate station locations. The maps shall include all current and disused sites (the disused sites will be those being active during the refinement period) and shall be annotated accordingly. If in the Consultants opinion this scale needs to be reviewed, then this should be discussed with the Project Manager.

The Consultant should also indicate how the actual recharge will be estimated. Special reference should be made to areas where the water table is deep, where the water table is high, when superficial deposits are present and the influence of surface water/groundwater interactions.

Task 8: River-flow Analysis

Purpose:

The interaction between rivers, streams or springs and the aquifer is crucial to the development of realistic flow balances. The nature and magnitude of the interaction is always difficult to identify and quantify. Information is available from continuous streamflow gauging and current meter readings. However, the interpretation of field readings is often complicated by poor quality records, poor siting of the gauging stations (for the purpose of identifying river-aquifer interaction) and unreliable information about inflows from Sewage Treatment Works or outflows for irrigation. These difficulties are compounded in urban areas. Nevertheless, imaginative and realistic interpretation of the available data can lead to insights into river-aquifer interaction. This should lead to estimates of the coefficients describing groundwater-surface water interaction.

Approach:

The daily river-flow records from up to ***[number]*** permanent gauging stations will be analysed using conventional baseflow separation techniques to establish the monthly baseflow and runoff contributions to each of the main water courses during the period of historical simulation. River and groundwater levels, drift geology and groundwater chemistry should also be inspected to identify areas of active surface water infiltration. Appropriate Agency hydrologists must be consulted in this work to ensure internal Agency consistency.

Each surface water hydrograph will be inspected and a full understanding of the hydrograph will be presented. Each description should indicate the quality of record and explain significant variations to the hydrograph, especially in terms of seasonal and climatic changes in rainfall, abstractions (either surface or groundwater) as well as artificial influences (e.g. effluent returns). The hydrograph should be quality checked and any anomalies should be corrected or removed following agreement with the Agency Project Manager. The Consultant shall provide an audit of any changes made and reasons for the changes. The audit shall document all Agency Project Manager approvals relating to the correction or removal of data.

The Consultant may propose a current metering programme which will assist in the interpretation of stream/aquifer interaction and hence a better definition of stream accretion. This shall only be done following discussions with and approval from the Agency Project Manager. The current metering programme shall be outside this Terms of Reference but will be based on the staff rates quoted for this Task.

Outputs:

The Consultant shall produce 1:50,000 scaled maps with OS background information (highlighting the river network) showing all surface water hydrometric locations. The maps shall include all current and disused gauging stations and current metering sites and will be annotated accordingly. If in the Consultants opinion this scale needs to be reviewed, then this should be discussed with the Project Manager. The Consultant shall review the need for and carry out as appropriate a river bed level survey and incorporate it onto the Agency's GIS system.

In its proposal the Consultant should demonstrate that it has an awareness (and an acceptance) of the problems that this Task is likely to involve.

Task 9: Calculation of a Preliminary Water Balances

Purpose:

The reason for preparing preliminary water balances is to check on the estimates of the inflow and outflow components. The flow balances should be designed to test different aspects. Flow balances for the whole study area and/or for smaller areas within the total area are equally valuable. Flow balances for the whole study period, for wet, dry and average years are also appropriate in certain situations. For aquifers which show a rapid seasonal response, a balance for a wet month and another for a dry month will help to understand whether aquifer properties change depending on water table elevations. It is unlikely that perfect balances will be achieved; however the inability to explain poor balances may indicate that there is insufficient reliable input data to justify proceeding with modelling.

Approach:

The Consultant is expected to calculate preliminary water balances for the likely model area prior to commencement of the historical modelling (Phase II). The consultant should advise on the appropriate time periods for water balances based on the data available. The water balances will indicate the general availability of water resources in the area and how conditions have changed during the period ***[HISTORICAL PERIOD]***. The Consultant should state in its proposal the assumptions that are likely to be made in the calculation of this preliminary water balance. The Agency attaches great importance to this step in the modelling procedure since it is the first indication of the viability of the conceptual model.

Outputs:

The Consultant shall produce either a single water balance or a series of water balances for different parts of the catchment. A number of water balances should be prepared covering different time periods. If water balances are calculated for sub-areas, then the aggregation of the parts shall cover the whole of the study area. Both total water balances and groundwater balances should be presented. It is unlikely that the numerical sum of the components will be zero, but the significance and reasons for any out of balance should be discussed.

Task 10: Development of a Surface Water/Groundwater Conceptual Model

Purpose:

Groundwater modelling is a cyclical process. From the field data it is necessary to formulate a simplified yet quantitative understanding of how the real flow system operates. This conceptual model forms the foundation upon which the numerical model will be built, therefore, the ideas it embodies need to be comprehensively tested prior to and during any numerical modelling. Prior to the commencement of the modelling, the Agency will require the Consultant to formulate its ideas concerning the dominant aquifer flow mechanisms and the degree of surface water-groundwater interaction into a conceptual model.

Approach:

To illustrate the system's behaviour, the Consultant shall produce relevant hydrogeological cross-sections (between 6 and 10 is typical), water balances at appropriate time scales, relevant river and water level hydrographs and plans showing the hydraulic gradients and the major changes in hydrogeology. Once the conceptual model has been agreed a generalised three-dimensional colour picture of the area should be produced, annotated to highlight key features.

Outputs:

The Agency will require the Consultant to present their ideas concerning the dominant aquifer flow mechanisms and the degree of surface water-groundwater interaction for discussion. The Consultant will:

1. define the extent of the study area and subdivide this into appropriate zones (vertically and horizontally) based on the hydrogeology
2. describe the hydrogeological conditions and flows at the boundaries of the study area
3. identify all inflows and outflows, estimate their size and illustrate their temporal variation
4. estimate the plausible range of all aquifer parameters in each hydrogeologically distinct zone
5. identify the limitations of the current conceptual understanding and the major sources of uncertainty

This conceptual model should include a description of the mechanisms operating in the area, the nature of the inflows and outflows, the number and types of boundaries, and should include a variety of different diagrams of the area, annotated to highlight key features (geological, hydrogeological and hydraulic) and to indicate average or typical flow quantities and aquifer parameter values.

Task 11: Proposed Development and Refinement of Numerical Model

Purpose:

Once a conceptual model has been agreed, the flow mechanisms identified can be represented numerically and the output compared with observed data and other information. The aim of this task is to construct a numerical model based on the conceptual model which is refined until it can can adequately simulate the field behaviour.

Approach:

The Consultant shall consider how the model will be set up based on the conceptual model and what features need to be successfully represented in order to give confidence that the model is adequate to answer the questions for which it has been developed. Acceptance criteria should be proposed and agreed with the Agency prior to building the numerical model.

The Consultant shall explain the method and rationale used to assign parameter values and inflows and outflows.

The Consultant shall clearly describe and justify the extent of the model and the location of the model boundaries, how space and time will be discretised, and the model layering. The layering shall be justified on the basis of the conceptual model by considering the flow system and the relationship between hydrogeological units. The hydrogeological conditions at the boundaries of the model shall be defined and their representation in the numerical model discussed. A figure shall be presented superimposing the model grid on the study area and shall highlight significant features, such as water bodies, geological features and physical boundaries. The dimensions of the grid blocks or elements and the number of nodes in the grid shall be clearly stated.

The location, value and associated tolerance for all head and flow targets shall be defined, justified and presented on a basemap. The Consultant shall propose acceptance criteria to define when the historical model has been sufficiently refined. These will pay due regard to groundwater levels, water level trends, groundwater horizontal and vertical flow patterns and hydraulic gradients, volumes of total river flow and surface/groundwater interactions including accretion profiles.

The Consultant shall include proposals for performing a model sensitivity analysis in order to establish the effect of uncertainty on the calibrated solution. Where appropriate the Consultant shall present the convergence criteria to be used during each model run.

Outputs:

The Consultant shall recommend and justify the following:

1. the extent, layers, orientation and nodal spacing of the model grid
2. the period of simulation and discretisation of time
3. the representation of boundary conditions and initial conditions
4. the aquifer types, geometry and properties
5. the spatial and temporal variation in recharge
6. the representation of abstraction
7. the representation of flow between model layers
8. the surface water-groundwater interactions
9. the choice of code

The model layering shall be justified on the basis of the conceptual model by considering the flow system and the relationship between hydrogeological units.

On completion of this Task the Consultant shall discuss with the Agency their proposals for constructing and testing all the above aspects of the historical model. The Agency Project Manager will require agreement on the proposed method for developing and refining the model prior to commencement of Phase II.

Task 12: Formulation of Phase I Report

Purpose:

The Phase I report is intended primarily for internal use by the Agency. The earlier sections will provide a record for the Agency of data and information relevant to the study area. The presentation should be in a suitable form for updating.

In addition the Phase I report will provide detailed information about the conceptual model and the associated parameter values. The uncertainties should be stated and possible methods of resolving them during subsequent phases of the work should be explained.

Approach:

The Phase I report with Appendices should provide a comprehensive record of the methodologies adopted and the findings of the Phase I study. It should be sufficiently complete for another consultant to carry out subsequent Phases of the work.

Outputs:

Four copies of a draft Phase I report (one each for the area, region, National Centre and external modelling advisor) should be presented. The report will include the following items:

1) Presentation in graphical and tabular form (where appropriate) the raw data as collated in Task 2 e.g. digitised (AutoCad) topographic, geological and piezometric maps, river-flow and groundwater hydrographs, tabulation of groundwater and surface water licence information;

2) Summary (in the form of an Appendix) of the key reference papers identified in Task 3, including a full reference of all relevant literature;

3) Interpretation and presentation (again preferably in graphical form) of data and information collated in Tasks 2, 4, 5, 6 and 8 e.g. maps and cross-sections showing the thickness and nature of Superficial Deposits deduced from borehole log information, results of baseflow separation analysis and interpretation of previous Agency low-flow surveys;

4) Presentation of the effective rainfall and water balance estimates from Tasks 7 and 9, and the proposed conceptual model from Task 10;

5) Indication of any extra data needs, especially river flow information, to enable the Agency to initiate a data collection programme; and

6) Formulation of the initial model design, including model dimensions, recharge and boundary conditions, general aquifer and riverbed characteristics, refinement and sensitivity analysis criteria from Task 11.

This draft report will be presented and discussed at a progress meeting between the Project Manager and Senior Modeller of the Consultant and the Project Review Panel. Prior to the meeting, the Consultant should allow up to six weeks for consideration by the Agency of the draft report and any modifications required for the final stage report. Any presentation materials used during the meeting should later be made available to the Agency. ***[NUMBER]*** hard copies of the final version of the report (including colour maps and cross-sections where appropriate) will be issued within one month of this meeting. The report should be produced to a high quality. It should be comb bound, laser printed and photocopied, unless otherwise agreed with the Agency. Colour photocopies shall be provided of relevant graphical outputs etc. The report should also be provided on computer diskette in a form compatible with Agency word processing systems i.e. Microsoft Word 97.

It is important to realise that the Consultant shall not proceed with Phase II of the Study unless or until the Agency has agreed in writing:-

1) the standard of data interpretation and details of the conceptual model (Phase I)

2) the methodology for development of the numerical model (Phase II).

Unless otherwise instructed, any progress prematurely undertaken in subsequent Phases will be done so at the consultant's own risk and cost. Should agreement not be reached at this stage, the Agency reserves the right to terminate the contract and payment will only be made for the work completed to that time.

Phase II: Development and Refinement of the Historical Model

Task 13: Construction of Model

Purpose:

The Consultant shall transpose their conceptual understanding into a time variant numerical model which fully represents the agreed flow behaviour of the aquifer system.

Approach:

The assumptions or modifications required in simplifying the conceptual understanding into the numerical model shall be fully documented. As a demonstration of the Consultant's modelling ability it should include in its proposal a brief discussion of the likely model boundary conditions for this Study and its suggestions as to the sort of refinement criteria that may be appropriate.

Outputs:

A groundwater model representing all the features listed under Task 11 and those documented in the Phase I conceptual model.

Task 14: Model Refinement

Purpose:

The model will be refined against the historical behaviour for the period ***[19?? to 20??]*** of the surface water and groundwater system until the acceptance criteria defined in Task 11 have been met or the Agency has agreed that further refinement runs are unnecessary.

Approach:

The Agency requires an initial testing of the sensitivity of the model results (outputs) to agreed changes in key mechanisms or parameters. A logical series of modifications to the model will then be agreed and carried out. The Agency will not accept arbitrary modifications to model mechanisms or parameters which cannot be justified by logical, physical explanations based on analysis of the observed data and other available information.

The Consultant shall maintain an audit of all refinement runs and shall keep the Agency informed of any problems or successes. The audit shall also include details of any changes to the conceptual model needed to effect a better match with the observed historical behaviour.

Appropriate numerical convergence criteria in terms of both head and flow will be agreed in consultation with the Agency. Typical values from previous modelling projects are given as guidance: a maximum head difference of around 10^{-4} m at any node and a flow imbalance of no more than 0.1 % of the recharge at any node

Outputs:

Comprehensive comparisons between field and modelled results will be made. These will include:

Groundwater Heads

- maps and cross-sections of groundwater heads
- hydrographs of groundwater head
- horizontal and vertical head gradients

Groundwater-Surface Water Interaction

- spring and river flow hydrographs
- river flow accretion diagrams
- plots showing gaining and losing reaches of streams

Water Balances (both total and groundwater alone)

- long-term average water balances for all components of the water budget
- time series of components of the water budget for the whole catchment and appropriate sub-catchments

Any other comparisons considered appropriate for testing whether the numerical model is able to represent the flow behaviour of the real system sufficient for the purpose of the study and the modelling objectives defined in Section 1.3)

Task 15: Model Sensitivity Analysis

Purpose:

The Consultant will undertake a rigorous sensitivity analysis of the behaviour of the model to determine the influence of uncertainty. This analysis may indicate the need for additional field investigation.

Approach:

The Consultant and the Agency will have identified the major sources of uncertainty in Task 11 and documented them in the Phase I conceptual model report. Uncertainty resulting from the following sources should be considered:

1. the field data
2. the adequacy of the conceptual model and possible alternative formulations
3. the mathematical and numerical representation of the flow mechanisms
4. the input parameters applied to the numerical model

The sources of uncertainty appropriate for investigation during sensitivity analysis will be agreed.

During the model refinement, the significance of the important model parameters in achieving an adequate match between field and modelled results will become apparent. In the sensitivity analysis, modifications to a single model parameter should be made (for complex models the changes may be made over a restricted area) and the effect on the simulation should be noted. Changes in horizontal hydraulic conductivity and specific yield should be of the order of 50 to 100%; for vertical hydraulic conductivity and confined storage coefficients, changes of one half to one order of magnitude should be made. The sensitivity to river coefficients should also be explored.

As a further demonstration of the Consultants modelling capabilities it is asked in its proposal to provide an indication of the parameters likely to require investigation in this way.

Outputs:

In the sensitivity analysis, many results will be obtained; skill is required in selecting comparisons between field and modelled results which demonstrate where greatest changes occur. Diagrams should be presented which clearly illustrate the influence which the sources of uncertainty have on the modelled results.

Task 16: Formulation of Phase II Report

Purpose:

The Phase II report is intended primarily for internal use by the Agency. The report will explain clearly how the model has been developed and refined. Any uncertainties or inadequacies of the model should be stated and possible methods of resolving these uncertainties (by field work and/or further model development) should be explained.

Approach:

The Phase II report with Appendices (such as the log of the important model runs and complete sets of figures showing how model refinement led to an improved simulation) should provide a comprehensive record of the methodologies adopted and the findings of the Phase II study. It should be sufficiently complete for the Agency or another consultant to update and improve the model.

Outputs:

Four copies of a draft Phase II report (one each for the Region, Area, National Centre and external modelling advisor) should be presented. The report will include the following items:

1) Presentation of details of the model refinement and sensitivity analysis including comparison of modelled and observed river and groundwater hydrographs, river-aquifer interactions and groundwater hydraulic gradients and flow directions;
2) Any revised understanding of the hydrogeology, recharge, surface water-groundwater interactions;
3) Model piezometric maps and groundwater cross-sections;
4) Deductions as to the impact of historical groundwater abstractions on surface water flows and regional groundwater levels.

The Consultant shall state clearly within the report the assumptions and limitations made within the calibrated model.

This draft report will be presented and discussed at a progress meeting between the Project Manager and Senior Modeller of the Consultant and the Project Review Panel. The Consultant should allow up to six weeks for consideration by the Agency of the draft report and any modifications required for the final Phase II report. Any presentation materials used during the meeting should later be made available to the Agency. ***[Number]*** hard copies of the final version of the report (including colour maps and cross-sections where appropriate) will be issued within one month of this meeting. The report should be produced to a high quality. It should be comb bound, laser printed and photocopied, unless otherwise agreed with the Agency. Colour photocopies shall be provided of relevant graphical outputs etc. The Consultant should make available the model input files and results of the refinement and sensitivity runs on computer diskette.

It is important to realise that the Consultant shall not proceed with subsequent Phases of the Task until receipt of written instruction from the Agency Project Manager. Unless otherwise instructed, any progress

prematurely undertaken in subsequent Phases will be done so at the Consultants own risk and cost. The Agency reserves the right to terminate the contract and payment will only be made for the work completed in Phases for which work has been instructed.

Phase III: Modelling of Resource Options

Task 17: Identification of Predictive Simulations

Purpose:

Predictive simulations will be carried out related to the specific problems identified in Section 1.3.

Approach:

The Consultant shall seek the advice of the Agency and other members of the Project Board to identify a baseline run and ***[ten]*** further predictive runs based on the options for the future management of the ***[CATCHMENT NAME]*** catchment. Written confirmation for at least ***[five]*** of these options will be provided during Phase II, while the remainder may be provided as a result of the initial prediction runs. Any additional predictive runs (including the associated sensitivity analyses) shall cost a maximum of one ***[tenth]*** of the Fixed Fee for this Activity per run.

In planning the predictive runs it is necessary to identify the period for which the predictive runs will be carried out and the starting conditions. ***[The approach generally adopted is to assume that rainfall, evapo-transpiration and potential recharge follow the historical sequence. For chalk and limestone aquifers which refill frequently, the starting conditions are as for the historical simulation but for sandstone aquifers the starting conditions are taken as the heads at the end of the historical simulation.]***

Task 18: Model Predictive Runs

Purpose:

To run the predictive simulations, carefully examine the outputs to identify the consequences of the management options and ascertain the reliability of the predictions.

Approach:

The refined model of Phase II will be used for each of the predictive runs listed in Task 17. The Consultant shall also identify the sensitivity of the findings due to the major sources of uncertainty as identified in Task 15.

Outputs:

Comprehensive comparisons of each run and results of the base run (and the other predictive simulations) will be made. All the outputs listed under Task 14 will be considered and conclusions drawn:

Deductions as to the impact of each of the proposed management options on surface water flows and regional groundwater levels. ***[Any other aspect of the system (e.g. water levels in a wetland) which the Agency requires to be considered should be defined here or agreed with the Consultant in writing during the project].***

Task 19: Formulation of Phase III Report

Purpose:

The Phase III report should provide a comprehensive account of the predictive simulations, summarise the results and highlight the findings.

Approach:

Four copies of a draft Phase III report should be presented. The report will include the following items:

1) Presentation of details of the resource option modelling, including comparison of historical, baseline and other predicted simulations for <u>Groundwater Heads</u>.
2) Presentation of corresponding results for <u>Groundwater-Surface Water Interaction</u>
3) For each of the simulations appropriate <u>Water Balances.</u>

This draft report will be presented and discussed at a progress meeting between the Project Manager and Senior Modeller of the Consultant and the Project Review Panel. Any presentation materials used during the meeting should later be made available to the Agency. Four copies of the final version of the report (including colour maps and cross-sections where appropriate) will be issued within one month of this meeting. The report should be produced to a high quality. It should be comb bound, laser printed and photocopied, unless otherwise agreed with the Agency. Colour photocopies shall be provided of relevant graphical outputs etc. The report shall also be provided on diskette in a form compatible with Agency Word Processing systems. The Consultant should make available the model input files and results of the predictive runs on computer diskette.

Phase IV: Final Report

Task 20: Final Report

Purpose:

Although individual reports have been prepared for each of the three preceeding tasks, a Final Report is required. Following the successful completion of Phase III, the consultant shall produce a final report which would be suitable for presentation at a Public Inquiry.

Approach:

The Final Report should cover all aspects of the study; it is anticipated the final report will consist of ***[50 – 100]*** pages of text. The Consultant shall agree with the Agency Project Manager the exact contents of the report at the end of Phase III

This will be an Agency report where the Consultant is writing on behalf of the Agency and, therefore, may require the incorporation of material or information external to this Task but needed by the Agency. All such additional information will be provided by the Agency. The report shall require a greater level of interchange between the Consultant and the Agency and as such the Consultant shall anticipate at least three draft versions of the report. The Consultant shall issue ***[four]*** copies of each draft version of the report. The title of the draft reports shall reflect the draft version number.

Following approval by the Agency Project Manager that further drafts are not required the Consultant shall issue within one month of approval ***[thirty]*** copies of the report, an unbound copy for duplication and diskettes of both text and maps.

Outputs:

As a minimum the report shall encompass the following:-

1) a description of the ***[CATCHMENT NAME]*** catchment and the various issues for long term management;
2) the purpose of the model and the specific objectives required of the modelling;
3) the development of the conceptual understanding of the aquifer system and detail any uncertainties and limitations in this understanding;
4) a summary of the model development and refinement. The assumptions and simplifications employed and their rationale will be discussed. The limitations of the model at this stage will be clearly stated. There should be sufficient detail in associated appendices for the Agency modelling staff to be able to repeat any model simulation run by the Consultant ;
5) implications of management option prediction runs;
6) a description of the computer model code and all utility routines;
7) an assessment of the influence which the uncertainties about the system are having on the behaviour of the model and the implications in terms of the model results and the conclusions drawn. The relative importance of the sources of uncertainty, identified in Task 15, should be considered.
8) the limitations of the model for predictive assessment; and,
9) the need for additional work/investigations.

Phase V: Training and User Support

Task 21: Compilation of a User Manual

Purpose:

The Agency should be able to use the User Manual to input the model data, repeat any simulation and process the results in the same way as the Consultant as well as providing the Agency's modelling staff with sufficient guidance to be able to extend the model by adding future data of the same type (e.g. future years abstractions and recharge distributions)

Approach:

The Consultant is expected to develop a User Manual (in addition to the standard guide that accompanies the software) which Agency staff can use to become acquainted with the key commands and error codes of the software and the model layout. The form of any ASCII data files should also be described, so that as the Agency becomes proficient in the use of the model they are able to can make data entries and modifications directly through a text editor.

Outputs:

The User Manual should be accompanied by copies of the model data files and the source code along with any executable programs which have been used to develop or run the model. The consultant will also supply any spreadsheets and databases developed during the Study. These files will be delivered on an appropriate medium.

Task 22: Provision of a Model Training Course

Purpose:

The aim of the Training Course is to ensure that the Agency can run the model(s) efficiently and confidently.

Approach:

The Consultant will run a two-day 'hands-on' course for up to four Agency staff at the Agency's ***[OFFICE LOCATION]*** offices to provide initial training on the setup and use of the model(s), on computers to be provided by the Agency. It is particularly important to demonstrate how other resource options can be investigated.

After the Agency's modellers have had opportunity to work with the mode, a further two days training will be provided.

Outputs:

The course shall be run within three months of the agreed satisfactory completion of Phase IV.

The Consultant shall install and test the software on Agency computers.

Task 23: Provision of Model Support

The Consultant will provide twelve months telephone support for the model, guaranteeing a two-day response time to Agency queries regarding the setup and running of the model.

Phase V does not require formal reporting. However, the Consultant will be expected to have completed Tasks 21 and 22 within ***[CONTRACT LENGTH]*** of the date of commission of the Consultant.

3 MODEL SPECIFICATION

The tender document will identify various aspects of the modelling requirements and the preferred approaches; reference will also be made to Documentation and User Manuals.

Currently work is being carried out by the Agency on the specification of models for the recharge, runoff and regional groundwater flow processes. Copies of this Chapter from previous tender documents are available (contact Paul Hulme at the Groundwater Centre) but considerable experience has been gained since the earlier documents were prepared.

4 PROPOSAL ITEMS

The proposal prepared by contractors will include a detailed technical proposal, a description of the staff who will carry out the project, the time allocated to each task, project management, quality assurance. fees and costs. Information will also be presented on the method of tender evaluation to be used by the Agency.

As with the model specification, significant developments in methods of management and tender evaluation are occurring within the Agency. This chapter on Proposal Items must be prepared very carefully to ensure that the contractor provides all the necessary information to allow a fair and consistent method of tender evaluation. Work is being carried out to prepare a template for the Proposal Items chapter; copies of previous documents for this item can be obtained through Paul Hulme.

Appendices may include

Appendix 1

Brief description of the aquifer(s) to be modelled

Appendix 2 - List of references

Note: This appendix lists published material relevant to this modelling study and is not exhaustive.

Appendix 3 - Known Problems for Conceptualisation

DETAILS OF PARTICULAR PROBLEMS IN THE AREA TO BE MODELLED WHICH NEED TO BE TAKEN INTO ACCOUNT BY THE MODEL.

Appendix 4 - Data available from the Agency

Within the Scope of Work the Consultant is required to collate and process various data for both conceptualisation (including water balances) as well as for model calibration. However, the data available from the Agency may not have been quality assured and will also be of variable duration and monitoring frequency. To assist the Consultant in developing an appreciation of the potential data available this Appendix has been provided to give an overall summary of four key data sources, namely groundwater levels, gauging stations, rainfall/climate stations and abstraction returns.

The summary of data available from the Agency is as follows (with no evaluation of the quality of data):-

Groundwater level monitoring sites	***[No.]***
Surface water level and flow monitoring	
Gauging stations	***[No.]***
Rainfall and climate stations	
Rainfall station - current	***[No.]***
Rainfall station - terminated	***[No.]***
Climate station	***[No.]***
Licence database	
Groundwater (PWS)	***[No.]***
Groundwater (Other)	***[No.]***
Surface water	***[No.]***
Impoundment	***[No.]***
Other	***[No.]***
Licences with abstraction returns	***[No.]***

Appendix 5 Functional Objectives

The modelling approach should satisfy the following capabilities:-

APPENDIX B

HYDROGEOLOGICAL INVESTIGATIONS IN THE KENNET VALLEY

1 Background

The Kennet Valley aquifer unit comprises a thick sequence of unconfined Chalk that forms the Berkshire and Marlborough Downs at the western end of the London Basin (Figure 1 – geology/cross-section). The basinal structure extends across the Kennet Valley unit along a WSW–ENE axis. The asymmetrical nature of the basin is such that to the north of the axis a pronounced Chalk dip-slope dips gently to the SSE from a marked escarpment that forms the NW boundary of the aquifer unit. The southern limb and boundary have been subjected to monoclinal folding associated with the Alpine orogeny that bring the underlying Upper Greensand and aquifer base to the surface. To the eastern end of the Kennet Valley the Chalk becomes confined beneath an increasing thickness of Tertiary clays of the London Basin proper. The western boundary is formed by an extension of the NW escarpment as the dip moves to a more easterly direction.

The aquifer unit comprises the Upper, Middle and Lower Chalk and the underlying Upper Greensand. Below this the Gault Clay marks the aquifer base. The aquifer is relatively free of drift, with minor deposits of clay with flints and plateau gravels marking the interfluves and fluvial deposits lining the rivers. Tertiary clays cap the higher ground towards the east of the aquifer unit.

The Kennet Valley Chalk is drained by the River Kennet system, a major tributary of the River Thames. The river flows in an easterly direction from springs in the Marlborough area and is almost entirely reliant on Chalk groundwater for its flow until it crosses onto the Tertiary clays at Newbury. Several south-flowing tributaries draining the northern dip slope, notably the Lambourn and Og, join the Kennet upstream of Newbury. All of these watercourses display a winterbourne nature typical of Chalk streams.

The north-eastern part of the aquifer drains to the River Pang, a direct tributary of the Thames. The scarp slopes at the northern, southern and eastern edges of the aquifer unit are drained by springs.

The Kennet Valley Chalk is heavily exploited for public water supply, with 31 sources of 0.35 Ml/d to 20 Ml/d being operated, principally, by Thames Water.

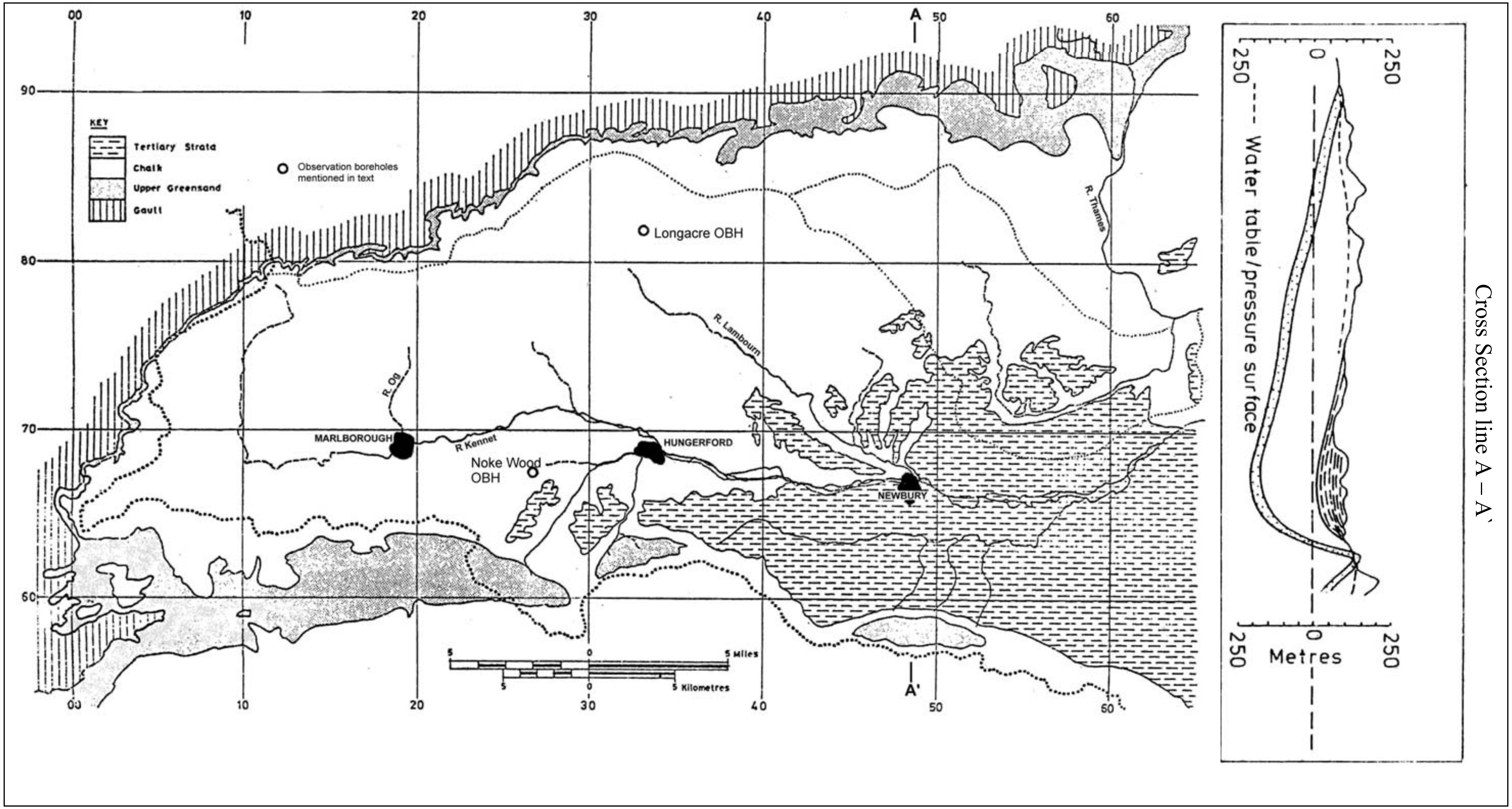


Figure 1. The Chalk-Upper Greensand aquifer in the Kennet Valley and adjoining areas

2 Thames Conservancy / Thames Water Investigation

In the 1950/60s the Thames Conservancy investigated the possibility of using groundwater to augment stream flows in extreme droughts, and ensure the security of large surface water abstractions from the Thames further downstream.

One recommendation of the investigation carried out by the Thames Conservancy was the development of Chalk groundwater resources in the catchment of the River Kennet. A Pilot Scheme was carried out in the Lambourn Valley during the period 1967 – 1969, the objectives of the scheme being:

- determination of the yield characteristics of the boreholes;
- determination of the hydraulic properties of the aquifer;
- determination of the effects of pumping on the aquifer/stream system;
- determination of the optimum mode of conjunctive operations with surface water resources.

The Pilot Scheme involved the drilling and testing of 9 augmentation boreholes, 5 of which were close to the perennial section of the Lambourn, 3 in the intermittent Winterbourne tributary valley, and 1 in the dry Boxford valley (for details see Figure 2).

The results of the testing (Thames Conservancy, 1971) showed there to be a good connection between the river and aquifer, and boreholes adjacent to flowing sections provided little net gain to the river as they recirculated river water rather than taking from aquifer storage. In the intermittent and dry valleys, the take from storage was more substantial and the net gain at Shaw gauging station, near the downstream limit of the Lambourn, was 43% of total abstracted water (Figure 2b). The perennial head of the Winterbourne stream was artificially maintained by the augmentation of flow, even though the natural head migrated rapidly downstream.

The testing also showed boreholes sited away from the perennial reaches to depart from the response of a homogeneous aquifer, with increased drawdowns and reduced yields. Short term testing of the boreholes in normal years was not indicative of drought performance and the requirement to locate at distance from perennial reaches needed to be balanced with the reduced transmissivity (T) and storage coefficient (S) values encountered at such locations.

The conclusions reached from the Pilot Scheme were:

- good hydraulic connection between river and aquifer
- need to site boreholes distant from perennial parts of stream in order to draw effectively on aquifer storage
- siting needs to be a compromise between net gain efficiency at distance from rivers and reductions in T and yield away from river valleys

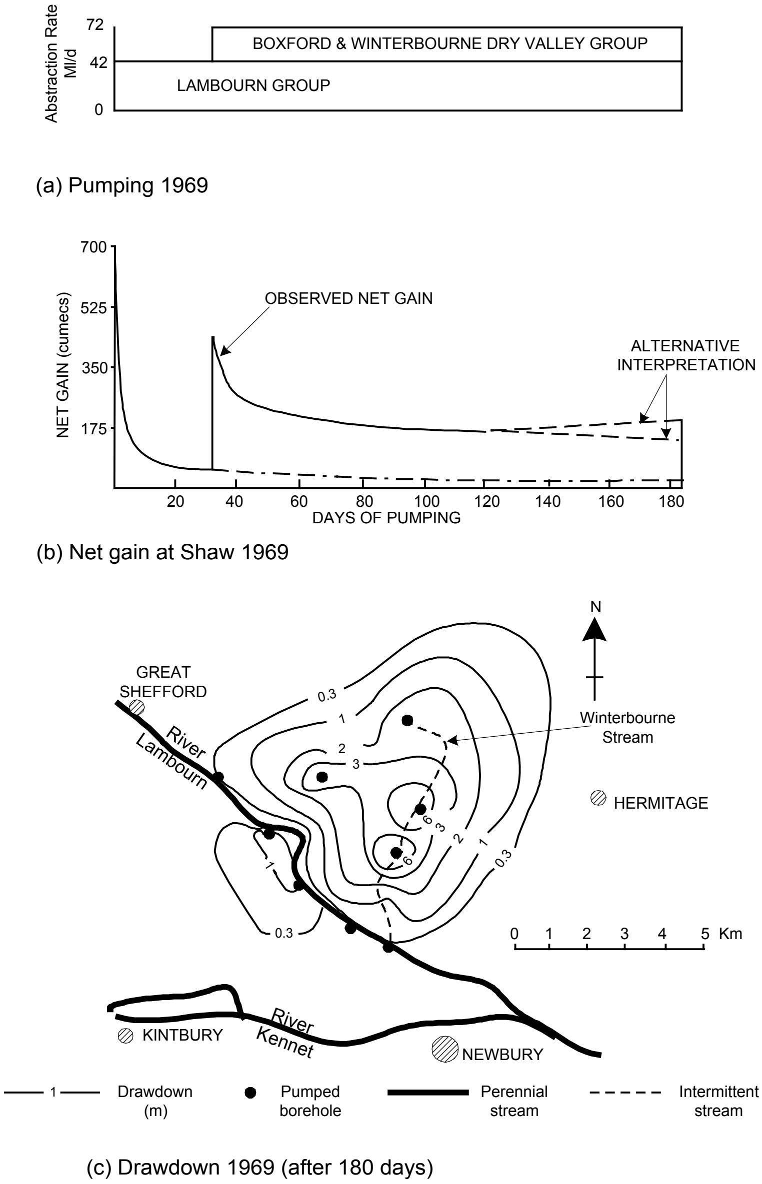


Figure 2. Lambourn Valley Pilot Scheme

At this time the recharge mechanisms at work in the Lambourn catchment were also considered. Evidence was obtained of rapid recharge to the water-table through cracks even when *SMDs* existed. A lumped model of the catchment that previously overestimated the extent of summer stream flow recessions provided much better reproduction of flow with the inclusion of summer recharge.

The information gained from the Pilot Scheme was fed into the development of Stage 1 of the Groundwater Scheme. Thirty-four abstraction boreholes were drilled and individually tested in 1973 -1974, and this provided the first indication of aquifer characteristics.

unconfined	$T = 50\text{-}2500\ m^2/d$	$S = 0.001 - 0.02$
confined	$T = 270\text{-}450\ m^2/d$	$S = 0.0002\text{-}0.00035$

In the unconfined aquifer the results indicated a strong correlation between aquifer parameters and topography, with high *T* and *S* in major valleys with perennial and winter flowing streams, reducing steadily up dry valleys, and rapidly reducing laterally away from the major valleys such that parameters are often 1-2 orders of magnitude lower on the interfluves.

Geophysical logging further revealed the picture of fissure development and showed the effective depth of aquifer to be generally of the order of 60m below valley bottoms in the unconfined Chalk.

In the Autumn of 1975 a group of 5 abstraction boreholes forming the Upper Lambourn wellfield were tested for 3 months under low groundwater level conditions. The yield of the wellfield declined throughout the test from an initial 25 Ml/d to 15 Ml/d, 33% below the estimated yield based on individual borehole tests. This indicated that yields were less than previously thought during drought conditions and analysis showed that low groundwater stage resulted in a significant reduction in *T* and *S* (i.e. *K* variation with depth).

To investigate the interfluvial aquifer areas, a number of observation boreholes were geophysically logged and tested in 1977-78. The location of the major yielding fissures suggested the effective aquifer thickness beneath the interfluves to be less than the 60m thickness beneath the valleys and that very few major fissures exist below minimum groundwater level.

Conclusions relevant to the unconfined Chalk:

- marked lateral and vertical variations in *T* and *S;*
- restricted depth of the effective part of the aquifer;
- fall off of yields in drought conditions.

From the various test results, Robinson (1976) developed a hypothetical map of *T* distribution for the Kennet Valley Chalk. By combining the depth to minimum water level, the saturated thickness of Lower Chalk and distance from a winter flowing stream, a reasonable fit of *T* compared to field data was obtained.

3 University of Birmingham Model Development

Whilst the investigative work was on-going, Thames Water developed a regional groundwater flow model of the augmentation scheme. However, this linear model did not allow for *K*-variation with saturated depth. The significant decrease in borehole yields during periods of low groundwater stage was not reproduced by the linear model. This non-linear response of the aquifer needed to be recreated for an accurate model simulation and a contract was let to the University of Birmingham for the development of a non-linear, *K*-variant depth model to better simulate drought yields.

The development of this model required accurate representation of the behaviour of the Chalk aquifer as identified in the trials and investigations above, particularly:

- representation of the variation of *T* and *S* with saturated depth
- simulation of perennial and non-perennial streams and springs
- lateral variations in effective aquifer depth
- inclusion of summer recharge
- flow between the Chalk and Upper Greensand

The mathematical model was based on finite difference programmes developed at the University of Birmingham (Rushton and Redshaw, 1979) and Thames Water (Connorton & Hanson, 1978). The model area is shown in Figure 3. It consists of a single layer with a mesh spacing of 1 km.

The northern, eastern and south-western boundaries roughly coincide with the base of the Chalk aquifer at the edge of the outcrop. The line of the River Thames forms the eastern boundary and the south-eastern boundary is located in the confined Chalk.

To accurately simulate the aquifer response, the development of the model was particularly focused on six areas:

- Recharge
- Variation of hydraulic conductivity (*K*) with saturated depth
- Variation of the unconfined storage (S_y) parameter
- Simulation of spring and stream flows
- Initial starting conditions
- Representation of the Upper Og catchment

These are discussed in detail in the following sections.

3.1 Recharge

Recharge has been estimated by Thames Water based on a daily soil moisture balance. The drying curve assumes 100% PE above the root constant and 30% PE below the root constant. The root constant is taken as 100 mm for chalk catchments. All summer rainfall transpires at the potential rate. To simulate the summer recharge required to accurately simulate streamflow recession curves, direct percolation to the aquifer was introduced at 15% of effective rainfall during periods when an *SMD* existed (see above).

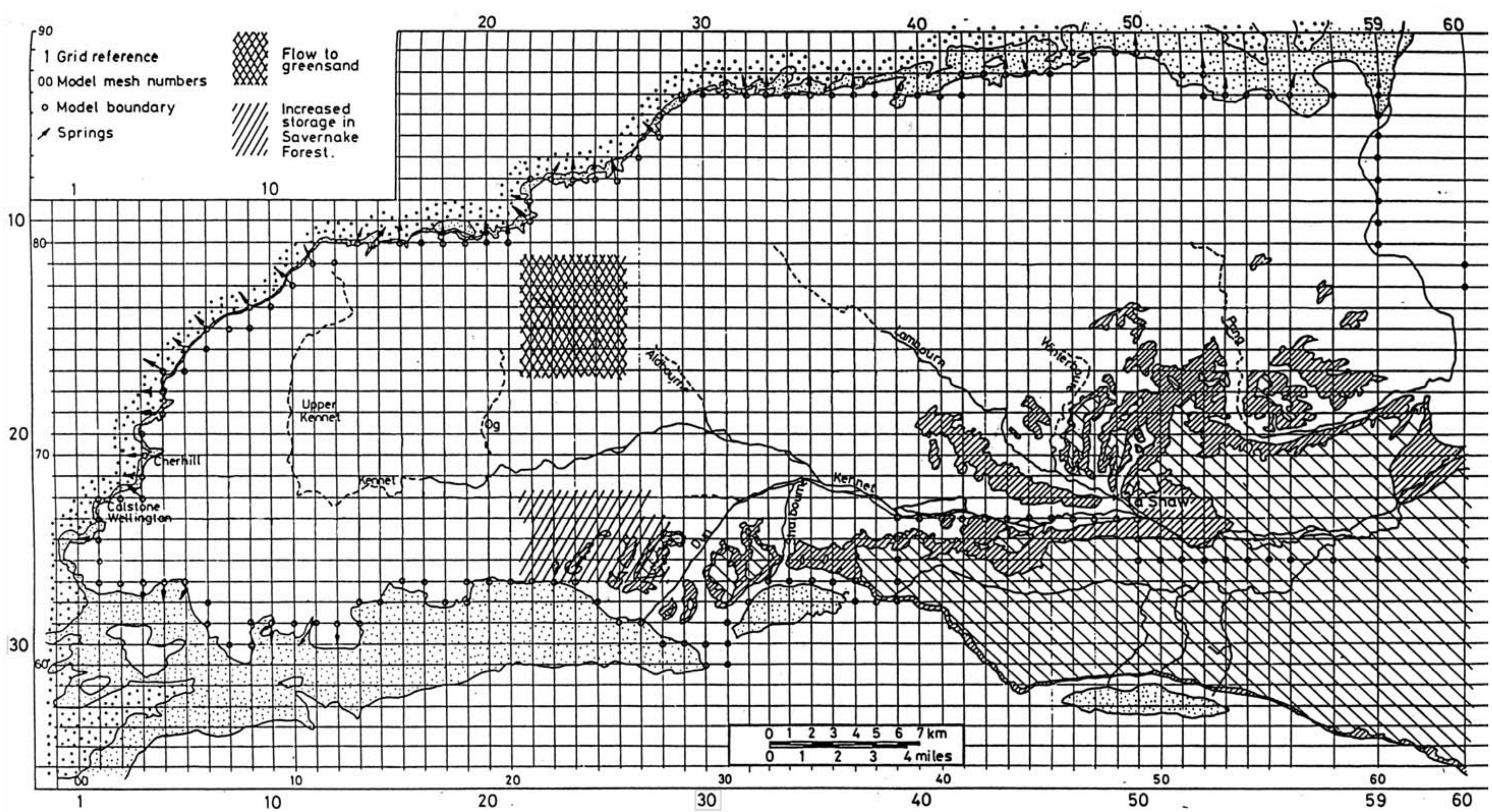


Figure 3. Region modelled, showing springs and streams

3.2 Variation of *K* with saturated depth

Previous models of the area have assumed a constant *K*. However the investigations discussed previously have identified the large variations in *K* that occur with saturated depth. The model was used to explore the magnitude by which *K* varied with depth.

4 parameters were used to explore *K*-variation with depth.

- *FACX* and *FACY*: rate at which *K* changes with depth in x and y directions
- h_d: level relative to initial conditions which represent average groundwater heads and flows
- h_z: thickness of aquifer with uniform *K*

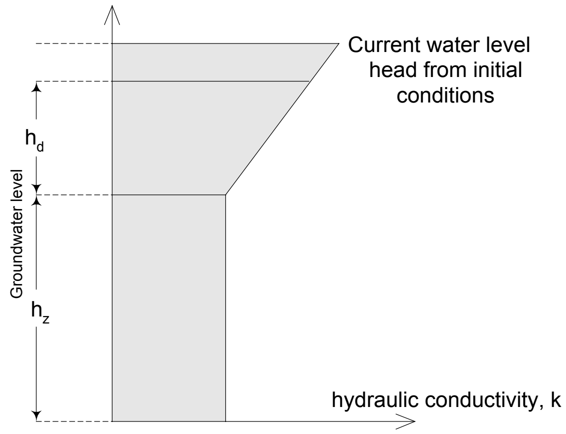


Figure 4. Variation of hydraulic conductivity with saturated depth

Experience of the Kennet Valley Chalk aquifer suggested that where initial *T* (for autumn) < 700m^2/d, winter *T* would not normally increase > 4 times this initial value. Where initial *T* > 700m^2/d, winter *T* does not extend to > 2 times the initial value. The setting of *FACX* and *FACY* were important in recreating this *T* distribution. Where these parameters are set too high, severe changes in *T* can occur leading to unrealistic head variation (see Figure 5).

Varying the spatial distribution of these *K*-variation parameters did not improve the simulation to any great degree. However, re-creation of the reduced aquifer depth below the interfluves, identified in the 1977-78 investigations, was included by reducing the thickness of the zone of constant *K* (h_z) from 40 to 20m where initial *T* was < 700 m^2/d.

The importance of using a depth variable *K* is seen in Figures 6a and 6b. Both stream flows and groundwater head fluctuations exert a much better approximation to field conditions when using a variable *K*.

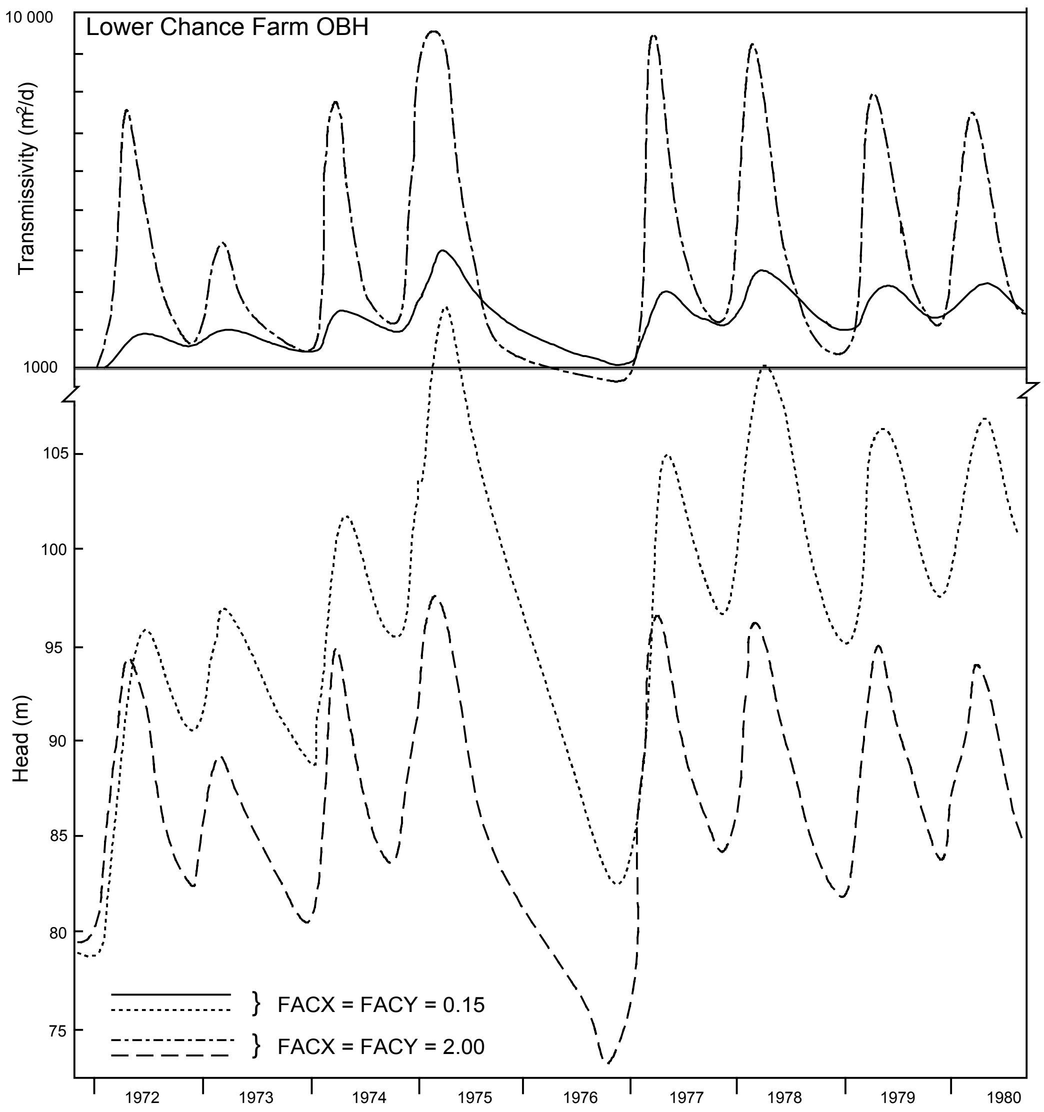
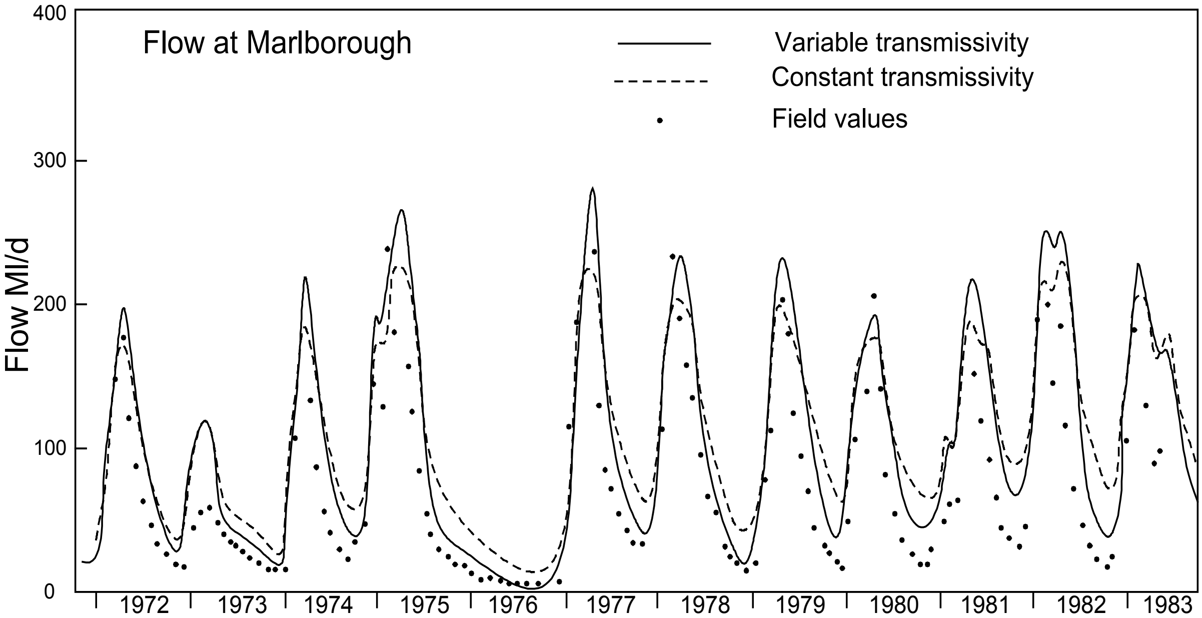


Figure 5. Effect on transmissivity and groundwater head variation of different values of *FACX* and *FACY*.

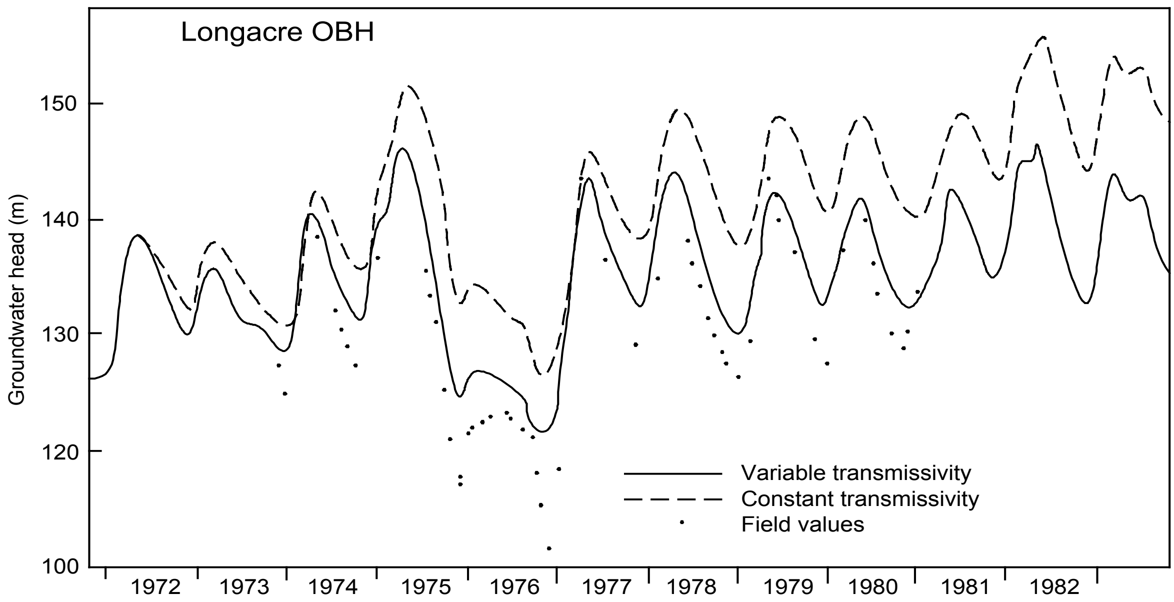
3.3 Variation of S_y

Values of S_y used in Thames Water's linear models were 2.5 times greater than the values obtained from pumping tests to account for the fact that the tests had been undertaken at low groundwater levels. A parameter, *SPARAM*, was incorporated to allow increases in S_y.

The variation of S_y with depth in line with *K* was tested, but this reduced the accuracy of modelled head fluctuations. Consequently, S_y remains constant with varying saturated depth in the model.



6(a). Effect on flow



6(b). Effect on groundwater heads distant from streams

Figure 6. Comparison between simulations with constant and varying transmissivity

Further investigation of the lateral variation in S_y was undertaken in an attempt to reduce modelled head variations to more accurately represent observed values. Uniform increases in S_y were modelled, but the enlarged aquifer storage dampened flow variations at Marlborough below that expected. Instead, *SPARAM* was varied non-uniformly in certain areas to better the simulation of modelled head variation. In particular *SPARAM* > 100 was used in the Noke Wood area to mimic the limited head fluctuation there (Figure 7). Subsequently, CCTV work undertaken by Thames Water revealed large fissures in the Noke Wood borehole to support the high S_y.

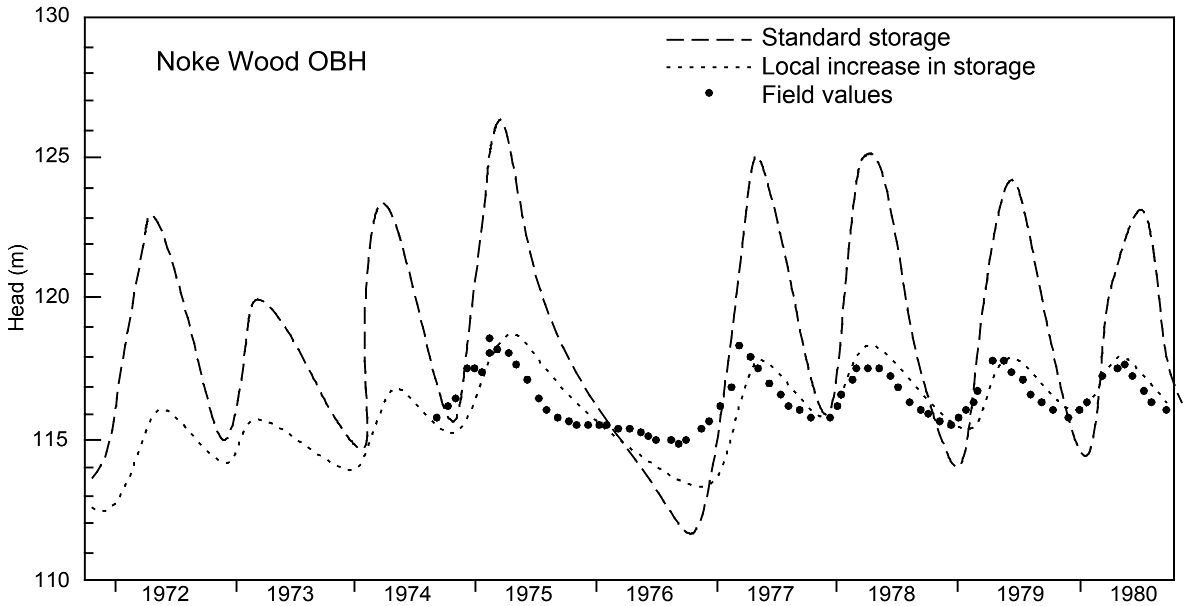


Figure 7. Improvement in simulation in Noke Wood area due to local increase in storage coefficient

3.4 Simulation of Springs and Streamflows

Numerous scarp springs bound the model area on the northern, southern and western sides. Most of these springs flow continuously throughout the year and are represented as constant groundwater heads. The *T* values in the vicinity of these springs are not great and the losses to the springs are not significant compared with the spring flows to the Kennet and Lambourn catchments.

Over the remainder of the model area the winterbourne nature of the Chalk streams means that they are partly perennial and partly non-perennial. The finite difference equations were modified to allow for four types of stream condition:

a) Non-Perennial Streams

For flowing non-perennial streams, the groundwater head, h, is above stream bed level, *SB*, and the stream bed level is assumed to coincide with the stream level, *SH*.

Groundwater flow to stream, *QS*, = *SPFAC* * (*h-SB*)

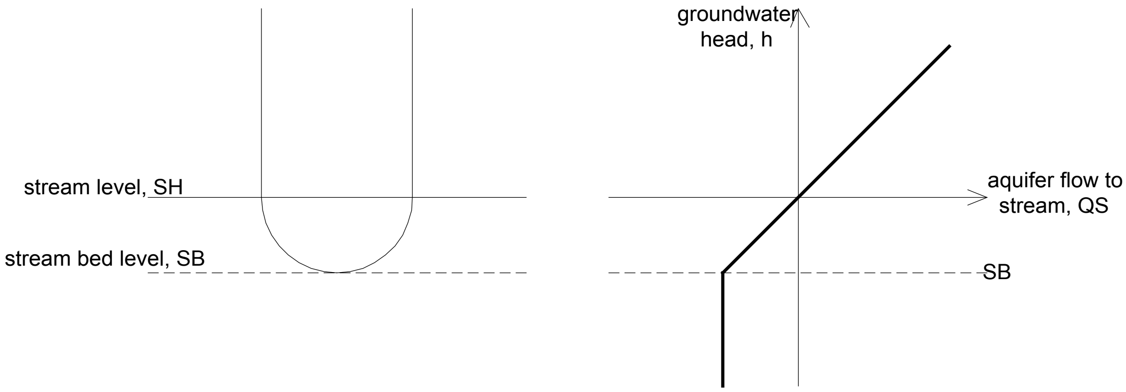
where *SPFAC* is a stream bed *K* factor.

Where non-perennial streams dry up the groundwater head drops below stream-bed level and no flow occurs:

$QS = 0$

b) Perennial Streams

For perennial streams, the stream level is assumed 1m above bed level and if the groundwater head is above stream bed level, flow occurs from the aquifer to the stream.



$$QS = SPFAC * (h - SH)$$

Where the groundwater head is less than stream bed level, no groundwater flow to the stream occurs, and any water flowing from upstream feeds the aquifer.

$$QS = SPFAC * (SH - SB)$$

The use of this approach to model streams resulted in modelled low flows along the Lambourn being too low, no matter what values of *SPFAC* were used. To achieve better approximations to actual flows, stream flows estimated from accretion graphs were used for initial conditions. After initial conditions were achieved, the stream calculation reverts to using the above methods of spring flow inclusion.

A negative aquifer loss of 500 m^3/d was applied to each non-perennial stream node, equating to a small recharge that ensured initial groundwater heads were above normal levels. These locally high groundwater heads were used as the stream bed levels. This negative loss equates to approximately 2% of total initial recharge and proved to be the only way of satisfactorily estimating stream bed levels in non-perennial reaches.

3.5 Initial Conditions

Initial model conditions are of great importance, particularly for a model with *K* variable saturated depth. An approach other than starting with average conditions and moving to a dynamic balance was developed. A time–instant technique was used for the Kennet Valley model, whereby the effective recharge (actual recharge + storage release) is distributed across the model by the aquifer *T*. For the autumn start month, effective recharge was estimated as approximately 40% of average annual recharge and this was distributed using a *TPARAM* = 1.0 since *T* values obtained from the autumn test pumps will be valid for the autumn initial conditions. After initial conditions were achieved, the recharge reverts to normal values.

3.6 Representation of the Upper Og Catchment

Modelled groundwater heads in a localised area north east of the River Og were 15 m higher than actual levels. The probable reason for this is the vertical transmission of recharge to the underlying Upper Greensand rather than lateral transmission through the Chalk. The water appears at nearby Upper Greensand springs. To model this response, a negative recharge of

350 m^3/d was applied to the Chalk nodes in the area (equivalent to half the annual recharge in this area). This reduced modelled groundwater heads by 10-15 m.

4 Conclusion

Several new methods and techniques were developed during the modelling to ensure that the various aquifer features of the Kennet Valley were simulated appropriately. This still necessitated a number of assumptions being made regarding certain aquifer parameters. Nevertheless, the numerical model does give a good overall representation of the aquifer response and reproduces groundwater head variations and stream flows with large annual baseflow variations effectively.

The nodal area of 1 km^2 limited the accuracy of river-aquifer interactions and modelled flows. The estimation of stream bed levels from initial groundwater heads leads to differences between field and modelled groundwater heads. However, this method allows more accurate representation of flows than if stream bed levels were specified and for the nature of this study, it was considered that the representation of flows was of greater importance.

Several improvements to the model were recommended for improved performance:-

- study of flow to the Upper Greensand and subsequent outflow at Upper Greensand springs.
- more detailed examination of recharge estimations, particularly during wetter years.
- better representation of stream flows by a denser mesh spacing and more knowledge of accretion.

The model is still operational and has so far been used to good effect for:-

- examination of major augmentation schemes associated with the Thames Groundwater Scheme.
- investigations of resources in the Upper Kennet area.
- calculation of stream flow responses for the Axford Public Inquiry.

5 References

Connorton, B.J. & Reed, R.N., 1978. A Numerical Model for the Prediction of Long Term Well Yield in an Unconfined Chalk Aquifer, *QJEG*, **11**, 127-138.

Institute of Civil Engineers, 1978. Thames Groundwater Scheme. *Proceedings of the Conference held at Reading University on 12-13 April 1978*.

Robinson, V.K., 1978. Test Pumping of Regional Observation Boreholes in the Kennet Valley Chalk. Thames Water.

Robinson, V.K., 1976. The Hydrogeological Model of the Kennet Valley Chalk Aquifer. Thames Water.

Rushton, K.R., Connorton, B.J. and Tomlinson, L.M., 1989. Estimation of the Groundwater Resources of the Berkshire Downs, *QJEG*, **22**, 329-341

Rushton, K.R. & Redshaw, S., 1979, *Seepage and Groundwater Flow*. Wiley (out of print).

Rushton, K.R. & Tomlinson, L.M., 1985. *Mathematical Model of the Non-Linear Response of the Chalk Aquifer of the Berkshire Downs*. University of Birmingham.

Thames Conservancy, 1971. *Report on the Lambourn Valley Pilot Scheme*, 1967-69.

APPENDIX C

THE FYLDE AQUIFER/WYRE CATCHMENT WATER RESOURCES STUDY

1 Background

The Fylde aquifer is located in central Lancashire (Figure 1). It underlies parts of the rivers Ribble and Wyre catchments. The Sherwood Sandstone of the Fylde aquifer is bounded in the east and underlain by Carboniferous rocks and overlain by younger Mercia Mudstones in the west (Figure 2). The aquifer is almost entirely covered by Drift deposits comprising interbedded Boulder Clay (till) and sands & gravels, ranging in thickness from 5m to over 30m. Their distribution and disposition are highly variable and complex.

The Fylde aquifer is heavily exploited for industrial and public water supply, forming part of North West Water's Lancashire Conjunctive Use Scheme (LCUS). Although these sources are not being operated at their full licensed rates, problems have become apparent both in terms of falling groundwater levels and depleted summer flows in the River Wyre and its tributaries as they cross the aquifer. This raised concerns over the long-term sustainability of water supply from the Fylde aquifer and the impact on surface waters and groundwater dependent features. A groundwater/surface water resource investigation was initiated in 1994; the main contract was let to Mott MacDonald.

2 Original LCUS Investigations

The LCUS was implemented in the early 1970's and includes abstraction boreholes at 16 sites on the Fylde aquifer.

Over 70 observation boreholes were sunk into the sandstone and 46 shallow boreholes were installed to monitor water levels in the overlying Drift deposits. The boreholes were subject to short-term individual testing and combined group testing for periods of up to three months.

Eight permanent flow measurement stations were constructed and a series of spot gaugings were used to identify gaining and losing stretches in the Wyre catchment.

The field studies were supplemented with the development of a groundwater model by WRc (WRc 1975). This model assumed 'fixed head' boundaries along the whole of the Carboniferous contact and in the south, as well as in Morecambe Bay. This implies that there is effectively an infinite source of water available in the Carboniferous to balance abstraction from the Fylde aquifer.

The results of these field investigations and groundwater modelling were used to define the licence conditions and abstraction rates for the groundwater components of the LCUS.

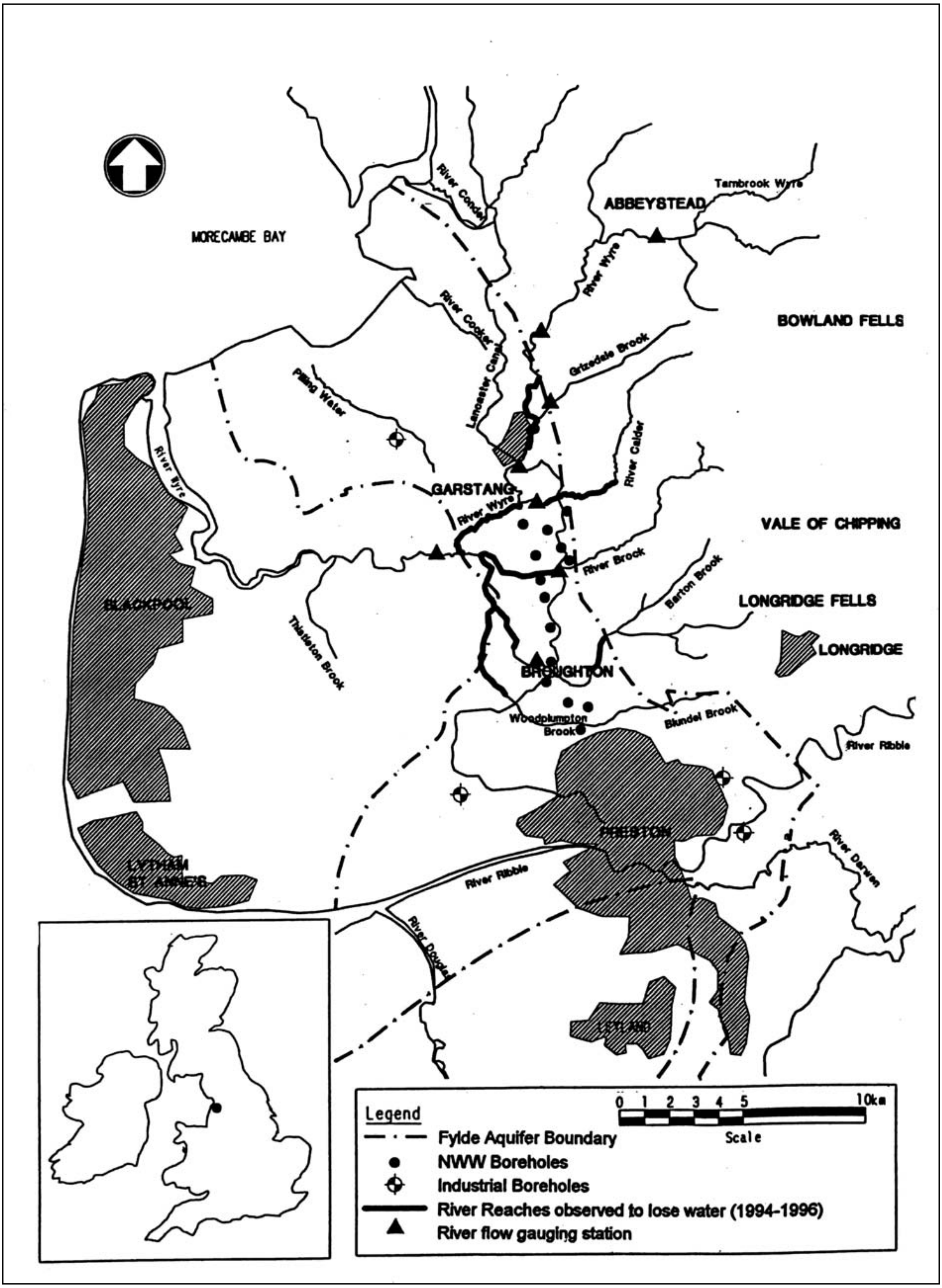


Figure 1. Location of the Fylde aquifer

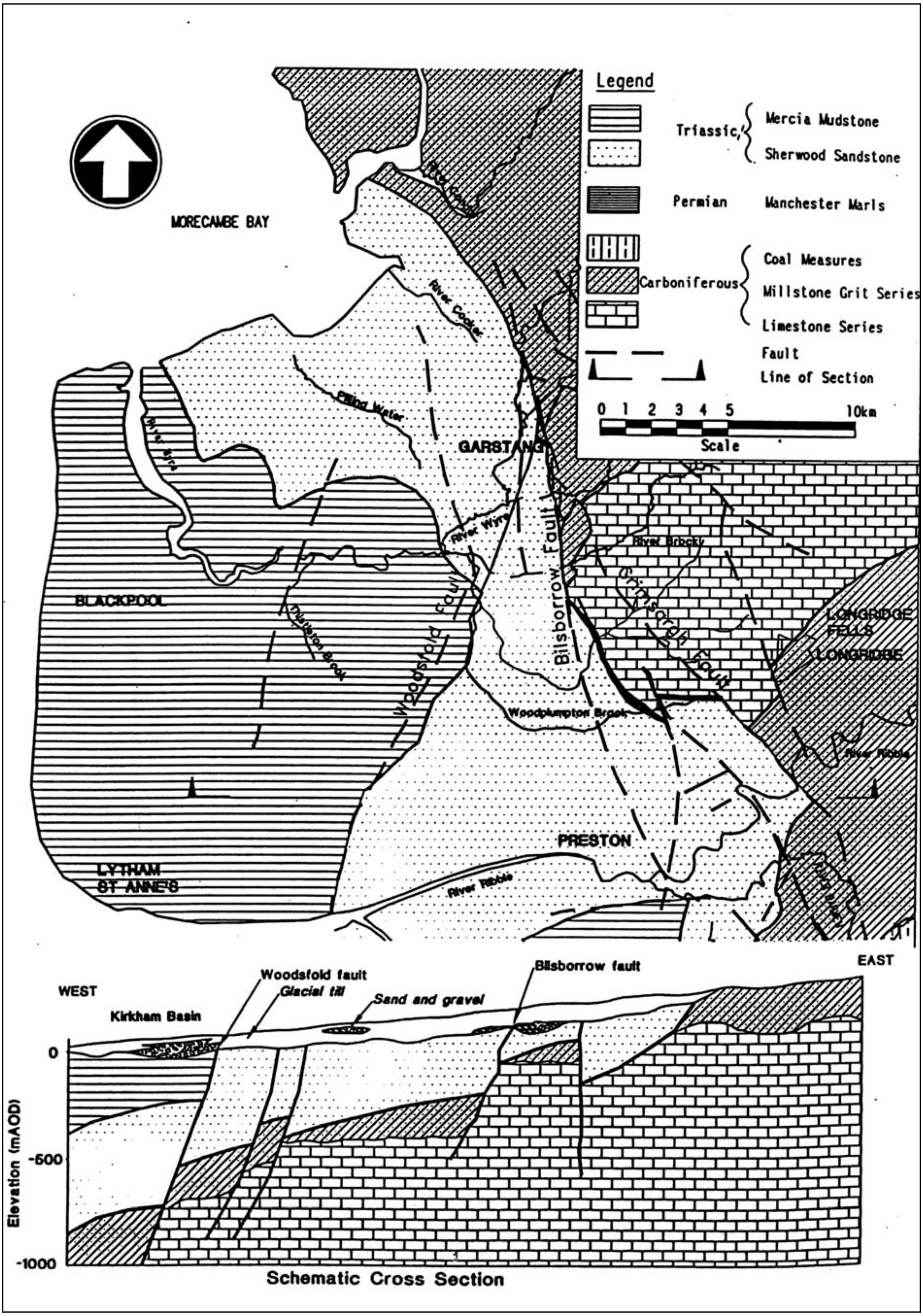


Figure 2. Geology of the Fylde aquifer

3 Fylde Aquifer/Wyre Catchment Water Resources Study

Objectives

Objectives of the study included:

- Reviewing the response of the Fylde aquifer to 20 years of operational use of the LCUS;
- Developing an integrated numerical model capable of representing both the groundwater and surface water environments which can be used as a tool for resource management and decision-making.

Project Structure

The study was carried out using a phased approach comprising:

- Phase 1 - Data collation, analysis and development of conceptual groundwater/surface water model.
- Phase 2 - Model Development and Calibration
- Phase 3 - Modelling of Resource Management/Demand Options
- Phase 4 - Model User & Training and Support.

3.1 Phase I - Data Collation and Conceptual Model

The Phase I studies included:

i. *Data Collation* - The temporal and spatial data (summarised in Table 3) were validated and entered into Mott MacDonalds database system (the Visual Display System - VDS) for ease of analysis, processing and presentation.

ii. *A Literature Review*

iii. *Interpretation of Lithological Logs* - production of plans (including rockhead topography, clay thickness, total Drift thickness) and numerous cross sections, particularly relating to the complicated Drift sequence, being relevant to recharge and river/groundwater interaction.

iv. *Calculation of Effective Rainfall*

v. *River Flow Analysis*

vi. *Preliminary Water Balance Assessment*

This information was used to develop a *simple* conceptual model of the groundwater/surface water system, which was then used to construct the numerical model. **However, although the data was processed by the consultant, insufficient thought was applied to understanding the basic geology and how the aquifer behaved before starting the modelling, a common failing of wanting to jump straight into the numerical modelling.**

The main geological, hydrogeological and hydrological study was complemented by a review of the ecological effects of low flows/water levels in the Fylde area.

Table 1. Data Collation

Hydrometric Data - over 25 years	
• Daily rainfall	- 27 sites
• Potential evaporation	- 12 gauging stations (300 station years)
• River flows	- spot gauging (38 sites) 1994-96
• Groundwater levels	- monthly records from 50 observation boreholes and 21 abstraction sites (1750 station years)
• Abstraction licence returns	
• Surface water augmentation and transfers	
Geological/Hydrogeological Data	
• Lithological logs	- From 700 boreholes (BGS & Agency archives)
• Published maps and memoirs	- From original LCUS and more recent pumping tests
• Aquifer characteristics	- From abstraction and observation boreholes
• geochemistry	

3.2 Phase II - Model Development and Calibration

The integrated surface water and groundwater model used Mott MacDonald's finite difference Integrated Catchment Management Model (ICMM)

Model Layers & Geometry:

- Initially a three layer model was established:
- a single layer representing the Sherwood Sandstone;
- a sands & gravels layer, where this directly overlies the sandstone (which acts as an additional storage reservoir);
- undifferentiated drift comprising varying proportions of sands & gravels and boulder clay.

However, it became apparent that it was necessary to split the sandstone into two layers separated by a "low permeability leakage interface" representing the marl bands within the sandstone. This more accurately represents the true vertical properties of the Sherwood Sandstones aquifers in the north west

Boundary Inflows:

Initially, inflows from the Carboniferous strata in the east were modelled as fixed heads (as in the original WRc model). These were subsequently represented as fixed gradients following more detailed consideration of the likely mechanisms of cross boundary flows, based on a series of geological long and cross sections of drawn by Agency staff (see section on geological framework).

River/Groundwater Interaction:

Interaction between the river and sandstone aquifer is dependent on the Drift coverage at the river. The mechanism of exchange was developed through analysis of river flow surveys and the Drift geology. In areas where significant thicknesses of Boulder Clay exist beneath the river (>15 m), no exchange of water between river and the sandstone was simulated. At the other extreme, there are areas within the Wyre catchment where Boulder Clay is absent beneath the river. In these circumstances the river is assumed to be in "direct" contact with the sandstone and significant leakage between river and sandstone is simulated, with the river effectively acting as a "recharge barrier". Detailed river flow surveys (spot gaugings) conducted between 1994 to 1996 helped identify 'losing stretches' and hence validate the model.

Recharge:

The *potential* recharge (representing the rate of vertical flow through the base of the root zone) was evaluated using the Penman-Grindley recharge model. Not all this recharge percolates through the Drift to the sandstone due to limitations in the ability of the Drift to transmit water vertically. The majority of potential recharge is rejected and is routed to the river system while a component flows within the Drift and discharges as baseflow to the river system. A small proportion is stored within the Drift (and in particular the sands & gravels) and is then slowly released into the sandstone aquifer in response to groundwater abstraction.

The recharge/leakage mechanism between ground surface and the sandstone aquifer is highly complex. The leakage mechanism used in the model simplifies the processes by averaging out the vertical thicknesses and permeabilities of the various sand and gravel and clay layers within the drift sequence, and representing them as a single 'drift' layer in the model. A 14 layer vertical strip model was subsequently used to assess the validity of this simplified recharge/leakage mechanism.

Calibration Period & Criteria:

The model was initially calibrated over the period 1969 to 1994, using monthly time steps. It was compared to:

- observed piezometery for selected time periods;
- groundwater hydrographs over the whole of the study area, for the full calibration period;
- observed river flows at six gauging stations;
- observed river losses and gains (from the spot gauging).

It was subsequently updated to include the severe drought of 1995/96 and to incorporate the findings of further geological investigations (see Section 3.4). These were initiated as a result of uncertainties in the conceptual model, which were highlighted during model calibration.

A total of 108 steady state simulations and 58 transient simulations were made during the model calibration process.

Sensitivity Analysis:

Additional model runs were carried out to assess the sensitivity of the calibration to variations in selected key parameters, including: vertical conductance and specific yield of the 'drift', permeability of the Carboniferous and Permo-Triassic sandstones, and the river bed resistance.

3.3 Further Investigations

Good agreement between the field and numerical values of river flows and groundwater levels were achieved in the north and central parts of the aquifer during the initial calibration. However, difficulties were encountered in simulating the consistent fall in groundwater levels that had occurred to the east and west of NWW's southernmost abstraction boreholes

(Figure 1) over the 20 years since the LCUS Fylde groundwater abstractions commenced. Various flow mechanisms were adopted in the model to improve the simulations. However, although relatively good simulations were achieved, it was necessary to reduce the model uncertainty through further desk and field studies.

Therefore, the available geological and hydrogeological evidence was critically reviewed by Agency staff. The possibility of a series of north-south 'horst and graben' (ridge and trough) structures was postulated. The Agency commissioned the British Geological Survey (BGS) to remap the study area using surface geophysical (seismic and gravity) data combined with a review of existing lithological logs. The resulting maps (BGS, 1995) showed the base of the Permo-Triassic sequence and presence and position of both major and previously unknown minor faults. This work, complemented by the drilling of two deep exploratory boreholes to confirm the geological structure around Preston, resulted in a fundamental revision and enhancement of understanding of the geological structure of the Fylde aquifer. It confirmed the dominance of north-south faulting and that there is a marked variation in aquifer thickness from east to west, i.e. the aquifer was acting as a series of north-south trending compartments (Figure 3.4.2). The revised geological structure was defined in the model, which helped to improve the simulation in the south.

Even with the improved understanding of the structure of the deep sandstone aquifer, it still proved difficult to account for the observed decline in groundwater levels in the south of the aquifer. Further examination of the overlying Drift cover indicated the existence of a deep glacial channel incised into rockhead. This was infilled by particularly low permeability Boulder Clay, albeit interbedded with occasional sand layers. The sandstone was clearly confined in this location and the clay was assumed to have a significant effect in limiting rainfall recharge. A reconceptualisation of the recharge mechanism, supported by two dimensional vertical strip modelling, enabled the observed piezometric decline in this area to be simulated.

3.4 Study Conclusions

The Fylde study has demonstrated the complexity and interlinked nature of groundwater/surface water systems and the difficulty in developing reliable or representative models based on limited data. Of particular importance to other resource assessment projects are:

- accurate representation of boundary conditions and recharge mechanisms;
- considering *all* available and relevant evidence (geological, hydrogeological, geochemical, geophysical, hydrological, ecological and modelling); effort can be wasted and conclusions can be unsound if insufficient effort is put into the conceptual modelling;
- adopting a collaborative, multifunctional approach including appropriate specialists and all stakeholders (to ensure shared ownership of the developed tool, if not the findings);
- maintaining accurate spatial and long-term temporal hydrometric records;
- ongoing review and updating of both conceptual and numerical models as new information is gained (an iterative loop).

3.5 References

Mott MacDonald (August 1997) - Fylde Aquifer/Wyre Catchment Water Resources Study (internal Agency report)

Seymour, Wyness and Rushton - The Fylde Aquifer - A case study in assessing sustainable use of Groundwater Resources. *In Hydrology in a Changing Environment.* - Vol.2 - Editors: Wheater & Kirby, J Wiley & Sons, 1998.