UNIVERSITY OF NEWCASTLE UPON TYNE
DEPARTMENT OF CIVIL ENGINEERING

STREAM - AQUIFER SYSTEMS OF THE THAMES BASIN: HYDROGEOLOGY, GEOCHEMISTRY AND MODELLING

by
PAUL L. YOUNGER

THESIS SUBMITTED IN FULFILMENT OF THE REQUIREMENTS
FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

MAY, 1990

ABSTRACT

The vulnerability of riverside wells in the Thames Basin to pollution by contaminated river water has been assessed by a programme of field characterisation and modelling. The Chalk, Quaternary river gravels and the modern streambed sediments control groundwater flow and solute transport in these stream-aquifer systems.

The Chalk is a fissured aquifer, in which matrix diffusion is an important cause of pollutant retardation. On the basis of new field evidence, it is proposed that the distribution of permeability within the Chalk reflects the configuration of Quaternary permafrost.

Flow in the highly permeable Quaternary river gravels is intergranular, and adsorption by organic matter and hydroxides may cause retardation of reactive contaminants.

The streambed sediments comprise lowly permeable carbonaceous muddy silts and peats. Slow advection and sorption of contaminants makes the sediments an effective barrier to pollution.

A mathematical model for flow and solute transport in stream - aquifer systems has been developed. Groundwater velocities are obtained by the solution of coupled flow equations (written in finite difference form) for up to three superposed aquifer layers. Vertical velocities are approximated using an interpolation scheme based upon the transmissivity of the constituent horizons of each layer. A 3-D particle tracking formulation (including a simple representation of matrix diffusion) is used for solute transport.

Hypothetical river spills of various duration were modelled for two sites (Dorney and Gatehampton). It was predicted that no wells would experience pollutant concentrations in

excess of EC limits after 20 - minute spills, although the Gatehampton wells would probably succumb after a 7-day event. Well water at both sites would breach EC limits after a 28-day event. Travel times to wells varied from 12 hours (chloride at Gatehampton) to many years (lindane at Dorney). Model performance was more sensitive to streambed parameters (permeability and sorption coefficient) than to aquifer parameters.

PREFACE

So many people have helped me during the course of this project that it seems somewhat churlish to thank so few by name. However, this thesis would be incomplete without a record of those people who were most helpful to me. In Newcastle, Professor P. Enda O'Connell, Rae Mackay, John Porter, Trevor Cooper and Professor Joe Cann all gave me invaluable advice at different stages in the project. At the Thames Water Authority, Reading, Brian Connorton, Vincent Robinson, Dave Banks, Mike Owen, Di Greenwood, Cathy Glenny, Dick Flavin and Mel Slingo all gave me great encouragement, and never seemed to tire of me pestering them for data! Paul and Sue Craddock were outstandingly hospitable towards me in Reading on many occasions. My family and friends have been supportive as ever, and it has especially fallen to my wife Louise to alternately egg me on, and then save me from myself when I was getting too uptight over work. To all of these people, and (to use a tired but essential formula) to all I have omitted to mention, I extend my warmest thanks. Finally, I would like to express my gratitude to the National Rivers Authority, Yorkshire Region, and in particular to John Aldrick and Dick Franklin, for allowing me the use of NRA photocopying facilities to produce multiple copies of the thesis.

"The force that drives the water through the rocks
Drives my red blood; that dries the mouthing streams
Turns mine to wax.
And I am dumb to mouth unto my veins
How at the mountain spring the same mouth sucks"

Dylan Thomas

Bless the Lord, my soul!
Lord God, how great you are,
Clothed in majesty and glory,
Wrapped in light as in a robe!

You stretch out the heavens like a tent.
Above the rains you build your dwelling.
From your dwelling you water the hills;
Earth drinks its fill of your gift.

You make springs gush forth in the valleys:
They flow in between the hills.
They give drink to all the beasts of the field;
The wild-asses quench their thirst.
On their banks dwell the birds of heaven;
From the branches they sing their song.

Psalm 104

TABLE OF CONTENTS

TABLE OF CONTENTS (Cont.)

TABLE OF CONTENTS (Cont.)

Page

TABLE OF CONTENTS (Cont.)

<u>TABLE OF CONTENTS (Cont.)</u>

Page

TABLE OF CONTENTS (Cont.)

TABLE OF CONTENTS (Cont.)

TABLE OF CONTENTS (Cont.)

LIST OF FIGURES

LIST OF FIGURES (Cont.)

LIST OF FIGURES (Cont.)

LIST OF FIGURES (Cont.)

LIST OF TABLES

LIST OF TABLES (Cont.)

LIST OF ABBREVIATIONS

1-D, 2-D, 3-D . . . . . Dimensions in Space

ABH . . . . Abstraction Borehole

ADI . . . . Alternating Direction Implicit *

ADMDR . . . . Advection, Dispersion and Matrix Diffusion Retardation

ADO . . . . Advection and Dispersion Only

AODN . . . . Above Ordnance Datum (Newlyn)

BE . . . . Boundary Element *

BPN . . . . Bedding Plane Normal

BPP . . . . Bedding Plane Parallel

DPRW . . . . Discrete - Parcel Random Walk

EC . . . . European Community

FD . . . . Finite Difference *

FE . . . . Finite Element *

IFD . . . . Integrated Finite Difference *

K . . . . Hydraulic Conductivity

LSOR . . . . Line-Successive Over-Relaxation

Ma . . . . Million Years Ago

MDRA . . . . Matrix Diffusion Range Approach

Ml/d . . . . Megalitres per Day (= TCMD)

MOC . . . . Method of Characteristics

MOM . . . . Method of Moments

OD . . . . Ordnance Datum

PAH . . . . Polycyclic Aromatic Hydrocarbon

PCB . . . . Polychlorinated Biphenyl

PTM . . . . Particle Tracking Method

RHC . . . . Relative Hydraulic Conductivity

LIST OF ABBREVIATIONS (Cont.)

RHS . . . . Right - Hand Side

RMSE . . . . Root Mean Square Error

SAI . . . . Stream - Aquifer Interactions

Sy . . . . Specific Yield

T . . . . Transmissivity

TCE . . . . Trichloroethylene

TCMD . . . . Thousand Cubic Metres per Day

TDS . . . . Total Dissolved Solids

ybp . . . . Years Before Present

Note: Those items marked with an asterisk are frequently used with the suffix 'M' in the text, standing for 'Method'.

CHAPTER ONE

INTRODUCTION

1.1 -- THE PROBLEM ADDRESSED IN THIS STUDY.

1.1.1 -- The Water Resources Setting.

In recent years, the vulnerability of surface water courses to pollution has become the focus of much attention. Where densely populated areas depend on streams for potable supplies, extensive water treatment is often required before the water can be released into the distribution system. Groundwater development has been traditionally viewed as a means of reducing dependence on vulnerable surface water supplies. Geochemical processes which occur during groundwater flow can remove or retard pollutant species. For this reason, groundwater has historically been regarded as having more dependable quality than surface water.

Unfortunately, groundwater development suffers from a number of drawbacks. Depending on the hydraulic characteristics of a given aquifer, for example, it may be difficult to obtain sustainable yields large enough to meet demand. Furthermore, instances of groundwater pollution have been reported with increasing frequency in the last few decades. Therefore the old assumption that groundwater quality will always be better than surface water quality no longer seems to hold true. While it is generally true that more chemical retardation will occur during groundwater flow than during surface flow, the main difference between surface and subsurface water pollution lies in the time scale over which quality problems will develop and dissipate. Streams and rivers can suffer the full effects of the onset of pollution within minutes or days, and, after the cessation of pollution input, recovery of water quality is usually fairly rapid (within days or months). On the other hand, groundwater flow and transport processes are so much slower than equivalent surface water processes that water wells may not display peak pollution until days, months or even years after the initial input occurs. Furthermore, once pollution is established in an aquifer, recovery may take years or even centuries. This distinction in time scales must be borne in mind when making water resource planning decisions.

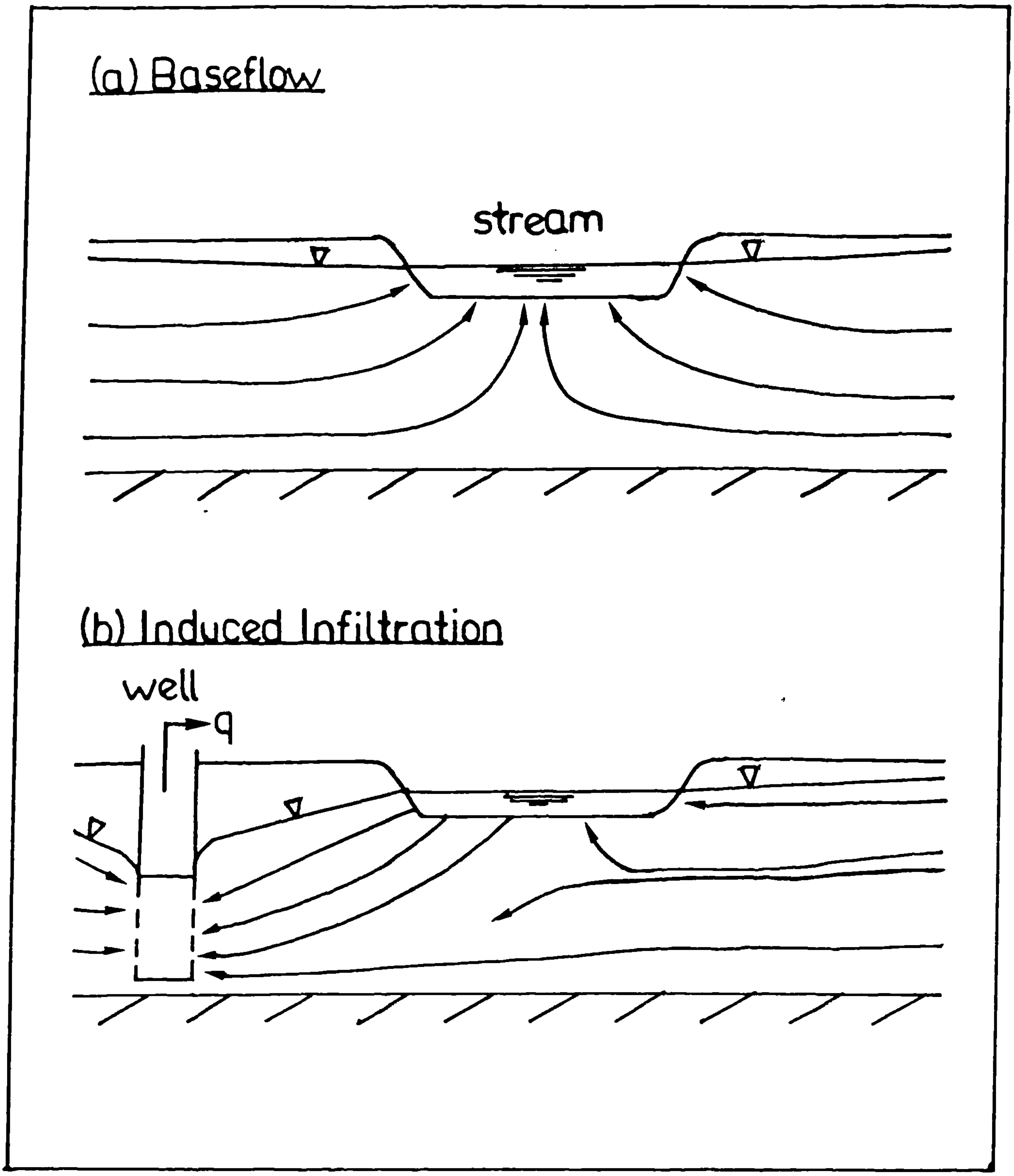
In the past, surface water studies and groundwater studies were usually conducted in isolation from each other. Since it has become clear that neither phase of the hydrological cycle is sufficient in itself to meet demand in many areas, integrated development of groundwater and surface water has become more common. For example, where surface water flows prove to be insufficient to meet demand during times of drought, groundwater can be used to augment river flows (Downing et al, 1981). In some instances, a well may be constructed close to a river in the hope that pumping of the well will cause water to flow from the river to the well. This process is termed 'induced infiltration' (Figure 1.1). Induced infiltration occurs at many sites throughout the world, often in wells that were not originally intended to cause river water ingress (cf Meinardi and Grakist, 1985).

During induced infiltration, river water moving into the subsurface may be improved in quality by filtration, dilution and a variety of chemical reactions. This amelioration in river water quality is usually termed 'bank filtration'. Frequently, contact - tank chlorination is the only treatment applied to bank - filtered water. Thus induced infiltration is often viewed as an economical first step in the treatment of surface water for use in public supply.

1.1.2 -- The Aims and Scope of the Present Study.

In the Thames Basin of southern England, which is the most densely populated area of its size in Britain, about 10% of the total public water supply is provided by wells which

Figure 1.1 -- Sketch to Illustrate the Definitions of (a) Baseflow and (b) Induced Infiltration.



lie within half a kilometre of the major rivers (Connorton, personal communication, 1989). For the most part, riverside wells in the Thames Basin have been free from pollution to date. This is no proof that bank filtration processes are working efficiently, however, since the quality of those river reaches adjacent to major riverside wells is generally high (cf Department of the Environment, 1986). Indeed, very little is known about the efficiency of bank filtration processes in the Thames Basin. Nonetheless, it is important for resource managers to be able to predict what impact a major pollution event in one of the major streams would have on riverside well sources. The questions which need to be answered include the following:

(a) If all surface water abstractions had to be turned off until river pollution had ceased, could the riverside wells be depended upon for pure water?

(b) Could a very short river pollution event lead to serious pollution at the wells?

(c) If pollution of the riverside wells could be expected, how soon after the onset of pollution in the river would peak pollution occur in the wells?

(d) Would processes of mixing and retardation in the subsurface reduce the concentration of a given pollutant in well water below a critical level (such as the EC limit)?

(e) How long would pollution entering from the river persist in the groundwater system?

The project described in this thesis was instituted to address such questions in the specific context of the Thames Basin. In pursuit of this objective, the following aims were identified:

(1) To gather together new and old data which throw light on induced infiltration and bank filtration in the major stream - aquifer systems of the Thames and Lea valleys (Figure 1.2).

(2) To derive a conceptual model summarising the major controls on flow and transport in these stream - aquifer

systems.

(3) To formulate a mathematical representation of this model.

(4) To solve this mathematical model in a predictive mode, so that assessments of the threats to riverside wells associated with accidental spills in the rivers can be made.

(5) To identify any deficiencies in our understanding of bank filtration processes in the stream - aquifer systems of the Thames Basin (which could be addressed in further studies), and to identify any findings which may have significance for stream-aquifer systems elsewhere in the world.

1.1.3 -- The Threat of River Pollution.

Before embarking upon a study of the vulnerability of riverside wells to pollution by infiltrating river water, it is important to assess the kinds of events which might occur in the Thames Basin. To date, no serious spills have occurred in the studied reaches of the Thames and the Lea, and it is therefore necessary to look a little further afield to identify the sort of accidents that could happen. As many events of this type are reported only in the popular press, references to specific events in the following paragraphs are rather informal. For details on the relative importance of the numerous toxic chemicals which have been found in rivers and streams, the excellent review by Hellawell (1988) should be consulted.

Recent pollution events in various European rivers have received wide coverage. Perhaps most notorious was the Sandoz fire at Basel, Switzerland, on November 1st 1986, in which 30 to 40 tonnes of toxic organo - metallic compounds entered the Rhine in fire - fighting water (Deininger, 1987; Capel et al, 1988). An estimated half a million fish, mostly eels, were killed as a direct result of the spill. Rapid co-ordinated responses by water supply authorities downstream of Basel (in West Germany and the

Netherlands) resulted in the shutdown of all river water intakes until the pollutant plume passed by, so that no polluted water was fed into public supply networks. Induced infiltration sources showed no detectable effects, suggesting that the bank filtration processes performed adequately. Other major spills of pesticides and metallic compounds occurred in the Rhine in West Germany, the Oder in Czechoslovakia, and the Rhone in Switzerland within six weeks of the Sandoz fire (see the New Scientist, 13-11-1986, p.19; 20-11-1986, p.13; 27-11-1986, p.17; 18-12-1986, p.5). More recently, in May 1988, the River Loire in central France was grossly polluted by chromium and cyanide after an explosion and fire at a chemical plant in the town of Azouer - en - Touraine (see The Guardian, 11-6-1988). 20,000 residents of the city of Tours, downstream of the plant, were without their regular supply of water for two days as a result of this accident (The Daily Telegraph, 13-6-1988).

Chemical spills of various kinds have afflicted many British rivers in recent years. A major river pollution event occurred in Cornwall on August 6th 1988 (see news reports in The Observer, 7-8-1988, p.2; and in the New Scientist, 18-8-1988, p.22). 20,000 homes were supplied with highly acidic water as a result of the erroneous addition of aluminium sulphate to a contact tank at a treatment works. Apart from the human health problems this caused, 30,000 fish were killed in the Rivers Camel and Allen when the mains were flushed to remove the poison. In Wales, the River Rhymney was polluted by factory chemical leaks three times in 1987/88 (see The Observer, 7-8-1988). Illegal releases of animal slurry and silage from farms accounted for 4,141 recorded incidents of river pollution throughout England and Wales in 1988 (Water Authorities Association, 1989). No mention of impacts on riverside wells was given in any of the reports cited above.

Even though the studied reaches of the Thames and Lea have not suffered major pollution as yet, damaging spills have recently affected at least two lesser rivers in the Thames Basin. In the early 1980s, a tanker carrying pesticides crashed into the River Roding near Bishops Stortford, releasing a pollutant dose which destroyed all life in the river for several years. More recently, a leakage of lindane and tributyltin oxide into the River Wey, near Godalming, Surrey, resulted in large fish - kills. Fortunately water intakes downstream of the spill site were switched off before the pollutant plume reached them (New Scientist, 25-2-1989), and no pollution has been detected at riverside wells to date.

From an interview conducted with a pollution officer at the Thames Water Authority (Nigel Marshall, personal communication, 1988), some potential sources of pollution in the studied reaches of the Thames and Lea have been identified. The most serious threats are felt to be posed by:

(1) Oil spills, from tankers on roads and from boats on the rivers.

(2) Pesticides (eg dieldrin, aldrin, lindane), from spills such as that which afflicted the River Roding in the early 1980s.

(3) Wood treatment chemicals (eg phenols, lindane etc), from one of the several factories producing these in the study area.

(4) Cyanides, which could be released from any of the light engineering plants which perform metal treatment (eg the Rover plant at Cowley).

(5) Radioactive nuclides, which could be released from military bases (RAF Brize Norton, RAF Greenham Common) or from research installations (eg AERE Harwell, AWRE Aldermaston).

It is worth noting that an event of the Sandoz type is unlikely in Britain, because of the strict implementation of a scheme known as BASIS (British Agrochemical Store

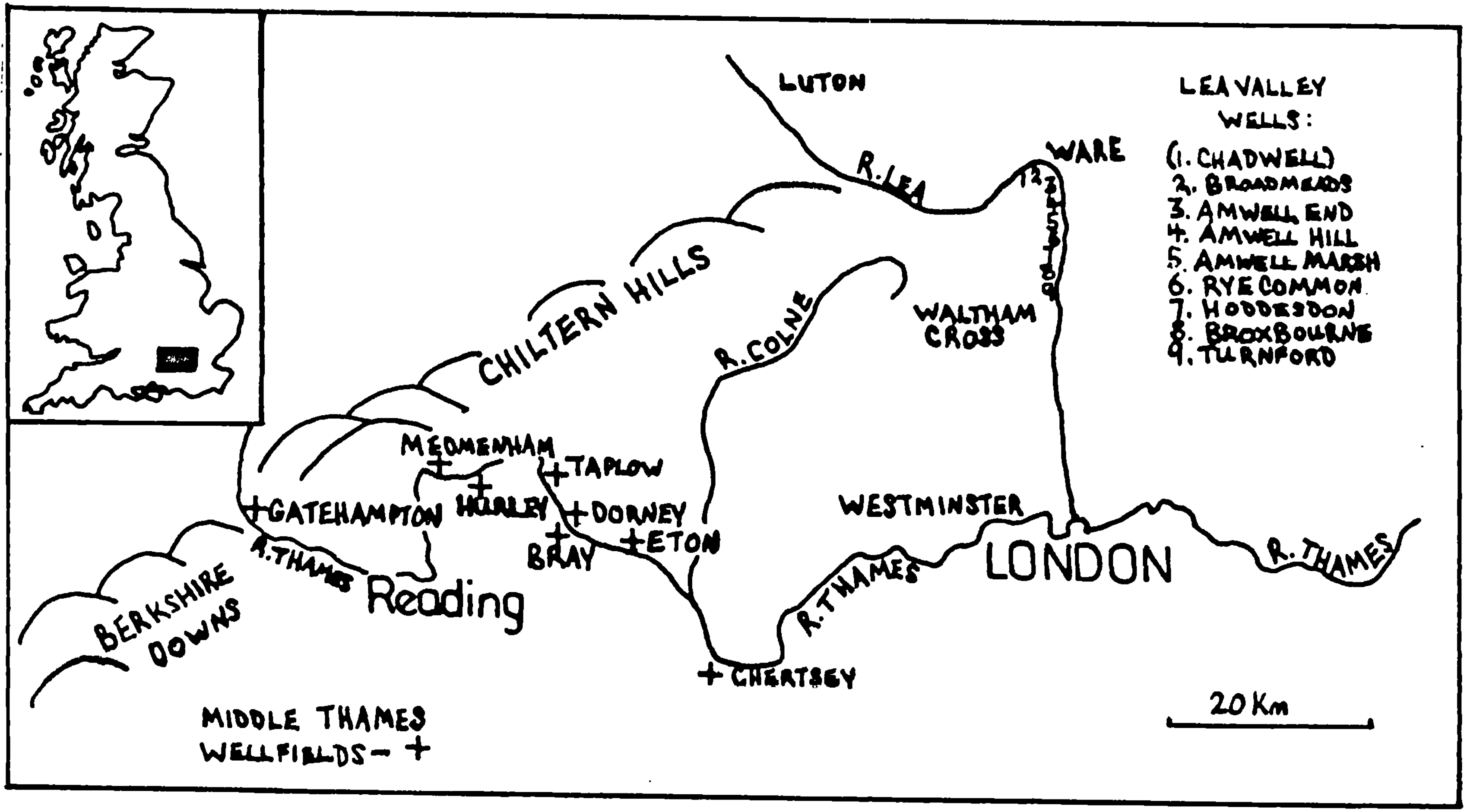


Figure 1.2 -- General Location of the Study Area.

Inspection Scheme), which includes provisions to prevent the escape of polluted fire-fighting waters to rivers. Nonetheless, there appears to be ample scope for short-term inputs of pollutants into the rivers from the sources noted above.

1.2 -- THE REGIONAL SETTING OF THE STUDY.

1.2.1 -- Topography and Climate.

The valleys of the Lea and the middle Thames lie in the northern and western districts of the Thames Basin respectively (Figure 1.2). The topography of the area is dominated by the Chalk escarpment, which forms the Chiltern Hills and the Berkshire Downs, and a number of deep valleys with perennial streams which breach the escarpment. Two such valleys are followed by the Thames and the Lea. In many places, the dry valleys of ephemeral streams occur as tributaries to the main valleys. On the upper heights of the Chalk escarpment, elevations up to 300m above ordnance datum Newlyn (AODN) are attained, while the valley floors lie at elevations between 40m AODN (Goring Gap and Ware) to 20m AODN (Dorney).

As might be expected, rainfall is higher over the elevated interfluves (up to 800mm per annum) than it is in the valleys (600 to 650mm per annum) (British Geological Survey, 1984). When evapotranspiration is taken into account, average recharge rates to the Chalk are in the range 200 to 350mm per annum (Brian Greenfield, Thames Water Authority, personal communication, 1988). Average rates mask seasonal variations in recharge, however, since rainfall is highest in the Autumn and Winter, and evapotranspiration peaks in the Summer.

1.2.2 -- Geology, Soils and Land Use.

The geology of the study area is discussed in great detail in Chapter 3, and therefore only a brief description is given here. Figure 3.1 and Table 3.1 summarise the stratigraphic succession. The dominating formation is the

Cretaceous Chalk (a pure micritic limestone), which is also the main aquifer in the area. Overlying the Chalk are a number of generally fine grained clastic formations, which are collectively referred to as the Lower London Tertiaries. Finally, outliers of Quaternary clastic deposits (including the residual soil known as the Clay-With - Flints; Catt, 1988, pp. 122 - 124) occur on many of the hills, and continuous bodies of gravel occupy the floors of most of the larger river valleys.

Soils in the study area correlate fairly closely with the underlying geology (Fenwick and Knapp, 1982, pp. 113-116). Rendzina soils, which are characterised by a thin calcareous humus - rich horizon (designated the letters Ah) overlying weathered Chalk bedrock (the C horizon), occur in the interfluve areas of the Chalk escarpment. In those places where the Chalk is overlain by clay - with - flints, leached brown soils (Udalfs) occur. These soils show a more complete profile, which, from the surface down, is typically:
(i) a humic upper (A) horizon;
(ii) a leached horizon (Eb), from which clays and organic matter have been largely winnowed;
(iii) a clay - rich horizon (B), deeply coloured by red iron oxides, and
(iv) weathered chalk (C), with infilled fissures containing flints and reddish clay.

While similar leached brown soils occur on some of the older gravel deposits, the soils of the modern floodplains are usually 'calcareous ground-water gleys' (Fenwick and Knapp, 1982, pp. 133 - 134). Because the water table is shallow beneath the floodplains, drainage and oxygen circulation are impeded in these soils, and iron compounds are frequently reduced, so that blue - grey stains (the so - called 'gley' effect) characterise the C horizon.

Land use is in general related to the geology and soil distribution. Where leached brown soils are dominant (over the clay - with flints and the higher river gravels), arable farming is practiced. Many poorly drained groundwater gleys adjacent to the rivers are used as rough pasture for cattle. In earlier times, the upland Chalk areas with thin rendzina cover were used as sheep pasture, but, with the advent of modern chemical fertilisers, cereal crops have replaced the sheep. Scattered stands of deciduous woodland occur throughout the area, both on the steeper hillsides and immediately adjacent to the rivers.

Sand and gravel quarries are extremely abundant in the river valleys, and environmental problems associated with these have been studied by several authors. During extraction, lowering of the water table can adversely affect sensitive wetland and hay meadow environments which owe their ecological diversity to shallow water table positions (Dixon et al, 1989). Landfilling in abandoned gravels pits has led to groundwater pollution in the Lower Colne Valley near Staines (Morgan - Jones et al, 1984) and in the Thames Valley near Chertsey (Naylor, 1974). Abandoned pits are often left unfilled, to act as lakes for recreational purposes, thus altering the hydrologic balance of an area.

1.3 -- A GENERAL INTRODUCTION TO STREAM - AQUIFER INTERACTIONS.

1.3.1 -- Introduction.

Studies of stream - aquifer interactions span the gap between the two disciplines of surface water hydrology and hydrogeology. For this reason, the terminology coined by one investigator to describe a specific stream - aquifer processes may seem clumsy or inappropriate to another investigator with a different background. Squabbles over terms such as 'baseflow' and 'bank storage' are frequently heard in hydrogeological circles, for instance, while the same terms are calmly accepted by most surface water

Figure 1.3 -- Hydraulic Connection and Disconnection.

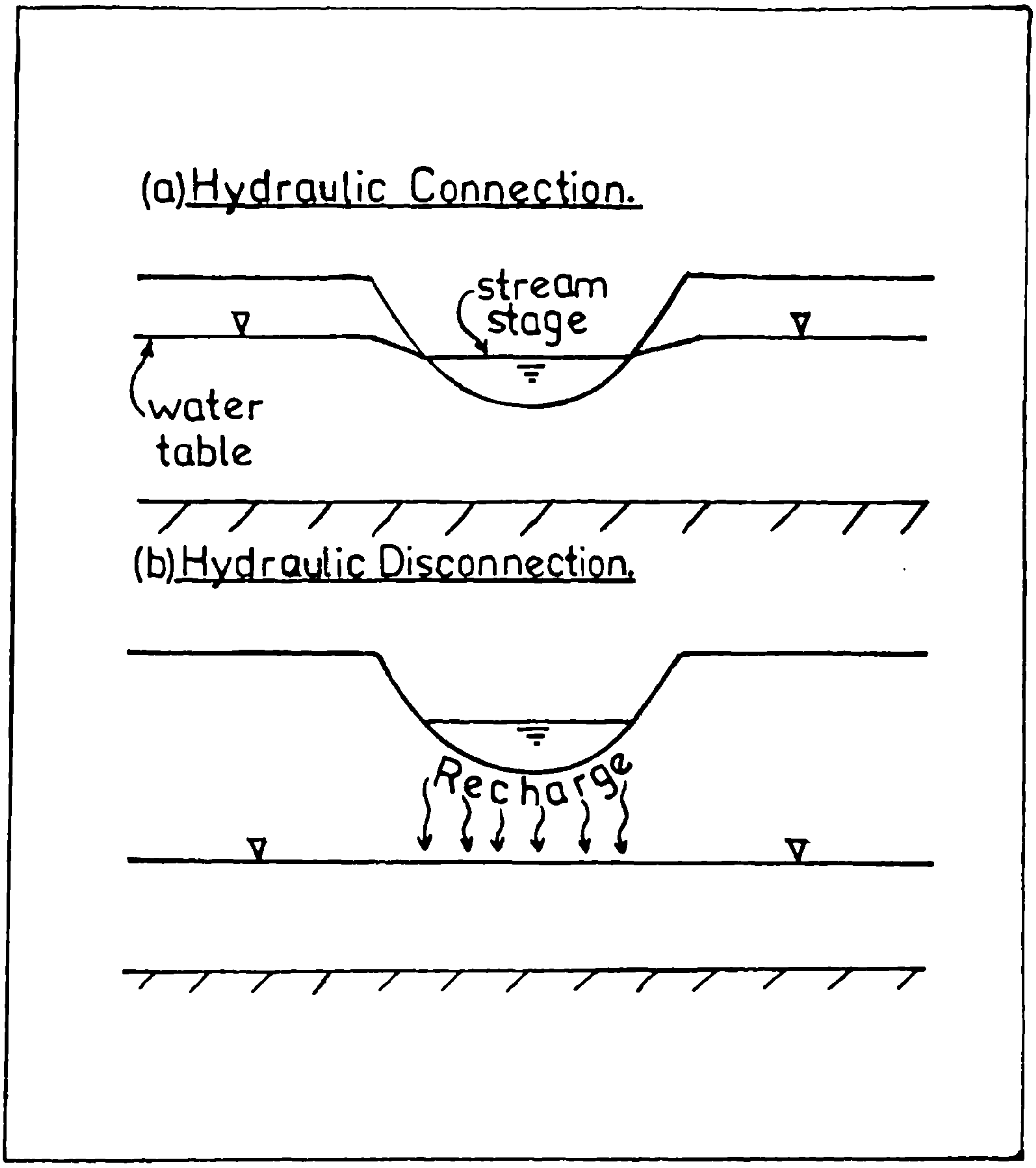
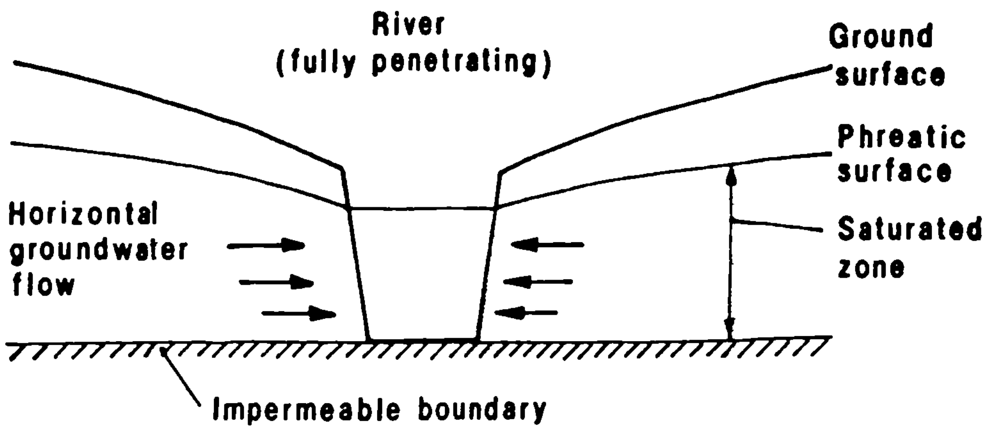


Figure 1.4 -- Degree of Penetration of an Aquifer by a Stream.
(a) Fully Penetrating (b) Partially Penetrating

(a)



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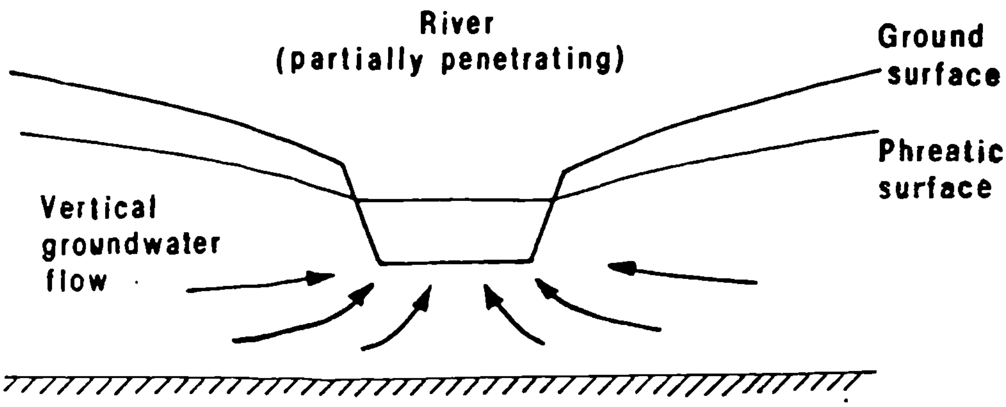


(Adapted from Bathurst, 1988).

hydrologists. The approach taken in the present study has been to use whichever term seems the most appropriate in a given context, while attempting to eliminate ambiguity.

The summary of major stream - aquifer processes which follows gives definitions for important terms along with key references. It is based upon a wide - ranging review of the literature on stream - aquifer interactions by Younger (1987).

1.3.2 -- Hydraulic Connection, Penetration and Baseflow.

A stream and an aquifer are said to be in hydraulic connection with each other if there is no unsaturated zone between the base of the streambed and the water table in the aquifer (Figure 1.3).

If a hydraulically connected stream completely penetrates the aquifer, so that the aquifer is effectively divided into two separate portions, then the stream is said to be fully penetrating (Figure 1.4a). Fully penetrating streams are seldom, if ever, found in nature (Sharp, 1977). More usually, a hydraulically connected stream will only impinge on a small amount of the saturated thickness of the aquifer. In this case the stream is said to be partially penetrating (Figure 1.4b).

Whenever the head in an aquifer exceeds the adjacent stage - head in a stream which is hydraulically connected to the aquifer, then groundwater will flow from the aquifer into the stream. This discharge of groundwater is normally referred to as baseflow, and it represents the natural unstressed state of many stream - aquifer systems (Figure 1.1). Under conditions of baseflow, with a net movement of water from the aquifer to the stream, the stream is said to be gaining (or "effluent") (Pettyjohn, 1985a, 1985b).

If the total distributed recharge to the aquifer remains lower than the rate of baseflow, then the aquifer will gradually drain, and the volume of baseflow discharged per unit time will also decrease. This decrease is called the 'baseflow recession' for a particular stream reach (Hall, 1968; Singh, 1968). After a certain amount of time this recession of baseflow may result in the stream stage having a greater elevation than the adjacent water table, so that water from the stream would flow into the aquifer. In such a case, the stream is described as a losing (or "influent") stream. Depending upon the rate of recharge from the stream to the aquifer, hydraulic connection may be broken, and further recharge will occur by flow through the unsaturated zone (Dillon and Liggett, 1983).

1.3.3 -- Bank Storage and the Rapid Response Phenomenon.

During a flood event, the stage in a hydraulically connected stream will usually rise above the adjacent groundwater head. When this happens, baseflow will be halted and water may flow from the stream into the aquifer, creating a recharge mound near to the stream. After the stage in the river drops at the end of the flood event, water from this recharge mound will flow back into the stream, causing an extended 'tail' on the stream hydrograph. This process of two - way exchange is known as bank storage (Pinder and Sauer, 1971; Sharp, 1977; Pettyjohn, 1985a, 1985b).

In some hydrogeological settings, bank storage does not operate and isotopic studies have revealed that peak stream discharges contain large amounts of recently - discharged baseflow. Studies of groundwater heads in such areas indicate that a 'ridge' appears in the water table near to the stream (where the water table is shallow) early in a flood event, and that this ridge leads to rapid groundwater flow through the stream - aquifer perimeter. This process, which is termed the rapid response phenomenon, is thought to be due to the rapid conversion of the capillary fringe (tension - saturated) above the shallow water table into rapidly flowing (pressure - saturated) groundwater. In this model, the conversion of the capillary fringe is attributed to the impulse of rapidly infiltrating recharge from above (Sklash and Farvolden, 1979; Gillham, 1984).

1.3.4 -- Conclusion.

Apart from the various features of stream - aquifer interfaces discussed above, there are many less prominent features which could also have been described. Where these are relevant to this study, some discussion is given elsewhere. For instance, the effect of streambed sediment on flow and solute transport is discussed in great detail in Chapters 2, 3, 5, 6 and 8. Moreover, a great deal could be said about induced infiltration (which was introduced in Section 1.1.1), particularly with regard to the various analytical models which are used to interpret pumping test data from riverside wells. However, since the present study is primarily concerned with numerical models of stream - aquifer systems, and since recent reviews of analytical models of induced infiltration are available (Sahuquillo, 1986; Younger, 1987), no further discussion on this topic is included here.

1.4 -- STRUCTURE OF THIS THESIS.

1.4.1 -- Order of Presentation.

The efforts and outcome of this study were fairly evenly divided between two foci:

(i) Description and interpretation of the field hydrogeology of Thames Basin stream - aquifer systems.

(ii) Development and application of a mathematical model of flow and solute transport in these systems.

The presentation and discussion of results in the following chapters is meant to reflect the equal importance of these two aspects. Indeed, the variety of topics covered in the literature review (Chapter 2) strongly reflects the bi-polar nature of this project. Nonetheless, since the mathematical modelling efforts are totally dependent on the hydrogeological work, the arrangement of material necessarily takes the form of a progression from field work (Chapters 3 and 4) to modelling (Chapters 5 to 8). In reality, much of the material in Chapters 3 and 4 was gathered for the sake of scientific curiosity, rather than because it was regarded as an essential pre-requisite for mathematical modelling. Ultimately, this 'extra' data proved invaluable in the development of the new geological model for the genesis of permeability in the Chalk which is presented in Chapter 4. If the emphasis of the entire study had been solely on mathematical modelling, Chapter 4 might never have been written. However, insights provided by the new geological model helped in the framing of the conceptual model for flow (Chapter 5).

In the end, the results of both aspects of the study proved equally instructive with regard to the processes of flow and solute transport in stream - aquifer systems of the Thames Basin. It is the purpose of Chapter 9 to draw both strands together into a harmonious summary of the new insights gained, and the new questions which arise, as a result of this study.

1.4.2 -- Organisation of Hydrogeological Information.

The hydrogeology of the Thames Basin has been extensively investigated by many earlier workers, and it is impossible to discuss any new findings without constant reference to what has gone before. For this reason, a rigorous division of field data into 'old' and 'new' is scarcely possible, let alone desirable. It was therefore decided to present the information on hydrogeology in Chapters 3 and 4 as a single account, whilst ensuring that the source of a given item is made obvious in context. Where substantial amounts of new data were obtained in the course of the present study, full details are given in various Appendices.

1.4.3 -- Organisation of Modelling Results.

When the time came to perform final modelling runs using real field data, two sites were selected for special attention. Rather than present all of the modelling results (flow and transport) for a given site in one chapter, it was decided that the flow results for both sites would be presented in Chapter 7, and the solute transport results for both sites in Chapter 8. This approach allows comparisons and contrasts between both sites to be drawn directly, without the need for tortuous references to other chapters. Abstraction of the results for a single site is facilitated by the careful ordering of those sections which refer to one site only.

1.4.4 -- A Note on Nomenclature.

Before proceeding with the main body of this thesis, it is as well to specify the particular meanings of some common terms as they are used here.

Firstly, the word 'stream' is used in a general hydrological sense to refer to any surface water channel, irrespective of its size. Thus the River Thames is a 'stream' for the purposes of general discussion. Because of the need to mention specific instances, however, the word 'river' frequently occurs in the narrative. This is not meant to imply any distinction from 'streams' discussed earlier.

In various chapters, discussion of the 'fissure system' of the Chalk is necessary. In this thesis, the word 'fissure' is taken to mean a widened, hydraulically significant, rock - mass discontinuity. A 'fracture', on the other hand, is taken to mean any rock - mass discontinuity, irrespective of whether or not it is widened or hydraulically significant. Thus all fissures are fractures, but not all fractures are fissures.

The term 'baseflow', which was defined in Section 1.3.2 above, is taken to mean groundwater discharge to a stream, irrespective of when this occurs in relation to surface runoff events. This clarification is necessary because of the common association of the term 'baseflow' with streamflow hydrograph analysis, where it is sometimes taken to mean the discharge of a stream between flood events.

The terms 'permeability' and 'hydraulic conductivity' have very similar meanings in this thesis, but a slight distinction must be made. Particularly in Chapter 4, the term 'permeability' is used to refer to the fluid-transmitting properties of the rock in general (a function of the porous medium alone), whereas the term 'hydraulic conductivity' is used whenever it is essential to remember that it is the transmission properties of the rock with respect to water that are being specified (eg when values are quoted).

A list of abbreviations appears at the front of this thesis to allow easy reference.

CHAPTER TWO

A REVIEW OF EARLIER WORK ON RELATED TOPICS

2.1 -- INTRODUCTION.

Because of its broad - based nature, there is a vast and varied body of literature dealing with the various aspects of this project. For this reason, it is not possible to restrict a review of previous work to a few key texts. In recognition of this fact, the review presented below is arranged in three separate sections. Firstly, the general groundwater modelling literature which proved to be of use in developing the model described in Chapters 5 and 6 is briefly reviewed; secondly, previous field studies of stream - aquifer water quality interactions are discussed; finally, numerical models of stream - aquifer interactions are reviewed. A further section could have been added to deal with earlier work on the hydrogeology of the Thames Basin (including stream - aquifer studies), but to avoid unnecessary repetition this information has been included together with new data in Chapters 3 and 4.

Stream - aquifer interactions (SAI) in general were reviewed at length by Younger (1987), in a report which covered the historical recognition of the various components of SAI, the assessment of large - scale SAI using hydrograph separation techniques etc, and the various analytical and numerical models of SAI which have appeared in the literature. However, as much of the information presented in that report is not directly relevant to the present discussion, only the two most relevant sections of that report (stream - aquifer water quality interactions, and numerical SAI models) have been expanded and updated for inclusion here.

Because the emphasis of this study is on the subsurface aspects of SAI, stream flow and transport modelling are not reviewed in any depth. Interested readers should consult the concise review of this topic presented by Bathurst

(1988), and the excellent series of papers by Chapman (1982), Bencala et al (1984), Bencala (1984), Kennedy et al (1984/1985) and Jackman et al (1984/1985), which describe case studies of the modelling of solute transport in rivers.

2.2 -- GROUNDWATER MODELLING.

2.2.1 -- Conceptual Aspects.

In conceptualising a specific hydrogeological system, choices must be made about the relative importance of various hydraulic and geochemical processes. A number of introductory groundwater texts share the advantage of offering a concise review of these processes to novice and practising hydrogeologists. Foremost amongst these works are those by Heath (1983) and Price (1985), in which largely qualitative discussions are given of all major aspects of hydrogeology.

Beyond these simplified discussions, the 'standard texts' of modern hydrogeology, notably those by Todd (1980) and Freeze and Cherry (1979), are indispensable. In addition to these texts, the collections of papers edited by Lloyd (1981) and Narasimhan (1982) contain an abundance of information on modern concepts in hydrogeology, from flow in fractures to flow in sedimentary basins.

Historically, groundwater flow has been studied more intensively than groundwater chemistry. Nonetheless, there is a large and rapidly growing hydrogeochemical literature. Simplified introductions to hydrogeochemical concepts have been presented by Edmunds (1981), Cherry et al (1984) and Anderson (1984). Amongst the book - length studies of this topic, those by Stumm and Morgan (1981) and Hem (1985) are rightly viewed as the classic accounts. A less exhaustive, though more readable, treatment of water chemistry has been produced by Drever (1982).

Three of the more important processes in solute transport and retardation are sorption, dispersion and biodegradation. Detailed discussions of the sorption of organic pollutants may be found in McCarty et al (1981), Karickhoff (1984) and Mackay et al (1985), while Hounslow (1983) discusses the effects of various aquifer compositions on inorganic contaminant sorption. Sorption non-equilibrium is discussed by Valocchi (1985), Goltz and Roberts (1988) and Bouchard et al (1988), amongst others. Dispersion remains a major area of research, and a vast literature is accumulating on this topic. Of the works consulted during this project, the most useful have been those by Mackay et al (1985) and Gillham and Cherry (1982), who both consider dispersion in unconsolidated sand and gravel aquifers. The molecular diffusion component of dispersion is discussed in the papers by Goodall and Quigley (1977) and Desaulniers et al (1981), who both describe cases of molecular diffusion of pollutants in silty clay deposits beneath landfills. The nature and geochemical function of microbes in the saturated zone have been discussed by Seppanen (1988) and McCarty et al (1981).

2.2.2 -- Mathematical Aspects.

For a full exposition of the development of mathematical models for groundwater flow and solute transport one need look no further than the classic treatise by Bear (1979). This work is summarised by Huyakorn and Pinder (1983) and by Bear and Verruijt (1987). Simplified derivations of governing equations may be found in Freeze and Cherry (1979) and in Mercer and Faust (1981), and an alternative derivation of the 2-D groundwater flow equation which pays particular attention to vertical flow components may be found in the paper by Connorton (1985). This last paper was inspirational to the mathematical approach taken in Chapter 6. Marsily (1986) includes detailed mathematical discussions of flow and transport, with clear and detailed discussions on the representation of sorption and dispersion.

2.2.3 -- Numerical Aspects.

A number of excellent reviews of state-of-the-art numerical groundwater modelling have appeared in the literature recently. These may be classified into review papers and text-books. Most review papers deal with flow and transport, but a few simpler papers concerned with flow modelling alone have appeared. Rushton (1981) produced a review of deterministic flow modelling which concentrates on British work. Lerner (1985) and Freyberg (1988) present case - studies which illustrate the dangers and ambiguities inherent in the application of such deterministic flow modelling techniques.

The earliest exhaustive review of solute transport modelling was produced by Anderson (1979). This review remains important for the insight it gives into the historical development of solute transport modelling. Plummer et al (1983) have presented methods for including thermodynamic effects (including dissolution, precipitation, speciation and redox effects) in solute transport models. Pinder (1984) reviewed finite - element models and Bedient et al (1985) reviewed migration processes as well as the mathematics of solute transport modelling. Stochastic solute transport modelling has been reviewed by Dagan (1983). Three recent reviews (Abriola, 1987; Naymik, 1987; Konikow and Mercer, 1988) cover both stochastic as well as deterministic models of subsurface solute transport. These latter reviews include useful analyses of probable future trends in solute transport modelling.

A number of useful text-books have been published which serve as practical introductions to numerical groundwater modelling. The book by Rushton and Redshaw (1979) is a good source of information on finite difference modelling of groundwater flow. Although hampered a little by an intermingling of information on numerical modelling with information on electrical analog modelling, it is nonetheless a very practical and useful book. Mercer and Faust (1981) give a good practical introduction to groundwater flow and transport modelling, but their slender book just falls short of being detailed enough to allow for guidance on use of the various numerical methods. Less clearly written but of more practical benefit is the book by Wang and Anderson (1982) which was found to be indispensable during the early stages of modelling in this project. It covers both finite difference and finite element methods, but gives only a brief introduction to solute transport modelling. Huyakorn and Pinder's (1983) book is far more mathematically sophisticated than any of the other books reviewed here, and as such it is hardly commendable for use by a novice modeller. It is also heavily biased in favour of the finite element method, and gives poor coverage of other techniques. Nonetheless it is a very good reference work. Marsily (1986) has produced a good mathematical hydrogeology text, which includes concise summaries of the finite difference and finite element methods, and practical hints for modellers. Finally, mention should be made of two excellent reports by the Illinois State Water Survey which give great insight into finite difference flow modelling (Prickett and Lonnquist, 1971) and "Random Walk" solute transport modelling (Prickett et al, 1981). Both reports include listings of FORTRAN programmes and worked examples.

2.3 -- STREAM - AQUIFER WATER QUALITY INTERACTIONS.

As might be expected, the principles governing solute transport during SAI are simply the sum of those which govern solute transport in the unsaturated and saturated zones, and in open channel flow.

In general, groundwater is more highly mineralised than direct runoff, simply because groundwater spends far more time in contact with soluble minerals than does direct runoff. It is this fact that lies behind so - called "chemical hydrograph separation" techniques reviewed by Younger (1987). If the total dissolved solids (TDS) content of groundwater and direct runoff in a catchment are known, the percentage of both components in total runoff during storms can be calculated using a pair of simultaneous equations similar to Equations (3.1) and (3.2), which are discussed in Section 3.5.1 below.

An important exception to the general rule of more highly mineralised groundwater occurs where a stream is subject to influx of sea water during high tides (eg the Lower Thames). In this case, flow of water from the stream to the aquifer may result in saline pollution of the aquifer (Connorton, personal communication, 1987).

Occasionally, various chemical species may be present in stream waters which are not found in as great abundance in the local groundwater. Such species are typically present as a result of human activities. Hellawell (1988) has reviewed the occurrence and origin of the main anthropogenic chemical species in rivers and streams. Induced infiltration aquifer tests occasionally involve a study of such species, since they can act as tracers, allowing the relative amounts of river water and aquifer water contributing to well discharge to be estimated (eg Edmunds, Owen and Tate, 1976; Ridings et al, 1977). In extreme cases, highly polluted rivers into which waste effluent is discharged may have a higher TDS concentration than the adjacent groundwater.

Processes of dilution may occur during SAI. Three basic scenarios may be envisaged:

(a) Groundwater which is more highly mineralised than the water in the connected stream is diluted by discharging into the stream and mixing with the stream water.

(b) Inflow of river water with a low TDS content into bank storage can lead to dilution of the groundwater adjacent to the stream.

(c) Baseflow may dilute a heavily polluted river.

Numerous chemical reactions may accompany these physico - chemical processes.

Very few workers have investigated the particular solute transport processes which characterise natural stream-aquifer interactions, such as baseflow. Three exceptions may be mentioned however:

(i) The pollution of streambed sediment in the Newlyn catchment, Cornwall, by dieldrin from baseflow, which is discussed in Section 3.4.4.1.

(ii) Reynolds et al (1986) have described the hydrochemistry of a catchment subject to acid precipitation. Acid rain falling on the Plynlimon Catchment in Mid - Wales generates direct runoff of such a low pH that ecological damage ought to be quite heavy. In fact the effects are less than might be expected due to buffering of the direct runoff by baseflow, originating from carbonate aquifers in the catchment.

(iii) Pinay and Decamps (1988) have studied the role of riverbank woodlands in reducing the nitrate content of baseflow which passes beneath them. Field investigations around the River Louge, near Toulouse, France, showed that all nitrate is removed from groundwater within 30m of flow beneath a riparian copse. The trees encourage the presence and activity of anaerobic bacteria, which utilise the nitrate as a source of oxygen.

Far more studies have been conducted into solute transport processes occurring during induced infiltration. The processes of retardation and degradation affecting solutes and suspended solids in water flowing from a stream into an aquifer are collectively known as bank filtration (cf Section 1.1.1). Although bank filtration is merely a special case of the attenuation processes which generally govern the movement of solutes in the saturated zone, the time taken for the water to travel from the stream to the well will often be so rapid that changes in water chemistry are less likely to reach completion than will be the case during "ordinary" saturated flow, where residence times are long.

A number of detailed field studies of bank filtration have recently appeared in the literature. Schwarzenbach et al (1983) have described the variable removal of organic pollutants during induced infiltration on the rivers Glatt and Aare, two tributaries of the Rhine in Switzerland. At the sites studied, organic carbon fractions in the streambed sediment (1 - 2%) and the aquifer (0.1%) are exceptionally low compared to their analogues in the Middle Thames valley (Appendix C). While some species, particularly aromatic hydrocarbons, were effectively removed from the infiltrating water by biodegradation, many others were not. Chloroform, trichloroethane, trichloroethylene and tetrachloroethylene all proved to be highly persistent, leading Schwarzenbach et al (1983) to conclude that 'with respect to such chemicals, bank filtration is inadequate as a first step in the treatment of river water for water supplies'.

Gay and Frimpter (1985) studied the distribution of polychlorinated biphenyls (PCBs) in the Housatonic River and its adjacent aquifer in Massachusetts, USA. Induced infiltration has been occurring at the study site since 1956, and the Housatonic River has frequently received discharges of PCB - bearing wastewater from an electrical components factory during this time. Up to a metre of black, organic rich sediment was found on the bed of the river in the study area. Examination of many water and sediment samples from the river and the aquifer showed that the PCBs were strongly sorbed to the streambed sediment, with no PCBs being detected in well water or on aquifer sediment.

If sorption onto streambed sediment can be a saviour from groundwater contamination, it can also contribute to pollution if contaminated sediment is dredged and disposed of carelessly. Salomons et al (1982) have described the groundwater pollution risk associated with the disposal of contaminated dredged sediment from the Rhine in landfills in the Netherlands. Their studies showed that heavy metals and pesticides were being leached from the dredged sediment under the reducing conditions prevailing in the landfill. Disposal of dredged sediment at sea, however, was not thought to pose a particularly high pollution risk.

Meinardi and Grakist (1985) have presented preliminary results from bank filtration studies in the Netherlands. Wells situated a kilometre or more from various rivers, and not intended to be induced infiltration sources, have shown a marked deterioration in quality after prolonged pumping, with induced flow of water rich in sulphate and chloride from the rivers. The proportions of river - derived water in the wells studied by Meinardi and Grakist (1985) did not exceed 10%.

A more detailed study of bank filtration in the Netherlands was presented by Stuyfzand (1989). He used ^{18}O data to calculate the proportion of river - derived water in well water, and also determined travel times and residence times for the water using tritium dating. The transport of a number of hazardous solutes from the River Rhine to nearby wells was then assessed in the light of these calculations. It was discovered that anoxic conditions were quickly established during induced infiltration, leading to mobilisation of iron and manganese, and the reduction of NO_3, DOC and O_2. Adsorption to streambed silts and disseminated clays in the aquifer removed many of the chlorinated hydrocarbons and trace metals, however, including some which are generally more mobile under reducing conditions. Physical filtration and biological processes removed bacteria and viruses from the bank filtrate so effectively that they were never detected in water from wells which were situated only 30m from the river.

Further upstream, in West Germany, the Rhine flows through the most densely populated area in Europe. Wastewater discharges from these areas profoundly affect the quality of water in the Rhine, and thus the quality of water from induced infiltration well sources. Wilderer et al (1985) have reviewed much of the German literature on bank filtration, noting that in 1979 about 6.5% of the drinking water supply of West Germany came from induced infiltration, which represents a significant decrease from 25% in 1960. This decrease has been attributed to the increased pollution of the Rhine over this period and to gradual clogging of the river bed with silt and chemical compounds. In a study cited by Wilderer et al (1985), the 'seal' on the bed of the Rhine at Dusseldorf was inspected using a diving bell, and was found to be composed of mineral oil, hydrocarbons, iron, manganese, copper, zinc and lead. This layer, which was up to 10cm thick, was so strongly indurated that it was difficult to remove even with a pneumatic drill. An area of $200m^2$ was eventually cleared, but the layer had re-formed within a year.

Wilderer et al (1985) also review studies of the 'efficiency' of bank filtration processes along the Rhine, where efficiency is measured as the percentage by which a given concentration of solute is reduced during induced infiltration. A study of selected trace organics showed that efficiencies can range from 0% (for chloroform) to 100% (for PCBs). These results conform closely to the findings of Schwarzenbach et al (1983) and Gay and Frimpter (1985), cited above. For heavy metals, the efficiency is also highly variable, and, as might be expected, it is critically dependent on the redox conditions of the system.

Laszlo and Hommonay (1986) have briefly summarised the effects of bank filtration on infiltrating river water in Hungary, where induced infiltration water sources account for 40% of the national water supply. Concentrations of ammonium, phosphate and the Chemical Oxygen Demand (COD - $KMnO_4$) were all found to be reduced by bank filtration.

Herrmann et al (1986) have studied the attenuation of selected organic micropollutants during bank filtration on the River Rotmain in Bavaria. The total dissolved organic carbon (DOC) concentration decreased drastically within the first few metres of infiltration. Trichloroethylene (TCE) was hardly attenuated at all, and where the aquifer medium was low in organic matter the chlorinated hydrocarbons showed high mobility. Polycyclic aromatic hydrocarbons (PAH; eg napthalene, two juxtaposed benzene rings) were totally removed in less than a metre of infiltration. It was thought that the PAHs may have been adsorbed onto suspended sediment in the river, reducing the possibility of infiltration. These findings showed good agreement with predictions based on retardation factor (Rd) values calculated from organic carbon partition coefficients (K_{oc}) and the organic carbon fraction of the streambed sediment (0.04).

Watt et al (1987) have described the first phase of an on-going study of induced infiltration and bank filtration in the Lower Spey Valley, near Fochabers, Scotland. Chemical analyses of 'native' groundwater, river water and mixed waters from riverside wells indicated that mixing of up to 80% river water with native groundwater could explain the concentrations of most species in water from riverside wells. However, the values of colour (a function of the concentration of organic acids in the water) and pH were much lower than the 80% mixing figure would suggest. Watt et al (1987) postulated that the attenuation of colour and pH was due to biochemical processes. Subsequent laboratory studies of gravel samples from the field site supported this postulation. Microbial activity was shown to account for all of the colour removal during flow of river water through laboratory columns packed with Spey gravels. When antibiotics were added to the columns, however, colour removal ceased. The changes in CO_2 activity consequent upon these biochemical transformations would cause a shift in the equilibrium of the Ca - H_2O - CO_2 system, which could explain the changes in pH.

2.4 -- NUMERICAL MODELLING OF STREAM - AQUIFER INTERACTIONS.

2.4.1 -- Introduction.

Two main obstacles hinder rigorous representations of stream - aquifer interactions in groundwater flow models:

(1) Transient processes generally occur much more rapidly in streams than they do in aquifers. As a consequence, time-steps of a few seconds may be appropriate in a surface water model, while steps of several days or even longer may be suitable in a groundwater model.

(2) Representation of partially penetrating streams (with or without low permeability streambed sediment layers) is difficult within the framework of 2-D areal groundwater flow and transport modelling. This is because of a marked discrepancy between the assumption of predominantly horizontal flow upon which such models are based and the significant vertical flow components common in the vicinity of partially penetrating streams.

Approaches to the first obstacle, the 'time factor', fall into two categories. Given certain field conditions, it can be useful to simultaneously solve stream and aquifer flow equations using an iterative approach. Convergence is usually accepted when the change in the stream - aquifer exchange flux between successive iterations falls below a predefined tolerance. This approach has been called 'internal coupling' (Freeze, 1972a; Dillon, 1983).

Several workers have used this approach, and their efforts are briefly reviewed below. Nonetheless, because of the time factor (1) mentioned above, it is easy to see that internally coupled stream - aquifer models can become very expensive to run. If solute transport processes are modelled as well, the expense may be out of all proportion to the amount of insight obtained from running the model. Indeed no internally coupled stream - aquifer models representing solute transport have appeared in the literature.

For more usual field conditions (such as in the Thames Basin, where the rivers are heavily controlled) it may be reasonable to assume that simultaneous solution of stream flow and groundwater flow equations is unnecessary, so that the results of either simulation may be used as input to the other without satisfying any coupling criterion. For instance, groundwater model output may be used to determine baseflow stream discharges without satisfying any interface boundary conditions. Such an approach is called 'external coupling' (Freeze, 1972a; Dillon, 1983). In this case, the modelling exercise reduces to a classical groundwater modelling exercise, with varying degrees of care taken over how to represent a lumped stream - aquifer exchange term.

Approaches to the partial penetration and streambed sediment effects (obstacle 2 above), are many and varied for flow modelling but virtually non-existent for solute transport modelling. Earlier attempts to model partially penetrating and sediment - lined stream - aquifer boundaries are reviewed below (Section 2.4.4).

Some recently published reviews concentrate on more specific aspects of stream - aquifer modelling than can be addressed here. Freeze (1982) discusses the interfacing of stochastic surface water models with groundwater models. Dillon (1983) addresses the issue of model structure in some detail. Winter (1984) assesses the applicability of stream - aquifer models to studies of acid precipitation. Finally Vasiliev (1987) discusses analytical models as well as numerical models.

In the review which follows, models are classified according to whether they are internally or externally coupled. The abbreviations used in this review are all listed at the front of the thesis.

2.4.2 -- Externally Coupled Numerical SAI models.

The first externally coupled numerical SAI model appears to have been that of Young and Bredehoeft (1972), in which an ADI - FD solution to the Boussinesq Equation (cf Bear, 1979, p. 113) was externally coupled with a stochastic input of surface water via the source / sink term in the Boussinesq groundwater flow equation. Young and Bredehoeft (1972) do not specify their streamflow routing technique. A complementary programme was developed to assess the economic / legal implications of management strategies proposed on the basis of the flow model simulation results. Satisfactory results were obtained when this economic / hydraulic pair of models was applied to data from the South Platte River Valley of north - eastern Colorado.

An externally coupled model which allows solute transport to be simulated along with flow was presented by Konikow and Bredehoeft (1974a, 1974b). This model has been used in the prediction of salinity changes over a decade in an irrigated stream - aquifer system near Lamar, south - eastern Colorado. As is often the case in semi - arid settings like the Lamar site, the salinity of the river water and shallow groundwater has increased, because of the exacerbated loss of water through evapotranspiration during use and reuse of groundwater and baseflow stream water for irrigation.

The Boussinesq Equation for groundwater flow was solved by Konikow and Bredehoeft (1974a) using ADI - FDM with a rectangular grid, and solute transport was represented by a MOC solution. The Konikow and Bredehoeft (1974a) model is externally coupled by modifying the streamflow by an amount equal to the source / sink term of the groundwater flow equation at stream nodes. Upstream stream discharge values are read into the model as input, and a simple mass balance equation is solved for each river node. Chemical concentration is coupled and routed in the same way. This is a very simple but effective external coupling technique.

Ten years after the original study, Konikow and Person (1985) compared Konikow and Bredehoeft's (1974a) predictions with the observed evolution of the system. Knoikow and Person (1985) reported that the original predictions of a 2 - 3% per annum increase in salinity appear to have been overly pessimistic. When the original calibration data were statistically analysed along with the more recent data for the site, it was found that a statistically significant increase in salinity had occurred during the year that was used for calibration (1971 - 72), while no comparable increase has occurred since. The 1971 - 72 increases were apparently caused by a drought - related reduction in river discharge over the same period. Hence assuming that the 1 - year trends used to calibrate the model were in fact long - term trends led to exaggerated predictions of long - term system behaviour. The system actually appears to have reached a dynamic equilibrium with respect to irrigation - related salinity (Konikow and Person, 1985).

In the light of the findings of Konikow and Person (1985), Person and Konikow (1986) improved the original model of Konikow and Bredehoeft (1974a) by incorporating expressions to represent salt transport through the unsaturated zone, and recalibrated it. It was found that 1 year's data were sufficient for the hydraulic calibration, but that at least 4 years of data were required to calibrate the solute transport model, if the dominant influence of short - term trends was to be avoided.

Knapp et al (1975) appear to have been the first to develop a "basin hydrology simulator" which can simulate all the land phases of the hydrological cycle (cf Refsgard and Stang, 1981; Miles and Rushton, 1983; Abbott et al, 1986). Four stacked horizontal layers are used in the Knapp et al (1975) model; the surface layer, upper soil zone layer, lower soil zone layer, and saturated zone layer. Fluxes between these are determined subsequent to solution of mass balance equations for each layer. Streamflow routing is accomplished using the analytical Muskingum method, and groundwater flow is represented by the Boussinesq Equation, solved using the ADI - FDM. The method of coupling resembles that used by Konikow and Bredehoeft (1974a). Reasonable correspondence between observed and computed values of stream discharge were obtained from a 25 - year simulation of the Little Arkansas River catchment northwest of Wichita, Kansas.

Morel - Seytoux (1975) presented a mathematically complex externally coupled model involving the Muskingum streamflow routing equation (solved using an explicit FDM) and the 2 - D Boussinesq groundwater flow equation (solved by ADI - FDM), both expressed in response function form. Although mathematically impressive, this model has been criticised by Dillon (1983) on the following grounds; (1) it is suitable for hydraulic connection only; (2) it requires large amounts of computer time and storage, and (3) it is a fairly crude description of SAI.

Refsgard and Stang (1981) devised a model to simulate all the land phases of the hydrological cycle for the Susa area, Zealand, Denmark. Their model involved solution of the 2 - D Boussinesq equation by the IFDM. However, Refsgard and Stang (1981) did not clearly describe the type of coupling employed, although it appears to have been external. Streamflow routing seems to have been carried out using a water balance technique such as that used by Konikow and Bredehoeft (1974a).

Oakes (1981) used an externally coupled model to investigate baseflow variations in a stream - chalk aquifer system in East Anglia. An explicit FDM was used to solve the equation describing transient unconfined 2 - D groundwater flow. The small time step demanded for the stability of explicit methods was deemed justifiable because of the ease with which non - linear boundary conditions at river nodes could be incorporated. No details of the coupling or streamflow routing techniques are given in Oakes' (1981) discussion, but the output of stream discharge hydrographs with monthly time steps suggests that an external coupling method was used along with routing by water balance techniques.

Miles and Rushton (1983) presented an integrated catchment model similar to that of Refsgard and Stang (1981) in which all of the major processes of the land phase of the hydrological cycle are represented. Precipitation and evapotranspiration data were input to the model, which gave river flows as output. Monthly time - stepping allowed streamflows to be routed by water balance techniques (cf Konikow and Bredehoeft, 1974a). Line successive over - relaxation (LSOR) FDM solutions were used in the groundwater module, and external coupling linked these solutions to the streamflow routing module. Application of the model to data from the River Worfe catchment in the West Midlands of England yielded interesting results, which were discussed further by Miles (1985a).

Under the acronym of SAMSON (Stream - Aquifer Model for Management by Simulation and OptimizatioN), Morel - Seytoux and Restrepo (1986) devised a two - component stream - aquifer management model (cf the model pair of Young and Bredehoeft, 1972). These two components were (1) an allocation model which used legal and economic data to compute the maximum permissible stresses on the system, and (2) a physical model, which could simulate the response of the aquifer system to the stresses proposed by the allocation model. Unfortunately, Morel - Seytoux and Restrepo (1975) gave no details of their solution methods or coupling procedures, though it seems that the model was based on earlier work by Morel - Seytoux (1975), which was reviewed above.

Abbott et al (1986) introduced a FD model for total catchment simulation (cf Knapp et al, 1975; Miles and Rushton, 1983) under the name SHE (Systeme Hydrologique Europeen; European Hydrological System). This system is still being expanded at the time of writing to include solute transport capabilities. A modular structure has been given to the SHE, with a central FRAME component governing the exchange of information between the various modules (precipitation / interception; unsaturated zone; saturated zone; overland and channel flow). The SHE simulates SAI for the following cases:

(1) Water table in contact with a flowing stream
(2) Water table in contact with a dry stream bed
(3) Water table lying below the bed of a flowing stream
(4) Water table lying below a dry stream bed

The SHE also allows for the streambed to be assigned a hydraulic conductivity value different from that of the surrounding aquifer. Groundwater flow is represented in the SHE by the 2 - D Boussinesq equation, of which an ADI - FDM solution is obtained. Open - channel flow is represented by a simplified version of the Saint - Venant equations, which are solved using an implicit FDM. Abbott et al (1986) did not specify the mode of SAI coupling in the SHE, but descriptions of the SHE coupling were given in

ASHE (1981). Four external coupling strategies are used, corresponding to the four cases listed above. For case (1), stream - aquifer interchange is represented by an expression developed by Preissmann at SOGREAH (the French member of the ASHE -- Association pour le SHE). This expression is essentially a radial - flow version of Darcy's Law, similar to those derived by Miles (1985a, 1985b, 1987a, 1987b). SAI for case (2) is represented by direct addition of an evapotranspiration component to the phreatic surface. Case (3) involves interchange from the stream to the phreatic surface via 1 - D vertical unsaturated flow, which (as elsewhere in the SHE) is calculated from the 1 - D form of the Richards equation using an implicit FD scheme. Case (4) is solved in a similar manner to case (3). Allowance for the presence of a lowly permeable lining is made using the methods described by Prickett and Lonnquist (1971).

Wald et al (1986) produced a curious hybrid analytical / numerical SAI model linking 1 - D groundwater flow with open channel flow. The groundwater equation was solved analytically using the convolution integral method of Hall and Moench (1972). A four - point fully implicit FD scheme was used to solve the full Saint - Venant equations. Coupling was external. After each time step, the solution of the Saint - Venant equations was modified by calling the groundwater module, which calculated a value for the groundwater source / sink term. An amount equal to this was then subtracted from the volume of routed streamflow. Suitable calibration of this model has not yet been accomplished and it seems unlikely to be of any practical use.

Hoque (1987) used the Galerkin FEM to independently solve the 2 - D groundwater flow equation and the kinematic flow model (derived from the Saint - Venant equations) for open channel flow. By regarding both of these solutions as independently correct, Hoque (1987) proposed that coupling can be accomplished by:

(1) Running the groundwater and open channel simulations separately for a given time period;

(2) comparing the stream node water levels from the groundwater and open channel solutions at the end of each time period;

(3) subtracting the smaller level from the greater level to give a stream - aquifer head difference, and

(4) calculating the exchange of water between the stream and the aquifer using Darcy's Law.

This coupling method avoids the difficulties of reconciling different time - stepping requirements for the groundwater and streamflow simulations (Vasiliev, 1987), but it does not appear to have a thoroughly physical basis. Hoque (1987) intended to apply this methodology to SAI investigations in the Ganges Kobadak irrigation project in Bangladesh. Results are not yet available.

An accidental spill of tritium in the Glatt River, Switzerland, allowed induced infiltration into the wells originally studied by Schwarzenbach et al (1983) to be monitored and modelled by Hoehn and Santschi (1987). The main focus of this study was in the estimation of dispersion parameters for the aquifer, which is composed of glaciofluvial sands and gravels. Instead of using the standard advection - dispersion equation, which assumes that dispersivities are constant in time and space, Hoehn and Santschi (1987) used the Method of Moments (MOM). In the MOM, simple algebraic expressions are used to define a local value for dispersivity according to the variance of a tracer distribution (in space or time). Using a constant groundwater velocity estimated from field data, dispersion of tritiated water in the aquifer was modelled using the MOM equations. While this study was an interesting exercise in the application of an alternative dispersion formulation, it did not reveal much about stream - aquifer interactions.

A simple externally coupled model for solute transport in stream - aquifer systems has been described by Gilliland and Nguyen (1987). The flow component of the model was based on the well - known PLASM model of Prickett and Lonnquist (1971), and solute transport was assumed to occur by advection only. Good reproductions of field data for both flow and nitrate migration were obtained when the model was applied to the Grand Island wellfield in Nebraska.

Guillet et al (1988) and Retrowski et al (1988) have described a stream - aquifer model of the Chalk aquifer near Aubergenville, France, where this is hydraulically connected to the Seine River. Unfortunately, neither paper explicitly revealed the numerical methods or coupling techniques used in the model, but the model seems to be a 2 - D areal groundwater model, externally coupled to a simple representation of streamflow partially separated from the aquifer by low - permeability streambed sediment. Solute transport seem to have been represented by numerical solution of the equation of hydrodynamic dispersion. The model has been used to assess the vulnerability of the Chalk aquifer to pollution from conjectural spills in the Seine, although the results of these studies were not reported.

Jorgensen et al (1989a, 1989b) have discussed methods for externally coupling the results of a 3-D finite difference model for unconfined groundwater flow to baseflow measurements, where the spatial scale of the groundwater model is such that model elements are far larger than the width of streams in the model domain. Essentially, SAI in this model is simply accounted for as a source/sink within a model element, with its magnitude determined explicitly by hydrograph separation techniques. Application of this simple model to a regional study of carbonate aquifers in the Ozark Plateau, USA, yielded a satisfactory match with field data.

Zipfel and Horalek (1989) used nested finite difference models to study long - term induced infiltration in the Upper Rhine Valley, Germany. A regional scale model was used to determine percentages of river - derived water in abstraction boreholes, while a 3-D model of a small portion of this regional domain was used to test some concepts of solute transport in the system. Unfortunately, the paper by Zipfel and Horalek (1989) does not include any real discussion of the aims or results of either modelling effort.

Kovar and Grakist (1989) used a 2-D areal finite element model of steady state groundwater flow to simulate the stream - aquifer systems in the Netherlands which were previously described by Meinardi and Grakist (1985). Using the information on velocities and heads obtained from this model, the MOC model of Konikow and Bredehoeft (1978) was used to calculate nitrate distributions in the aquifer. A reasonable agreement between observed and predicted nitrate concentrations was reported.

2.4.3 -- Internally Coupled Numerical SAI Models.

Pinder and Sauer (1971) appear to have been the first to produce an internally coupled SAI model, in which 1 - D open channel flow was internally coupled with 2 - D transient, unconfined groundwater flow. The interface boundary conditions were framed in terms of Darcy's Law. The internal coupling methods used by Pinder and Sauer (1971) have been borrowed by many later workers, but never bettered. The main drawback with the Pinder and Sauer (1971) model is that it employs incongruous numerical schemes for the open - channel and groundwater solutions. An explicit FDM is used for the open - channel solutions, which requires far shorter time steps for stability than the ADI - FDM used for the groundwater solutions. Of course the time - scale difference between stream- and groundwater flow is such that these solutions are satisfactory in isolation (Vasiliev, 1987), but practical coupling of the two schemes in a computer programme is cumbersome.

Pinder and Sauer (1971) did not apply their model to real - world data, but used it to investigate the theoretical effects of bank storage phenomena on stream flood waves. However, Pogge and Chiang (1977) did apply the Pinder and Sauer (1971) model to data from a site in west - central Kansas, concluding that "the model performs adequately in simulating the response of the stream / aquifer system to the passage of a flood wave". They also noted the critical importance of selecting a suitable value for the Manning roughness coefficient in the streamflow routing equations: " . . . the bank storage occurring in the study area will be reduced by about 50% if the value of n [the roughness coefficient] is decreased from 0.055 to 0.035. This is because of the shorter duration of the flood peaks when n is equal to 0.035 . . ." (Pogge and Chiang, 1977, p. 98).

Zitta and Wiggert (1971) independently derived an internal coupling method very similar to that of Pinder and Sauer (1971) and used it to combine 1 - D unsteady streamflow routing (using the Saint - Venant equations) with 1 - D transient unconfined groundwater flow simulation (using the Boussinesq equation). Both the surface and subsurface flow equations were solved using explicit FDMs, and thus suffered from timestep length restrictions. Like Pinder and Sauer (1971), Zitta and Wiggert (1971) used their model only for theoretical investigations of bank storage effects on streamflow hydrographs, doing a number of sensitivity analyses on the influence of channel geometry. However, the Zitta and Wiggert (1971) model is more limited in scope than the Pinder and Sauer (1971) model because of numerical stability problems and because it only considers 1 - D groundwater flow.

Freeze (1972a) went further than Pinder and Sauer (1971) by including unsaturated flow and 3 - D groundwater flow in an SAI model. Internal coupling was used to combined the Jacob - Richards Equation for 3 - D, saturated - unsaturated transient groundwater flow with equations describing 1 - D gradually varied, unsteady, turbulent, subcritical flow in an open rectangular channel of variable width. The groundwater flow solutions were procured by LSOR and the streamflow solutions by the single - step Lax - Wendroff explicit FD scheme.

This model was not tested for real - world data, but was used by Freeze (1972b) to investigate streamflow generation in upland source areas, yielding useful insights into processes of interflow and baseflow discharge.

Rovey (1975) developed an internally coupled FD SAI model which had a number of unique features. Most outstanding of these was the division of the groundwater module into two interfaced simulation zones; a 3 - D zone in the vicinity of stream nodes (where vertical flows will dominate if the stream is partially penetrating), and a 2 - D zone for parts of the aquifer distant from the stream (where saturated flow would be approximately horizontal).

Streamflow routing in the Rovey (1975) model was accomplished by use of the Manning formula, and the 3 - D groundwater simulation subroutine solved the Richards equation for saturated / unsaturated flow, thus allowing for the passage of the water table out of hydraulic connection with the stream. The 2 - D groundwater simulation subroutine solved the Boussinesq equation.

Rovey (1975) paid much attention to the effects of streambed sediment on flow across the stream / aquifer interface. Unpublished studies cited by her suggested that siltation was a perennial limitation on SAI in the modelled system.

Application of the Rovey (1975) model to data from the Arkansas River Valley, near Lamar, Colorado, produced satisfactory results for dry weather periods. Failure to predict flood flows correctly prompted Rovey (1975, p. 39) to suggest modification of the model to allow representation of overland flow, flow in minor tributaries and unsteady non - uniform streamflow.

Cunningham and Sinclair (1979) developed and tested a Galerkin FE model in which open channel flow, represented by the Saint - Venant equations, was internally coupled with 2 - D transient saturated groundwater flow, represented by the Boussinesq equation. In many respects the Cunningham and Sinclair (1979) model was nothing other than a refined FE version of the earlier FD model of Pinder and Sauer (1971).

In a number of sensitivity analyses, Cunningham and Sinclair (1979) indicated that model output (stage hydrographs) was most sensitive to changes in the Manning roughness coefficient (cf Pogge and Chiang, 1977), and the channel bed slope. Next in importance was the hydraulic conductivity of the channel perimeter. Variations in aquifer parameters (K and S) had the least effect on model output. In an application to two years of data from the Truckee River, northern Nevada, model predictions showed fairly good agreement with reality.

PREDIS (an acronym of Precipitation - Discharge) is an integrated catchment model similar to that of Knapp et al (1975), save that it is internally coupled. PREDIS has a modular structure. When the open - channel flow and groundwater flow modules are operated together an SAI model bearing the name GRODRA (Groundwater - Drainage) is formed (Wesseling and Jansen, 1986). GRODRA was developed at Delft Hydraulics Laboratory in the Netherlands, and has been described by Crebas et al (1984).

In the groundwater module, the Boussinesq Equation was solved using a Galerkin FEM (with Crank - Nicolson implicit FD time - stepping). The open - channel flow module was based upon a FD solution of the 1 - D form of the Saint - Venant equations. Crebas et al (1984) reconciled the different numerical schemes used in the solution of these two modules by arranging the stream along inter - element boundaries, thus making the computational nodes of the two schemes coincident. Internal coupling was accomplished by a complex iterative procedure in which the source / sink functions of the groundwater and open - channel flow equations were linearised in the form of Taylor expansions and solved as integrals involving terms for both groundwater head and stream stage. A conservative water balance was maintained using this approach. Unfortunately, Crebas et al (1984) omitted many steps in their mathematical formulation, and made no attempt to justify abandoning the more usual internal coupling techniques in favour of their own more complex (but less physically meaningful) approach. Wesseling and Jansen (1986) have applied the GRODRA model to a drainage control and land conservation project in the Netherlands. Early results indicated good agreement between predictions and reality.

2.4.4 -- Representing Partially Penetrating and Sediment-Lined Streams.

When stream - aquifer interactions are not the main focus of a study, modellers have tended to use a very simple representation for the stream - aquifer boundary conditions. In regional groundwater modelling, for example, rivers are frequently represented as lines of fixed head, which therefore act as flow boundaries so that no groundwater flow passes them. Such fixed head river boundaries are conceptually equivalent to rivers which fully penetrate the aquifer. Fully penetrating rivers are rarely found in nature. More usually, the river partially penetrates the aquifer such that there is the opportunity for exchange flow between the portions of the aquifer on opposite sides of the river (Figure 1.4a). Partially penetrating rivers drain groundwater storage less efficiently than do fully penetrating rivers (Singh, 1968). Furthermore, they induce considerable vertical components of flow in contiguous aquifers, in contrast to the horizontal flow adjacent to fully penetrating rivers (Figure 1.4b). For these reasons, the representation of rivers by fixed head nodes can introduce significant errors into groundwater models.

To avoid the errors associated with the assumption of full penetration, the river can be represented by a leakage boundary (eg Prickett et al, 1971). This is generally accomplished by assigning known 'head' values to nodes in a model layer overlying the aquifer model at "river nodes", and then calculating a flux from the river to the aquifer (or vice versa) at each node. This method does not divide the aquifer into separate domains, and as such it is more consistent with the geometry of most natural stream-aquifer systems. The stream - aquifer exchange flux (qsa) is usually calculated by a modified version of Darcy's Law such as:

$$qsa = Ks(hs - ha) / bs \quad . \; . \; . \; . \; . \; . \; . \; . \quad (2.1)$$

where:

qsa = stream aquifer exchange flux (L/T)

Ks = hydraulic conductivity of the streambed sediment (L/T)

hs = stream stage 'head' (L)

ha = aquifer head immediately below the river node (L)

bs = thickness of the streambed sediment (L)

The definition of these terms is clarified by Figure 2.1.

Equation (2.1) is formulated for 1- D flow, whereas the true exchange with a river is likely to be more akin to radial flow (cf Figure 1.4). In recognition of this fact several workers have produced empirical expressions which relate the geometry of the stream perimeter to the flow of water between the aquifer and the river. The simplest of these may be written (Miles, 1985a):

$$Qsa = C\ L\ (hs - ha) \quad \ldots\ldots\ldots \quad (2.2)$$

Where C is a coefficient of resistance to the flow and L is the length of the stream reach modelled. Qsa is equal to qsa*A, where A is the area through which the exchange flow occurs. The coefficient C has been variously defined:

$$C = [5.0\ Ka\ P\ /\ (D + d + s)] \quad \ldots\ldots\ldots \quad (2.3)$$

(Miles, 1985b)

$$C = \pi Ka\ /\ \ln\ ([0.5D + r]\ /\ r) \quad \ldots\ldots \quad (2.4)$$

(Herbert, 1970)

$$C = 1\ /\ [(1/\pi Ka)\ln(zD/P) + p/P] \quad \ldots\ldots \quad (2.5)$$

(Crebas et al, 1984)

where:

Ka = aquifer hydraulic conductivity

D = aquifer saturated thickness below the stream

d = depth of stream

s = height of seepage face above stream stage (if any)

w = width of stream

P = w + d + s (i.e. perimeter term).

z = some dimensionless coefficient (see Crebas et al, 1984)

p = 'hydraulic impedance' (see Crebas et al, 1984)

r = radius of channel (assumed to be semi - circular)

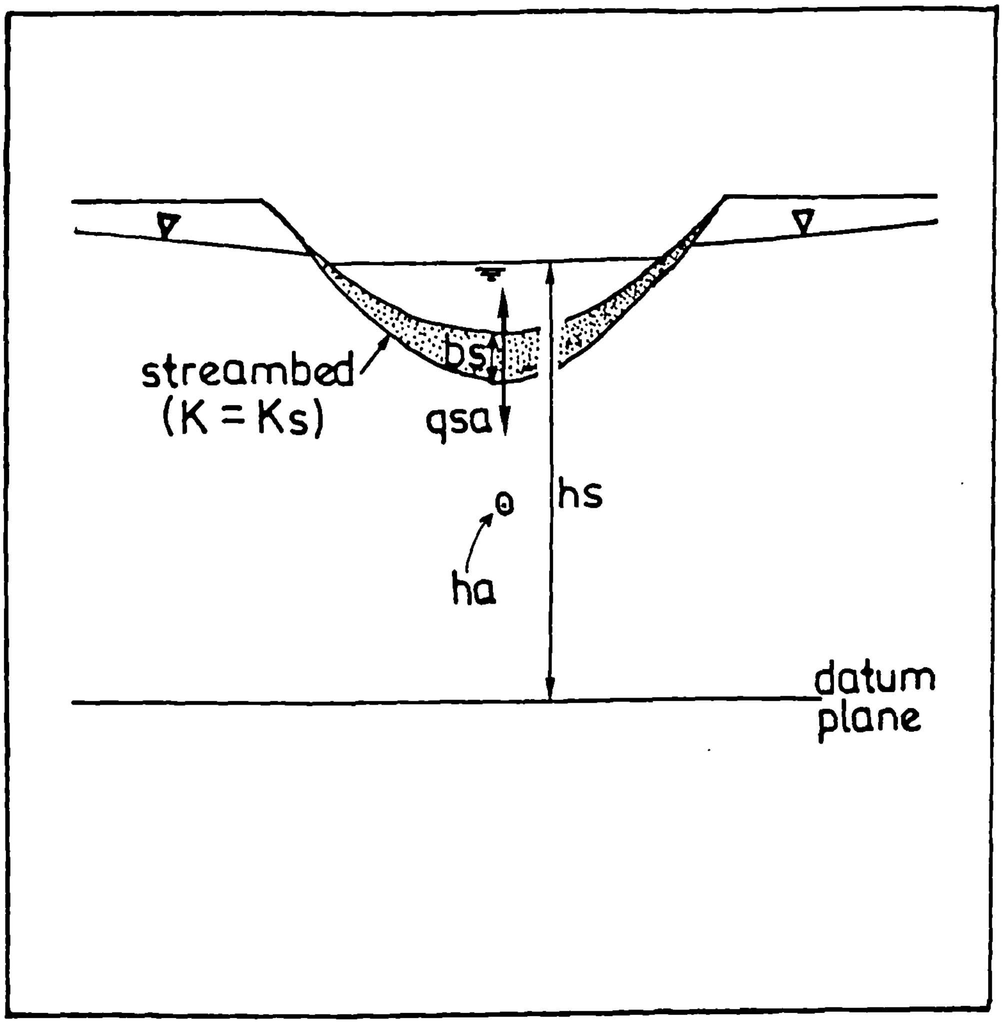
Miles (1985b) has also redefined the parameter 'r' in (2.4) as:

$$r = w(s + d)\ /\ P.$$

Further versions of Equation (2.2) are presented by Rushton and Tomlinson (1979), and Miles (1987a, 1987b) has devised methods for calculating a 'prevailing' value for Ka when convergent flow towards a stream occurs through an aquifer which is layered and/or anisotropic.

All of the definitions for C and Equation (2.2) mentioned above suffer from the same drawback; they fail to consider the effect of a lowly permeable streambed sediment layer on the stream - aquifer exchange. In most systems, vertical

Figure 2.1 -- Diagram Illustrating the Terms in Equation 2.1.



differences in head are likely to be even more profoundly affected by the latter phenomenon than by the geometry of the stream boundary. For this reason, the simple approach of Prickett et al (1971), as represented in Equation (2.1) above, remains the most useful for most modelling scenarios. As will be seen in subsequent chapters, however, even this approach may be insufficiently detailed when the output from a stream - aquifer flow model is to be used in the modelling of non-conservative solute transport. In such a case, explicit representation of flow in the streambed sediment may be necessary.

2.4.5 -- Summary and Conclusions on Numerical SAI Models.

Numerous externally and internally coupled stream - aquifer flow models have been developed, and techniques for representing partially penetrating streams in such models are well established. The effects of a lowly permeable streambed sediment layer on stream - aquifer exchange can be incorporated into a flow model quite readily. However, very few models for solute transport in stream - aquifer systems have been described, and none of these has included any assessment of the geochemical effects of streambed sediment, or the full spatial implications of vertical flow components as these apply to solute transport. It would thus seem that development of suitable methodologies for modelling the effects of stream - aquifer interface processes on solute transport is an important avenue for future research in the field of stream - aquifer modelling.

CHAPTER THREE

HYDROGEOLOGY OF STREAM - AQUIFER SYSTEMS IN THE THAMES BASIN.

3.1 -- INTRODUCTION.

In describing the hydrogeology of stream - aquifer systems in the Thames Basin it is essential that the ingredients of the system are first described. Thus the first section of this chapter is an account of those hydrostratigraphic units which occur in stream - aquifer settings, while the particulars of their behaviour with respect to streams are reserved to the second section.

The general study area for this project is shown in Figure 1.2, and basic information on the named sites is given in Appendix A. As shown in Figure 3.1, the Thames Basin is a synclinorium developed in a succession of Mesozoic and Cenozoic sedimentary units. Table 3.1 summarises the stratigraphy of the part of the Thames Basin studied in this project.

3.2 -- THE HYDROGEOLOGY OF THE CHALK.

3.2.1 -- Introduction.

No complete review of the various aspects of Chalk geology has yet been published, doubtless due to the breadth of research areas involved and to the sheer volume of material available. Partial reviews covering the petrology and diagenetic features of the Chalk have been presented by Hancock (1975) and Scholle (1977) respectively, while Price (1987) has reviewed fluid flow in the Chalk. In the following sections, a broad ranging but selective review of Chalk properties is given, along with some new data from field studies conducted by the present author.

3.2.2 -- Geology. Because of the proximity of its main outcrop areas to London, and because of its importance in the water supply of that city, the Chalk has been

TABLE 3.1 -- Stratigraphy of the North West Thames Basin.[1]

AGE[2]	UNIT	THICKNESS (m)	HYDROLOGICAL CLASSIFICATION[3]	LITHOLOGY
Q	GLACIAL DEPOSITS	0 - 50	aquitard/fer	till, sands and gravels
Q	CLAY-WITH -FLINTS	0 - 10	aquitard	as named
Q	RIVER GRAVELS	2 - 13	aquifer	sands and gravels with some silts
			UNCONFORMITIES	
T	LONDON CLAY	up to 100	aquitard	mudstone
T	READING BEDS	8 - 35	aquitard	mudstones and silty sandstones
			UNCONFORMITY	
T	THANET BEDS	0 - 16	aquifer	fine - grained sandstones and siltstones
			UNCONFORMITY	
K	UPPER CHALK	50 - 120	aquifer	soft white chalk with horizons of flint nodules
K	MIDDLE CHALK	50 - 100	aquifer	dense white chalk; few flints.
K	LOWER CHALK	40 - 80	aquifer/tard	greyish marly chalk

[1]Derived from data in British Geological Survey (1984)

[2]Q = Quaternary; T = Tertiary; K = Cretaceous.

[3]i.e. aquifer (stores and transmits significant quantities of water) or aquitard (low storage, low transmissivity unit). Classifications with a / denote local variations, not a compromise.

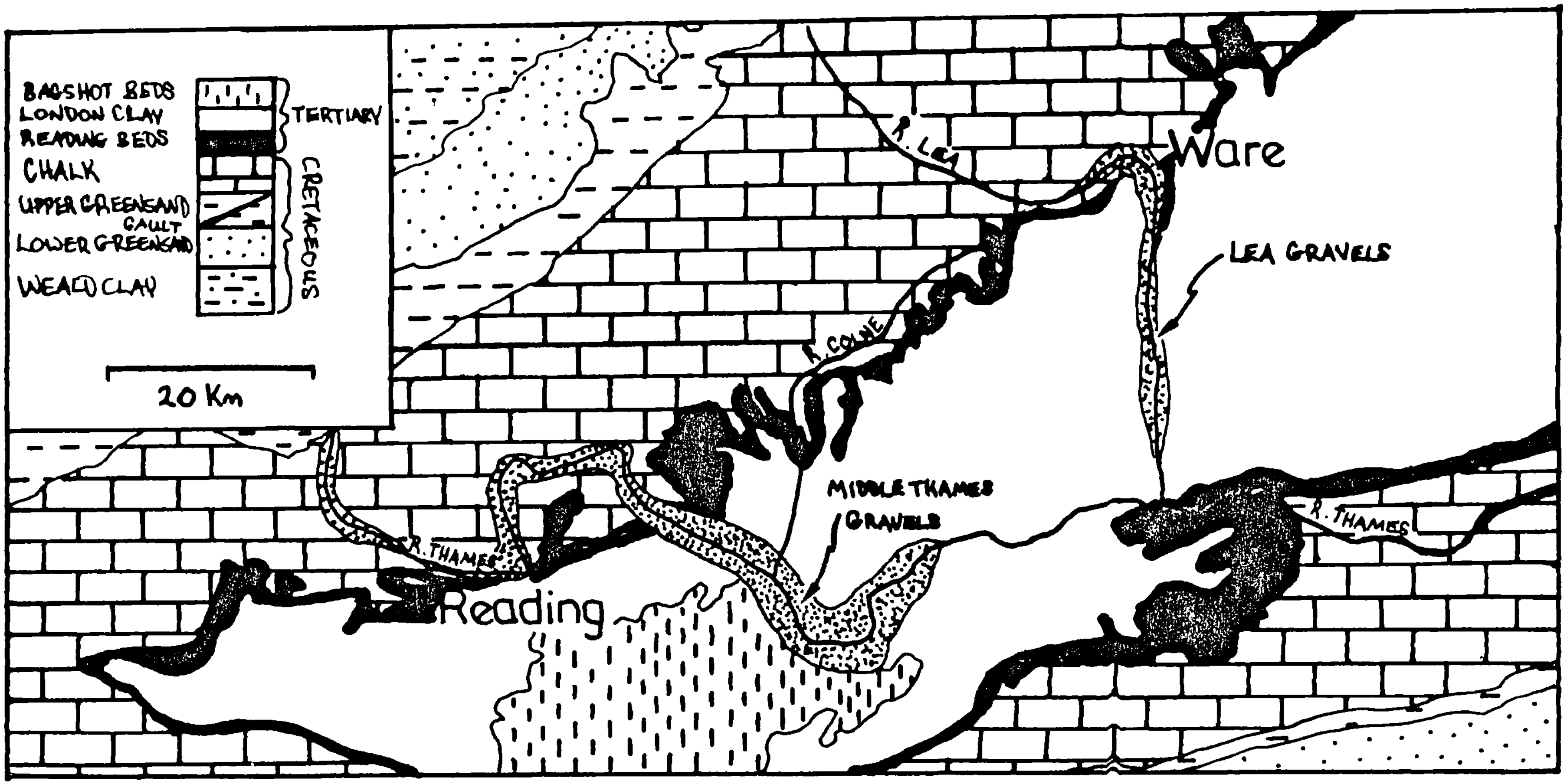


Figure 3.1 -- Geology of the Northwest Thames Basin.

intensively studied since the earliest days of geology.

The Upper Cretaceous Chalk of southern England is a soft, brilliant white, fine - grained, microporous limestone. Its three most distinctive features are (Hancock, 1975):

(1) Purity -- More than 96% $CaCO_3$, with trace amounts of Al_2O_3, MgO, Fe_2O_3 and SiO_2. This mineralogical and chemical purity is reflected in the remarkable whiteness of the Chalk.

(2) Friability -- because the Chalk was initially deposited as very stable low - magnesium calcite, it has undergone relatively little cementation.

(3) Lateral and Vertical Extent -- during the Upper Cretaceous, the Chalk was deposited over several continents during 27 million years (from 95 Ma to 68 Ma).

Petrologically, the Chalk is a micrite (ie a carbonate mudstone), and is largely composed of the calcitic plates of planktonic algae (Hancock, 1975). These plates show a bimodal grain - size distribution, with two principal ranges of 0.5 - 4 microns and 10 - 100 microns. The finer range accounts for 75 - 90% of white Chalk sediment, and the coarser fraction for some 0 - 15%. While the plankton plates dominate the fine range, the coarser range is mostly composed of echinoderm plates and bivalve and bryozoan fragments.

Original depositional features of the Chalk include:

(a) Bedding -- best seen where the clay content of the Chalk is at its highest (eg in the Lower Chalk), leading to the development of alternating beds of marl and pure chalk. In pure Chalk, the bedding planes are often marked by undulating fracture planes, and / or courses of flints. Whilst lamination is occasionally seen within beds, it has generally been obliterated by bioturbation.

(b) Burrows and borings, relict bioturbation structures, are widespread in Chalks (Hancock, 1975; Scholle, 1977), but are frequently only visible when special staining techniques are used. Flints occasionally occur as casts of the horizontal burrow trace fossil Thalassinoides.

Diagenesis of Chalks has been categorised as early ("intrinsic") diagenesis or later ("non-intrinsic") diagenesis (Scholle, 1977; Clayton, 1983). Early diagenesis mainly involved compactional dewatering of the unconsolidated Chalk sediment, with some sea - floor cementation (by recrystallisation of calcite and precipitation of phosphate from reworked fish skeletons and coprolites) leading to the development of hardgrounds (Willcox, 1953; Clayton, 1983).

Later diagenesis involved precipitation of flint nodules and induration of the Chalk. Flint, which is a form of chert, is a microcrystalline random mosaic of quartz, in this case believed to be formed from silica released by dissolving sponge spicules. Induration of the Chalk (which is more marked in the northern province in Yorkshire and Ulster) resulted from pressure solution and re - cementation, which has been variously attributed to burial, tectonic compaction, or thermal hardening.

Chalk stratigraphy has been described by various authors in both litho- and bio- stratigraphic terms. The lithostratigraphic subdivision has always been the most hydrogeologically useful. Lithological properties (such as colouring, hardness, the presence or absence of flints and the position of certain laterally persistent hardgrounds) are used to divide the Chalk into three major units (Table 3.1). In particular, three hardgrounds form major markers in this scheme. The Upper / Middle Chalk boundary is marked by the Chalk Rock, the Middle / Lower Chalk boundary by the Melbourn Rock, and the Lower Chalk is subdivided into upper and lower divisions by the Totternhoe Stone. In general, the Lower Chalk is more marly than the other two divisions. The Middle and Upper Chalk divisions are very similar to each other, save that the Upper Chalk is characterised by the widespread development of courses of flints along bedding planes, whereas flints are less abundant and more randomly distributed within the Middle Chalk.

Weathering of the Chalk is well displayed at many sites in the study area. Karst features, such as solution pipes and swallow holes, are reasonably common, especially in the Lea catchment, and have been described by Kirkaldy (1950), West and Dumbleton (1972), Walsh and Ockenden (1982) and Edmonds (1983), amongst others. During the course of this study, a major collapse hollow appeared near the Lea at Darnicle Hill (TL 308046), where the Chalk is confined by about 25m of Lower London Tertiaries. Within a few weeks, the hole was about 5m deep and 25m in diameter, dramatically illustrating the ongoing nature of karst erosion.

Fossil periglacial weathering features are also common, and three examples are frequently encountered; ice - wedge casts, gelifluction lobes and debris fans. Examples of ice wedge casts cutting the upper surface of the Chalk at Playhatch Quarry (SU 742765) near Reading are shown in Figure 3.2. In aerial photographs of areas such as Playhatch, ice wedge casts are often seen to produce polygonal patterned ground networks in the crop marks (eg Catt, 1988; p. 100). "Gelifluction", which is defined by Washburn (1979) as solifluction in the presence of permafrost, has resulted in the mass wasting of Chalk throughout the study area. A particularly striking example of a gelifluction lobe was observed by the author at Hindhay Quarry (SU 868828). In this location, the upper surface of the Chalk (beneath the modern soil) has been pulverised (probably by freeze - thaw processes; Williams, 1987) into pasty grey 'putty chalk' with scattered flint clasts. Some of this putty chalk, along with remnants of a palaeosol ('clay-with -flints'), has slid down the palaeoslope to form a large lobe of debris (Figure 3.3).

(Cross-Sectional View Exposed in Quarry Face)

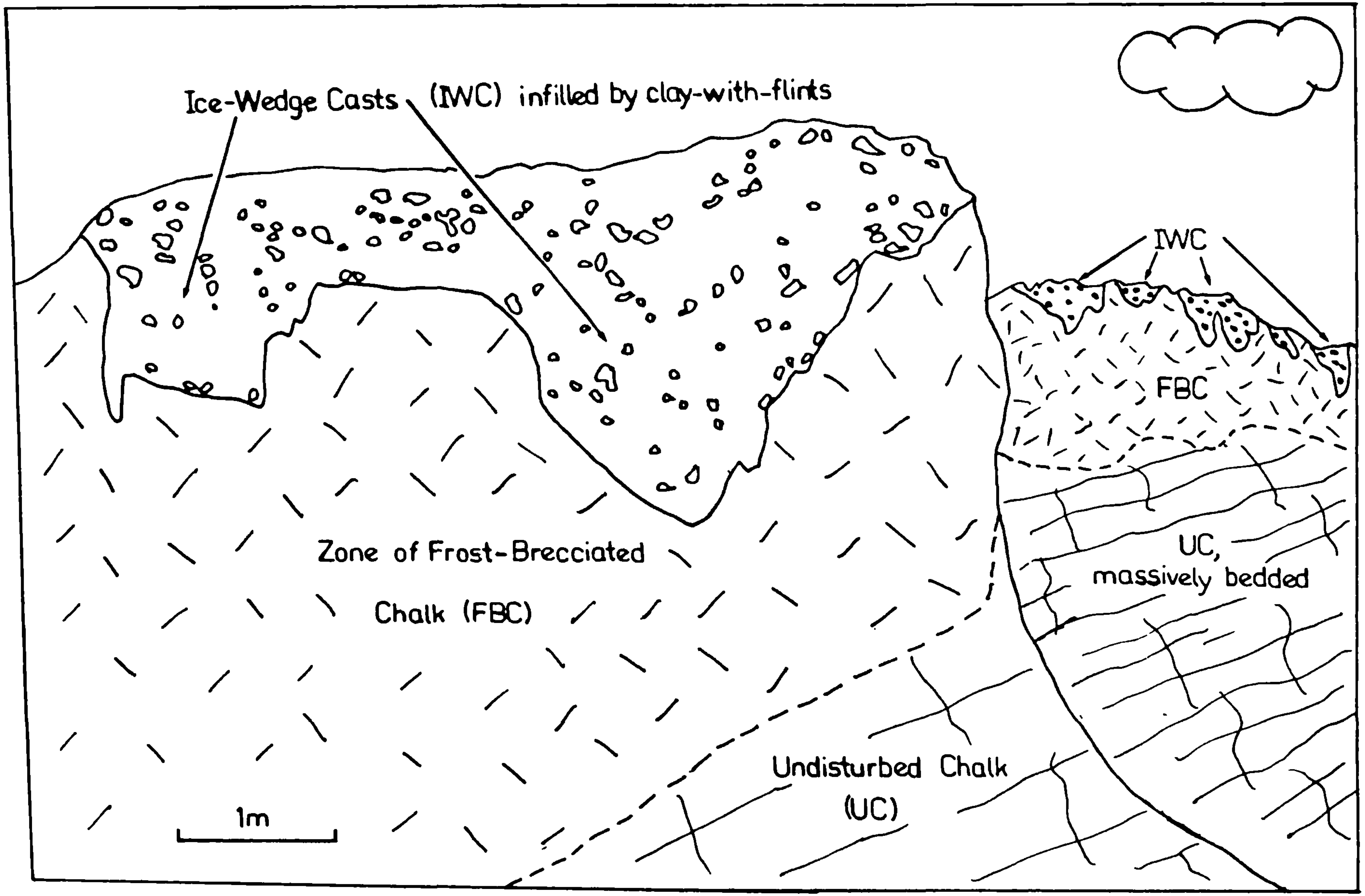


Figure 3.2 -- Field Sketch of Ice - Wedge Casts at Playhatch.

Debris fans emerging from the mouths of modern dry valleys are ancient analogues for modern alluvial fans in periglacial Canada and Alaska. A large complex of fans enters the Middle Thames Valley near Medmenham, constricting the valley considerably (Gibbard, 1985, p.77). The significance of these periglacial features will be discussed further in the next section and in Chapter 4.

3.2.3 -- Hydraulic Properties.

Fine grained sediments like the Chalk often have high matrix porosities (eg 41 - 50 % for Upper and Middle Chalk, 21 - 30 % for Lower Chalk) but very low matrix hydraulic conductivities (eg 10^{-2} m/d to 10^{-3} m/d for the Chalk; Price, 1985) due to the restricted size of pore necks.

Field tests of the bulk hydraulic conductivity (K) and transmissivity (T) of the Chalk, however, typically yield much higher values. For example, in river valleys (where Chalk T is typically highest) T values of 1000 m^2/d are common (British Geological Survey, 1984), implying K values of around 20 m/d, if a saturated thickness of 50m is assumed. Indeed Foster and Milton (1974) quote T values of 2500 m^2/d and K values of 170 m/d for the Chalk in Yorkshire.

The great discrepancy between laboratory and field K values is due to the widespread development of fissures in the Chalk. Indeed the chalk is a classic example of a dual-porosity medium, with both fissure porosity and matrix porosity.

Fissure permeability in the Chalk varies laterally and vertically, and is known to broadly correlate with four major factors:
(1) Topography -- fissure permeability is best developed in the river valleys (cf T = 75 m^2/d in interfluve areas; 2500 m^2/d in river valleys; Ineson, 1962; British Geological Survey, 1984).

(Cross-Sectional View Exposed in Quarry Face)

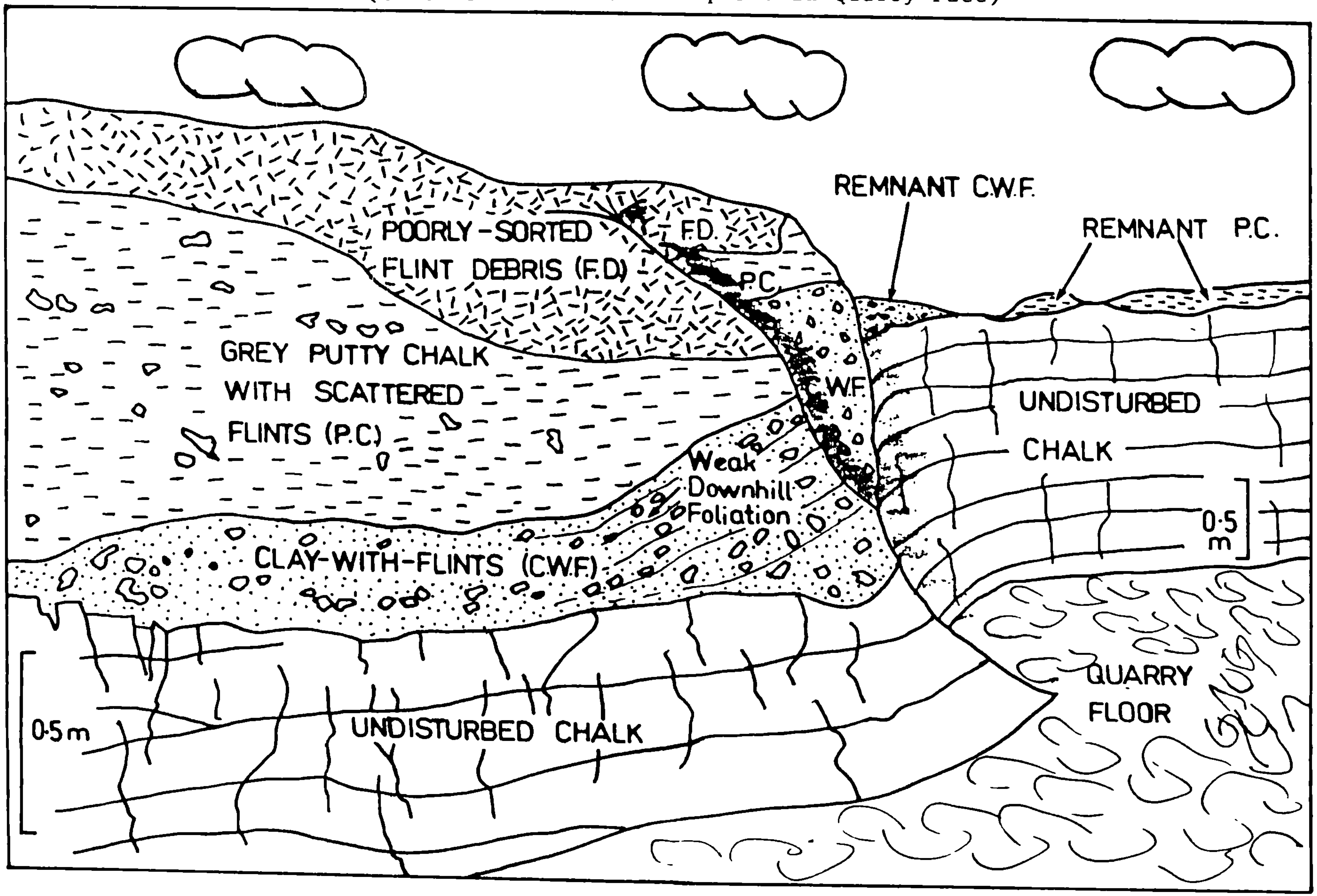


Figure 3.3 -- Field Sketch of an Exhumed Geliflucion Lobe at Hindhay Quarry.

(2) Structural and Diagenetic Features -- In confined Chalk, fissuring is often associated with the crests of anticlines; by the same token, the compressional zones in the axes of synclines tend to be tight and unfractured (Ineson, 1962; Toynton, 1983). Hardgrounds (e.g. the Chalk Rock, Melbourn Rock and Totternhoe Stone) are usually more competent than the surrounding Chalk and tend to have better developed fractures (Ineson, 1962).

(3) Palaeohydrology -- present and former zones of water table fluctuation (and as will be argued in Chapter Four, former periglacial river taliks) tend to be zones of fissure enlargement (see for example Connorton and Reed, 1978; Headworth et al, 1982; Foster and Milton, 1974).

(4) Depth -- the extent of solutional enlargement of fractures decreases non - linearly with depth (Connorton and Reed, 1978; Headworth et al, 1982). Because of this, the effective saturated thickness of the Chalk rarely exceeds 75m, even though the Chalk itself may extend to much greater depths below the water table.

Until recently, the association between river valley axes and high Chalk permeabilities was thought to be absolute. Evidence which has accumulated during the present project, however, shows that the reality is rather more complex. Zones of 'tight' Chalk have been discovered in the Middle Thames Valley, associated with deposits of 'putty chalk' at the Chalk / gravel interface. This discovery prompted some geological modelling work on the part of the author, which is presented in Chapter 4. Hence no further comment on the nature and significance of the 'putty chalk problem' will be given here.

Even though the fissures in the Chalk account for only 1 - 2 % of the bulk rock volume, they supply nearly all of its available storage capacity, which is therefore rather low. For example Foster and Milton (1974) quote a range of specific yield values of 0.005 - 0.01 for unconfined Chalk in Yorkshire, although values up to 0.07 were reported by

Headworth et al (1982) from Hampshire. Since storage capacity is dependent on the development of fissuring, it decreases with depth in a manner similar to hydraulic conductivity (Connorton and Reed, 1978).

Because of the critical control which the fracture system exerts on the aquifer properties of the Chalk, the present author made a special study of this feature. Details of this study are given in Appendix B. The main conclusions of this study are:

(i) In the Thames Basin the bedding plane parallel (BPP) fracture set shows the greatest frequency (mean 9.4/m) and lateral persistence (at least several kilometres on average), while the bedding plane normal (BPN) sets are less frequent (6.3/m) and less persistent (traces rarely extend beyond 3 metres).

(ii) There is a difference in absolute and relative frequencies of BPP and BPN sets between the Thames Basin and the Kent area (North Downs, South Downs and Isle of Thanet). This illustrates the dangers of any application of Chalk fracture system data beyond the Thames Basin. Within the Thames and Kent areas, however, frequencies are fairly homogeneous.

(iii) Correlation tests on data from the valleys of the Thames, the Cam and the Medway do not show the inverse correlation between fracture frequency and the distance from a valley centre which has been postulated in the past (Ineson, 1962). Thus one of the main props of the old model for the development of Chalk permeability is found to be wanting. This finding paves the way for the new hydrogeological model for the development of Chalk permeability proposed in Chapter 4.

Recharge to the Chalk aquifer is sometimes difficult to assess due to the complex stratigraphy of the overlying deposits. Nonetheless, the relatively high proportion of baseflow in total runoff hydrographs from Chalk catchments (50% - 95%; Foster, 1974) suggests that recharge to the

Chalk is a fairly efficient process. Detailed studies of Chalk recharge have been presented by Lloyd et al (1984), Senarath and Rushton (1984), and Jackson and Rushton (1987).

Flow mechanisms in the Chalk differ somewhat between the unsaturated and saturated zones. In the unsaturated zone, most flow seems to occur in microfractures and the larger intergranular pores of the matrix blocks (Geake and Foster, 1989), with downward flow in the main fissures only occurring when rainfall intensity exceeds the infiltration capacity of the matrix blocks. In the saturated zone, on the other hand, most flow occurs in the fissures, with negligible volumes of water moving in the matrix blocks (Downing et al, 1979).

Where the Chalk is karstified, flow mechanisms differ from those just described. Two studies have considered the hydraulic effects of Chalk karst features. Harold (1937) noted rapid flow (up to 5.5 km/d) in fissures from the sink-holes near Water End, Herts, to wells in the Lea Valley (Broad*meads, the Amwells and Rye Common). Atkin*son and Smith (1974) described rapid groundwater flow, demonstrated by tracer tests, between swallow holes and public supply wells in the Chalk of southern Hampshire. Velocities of 2 km/d were recorded, which Atkinson and Smith (1974) argued could only have been achieved by turbulent flow under the prevailing hydrogeological conditions.

3.2.4 -- Geochemical Properties.

Geochemical processes of importance in the Chalk include matrix diffusion, carbonate dissolution, ion exchange and redox reactions. All of these processes affect the natural hydrochemistry of the Chalk, as well as having important implications for contaminant transport (see Edmunds et al, 1987, for a review of the literature on this subject). Examples are given below.

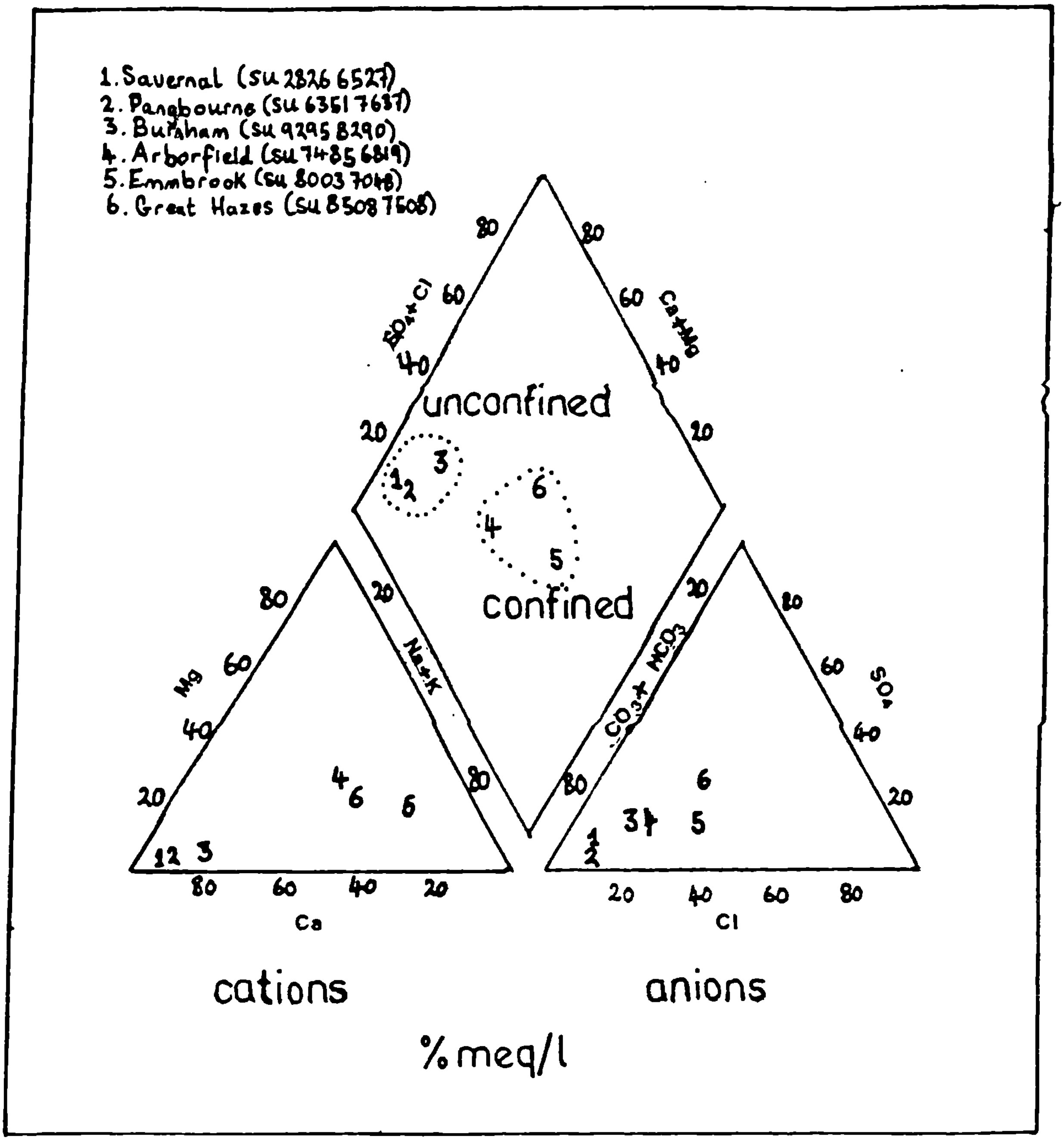
(i) Matrix Diffusion. Matrix diffusion is defined as the exchange of solutes between advecting water in fissures and stagnant water in porous blocks between these fissures ('matrix blocks') by molecular diffusion (Lever et al, 1983). The effects of matrix diffusion on the quality of water in the Chalk are well documented.

In the deepest parts of the Chalk aquifer, the chemistry of water in the smallest pores of the matrix blocks is quite different from that of the main body of advecting groundwater in the fractures. Exchange of solutes by matrix diffusion alters the composition of water nearest to the fractures, but water in the centre of the matrix blocks sometimes has a marine composition (Bath and Edmunds, 1981). In matrix blocks near the water table, however, the greater through - put of "fresh" meteoric waters in adjacent fissures has resulted in greater dilution of water in the centre of the blocks (Edmunds et al, 1973).

Numerous authors have identified matrix diffusion as a major control on pollutant migration in the Chalk (for reviews, see Black and Kipp, 1983, and Müller, 1987). In general, matrix diffusion results in increased retardation and dispersion of pollutants.

(ii) Carbonate dissolution. Variations in the natural chemistry of Chalk groundwater between the unconfined and confined parts of the aquifer have been attributed to differing carbonate dissolution regimes and to ion exchange processes (Ineson and Downing, 1963; Flavin and Joseph, 1983; British Geological Survey, 1984). Figure 3.4 is a plot of six Chalk water analyses which illustrate these differences. Unconfined Chalk water (Samples 1 - 3) is of Calcium - Bicarbonate Type, and generally of low total dissolved solids (TDS) content (about 400 mg/l), with up to 30 mg/l chloride and 50 mg/l sulphate. Nitrate is typically around 30 - 40 mg/l in this setting. Confined

Figure 3.4 -- Piper Plot of Chalk Groundwaters.



Chalk water is generally of Sodium - Bicarbonate Type, with elevated Cl (up to 500 mg/l) and SO_4 (up to 150 mg/l). Nitrate is generally negligible in confined Chalk waters.

The reasons for these differences are fairly well understood. The Ca - HCO_3 type water in the unconfined Chalk is typical of waters subject to "closed - system" carbonate dissolution, in which the water first equilibrates with a CO_2 gaseous phase, then reacts with the rock in the absence of a gas phase (Garrels and Christ, 1965; Connorton, 1976; Heathcote, 1985; Pitman, 1986). Occasionally, "open - system" dissolution (in which a gas phase of fixed pCO_2 is present throughout the rock - water interactions; eg in the unsaturated zone) can be shown to account for the chemistry of shallow unconfined water, and, even more rarely, for deeper (ie more than 60m) unconfined waters (Heathcote, 1985). Distinction between the products of these two pathways is made on the basis of solute mass balance calculations (Plummer and Back, 1980) and stable carbon isotope ratios (Deines et al, 1974).

(iii) Ion Exchange. The elevated sodium concentrations seen in the confined Chalk are due to cation exchange reactions (Ineson and Downing, 1963), with clay minerals and iron hydroxides in the Chalk, and, more importantly, in the overlying and underlying fine - grained clastic formations.

(iv) Redox Processes. The high sulphate concentrations in the confined Chalk are probably due to oxidation of pyrite in overlying clastic formations, in particular the London Clay (Ineson and Downing, 1963) and the Quaternary boulder clay (Heathcote and Lloyd, 1984, p. 148), through which water enters the Chalk by leakage. Magnesium is also thought to enter the Chalk from the London Clay in the same way (Ineson and Downing, 1963). Any nitrate entering the confined Chalk suffers reduction to nitrogen gas as it encounters the anoxic regime deep within the aquifer.

(v) Baseflow Quality. The chemistry of streams draining Chalk catchments tends to closely reflect the groundwater quality of the Chalk (Casey, 1969; Hydrotechnica, 1988), although distinguishing differences between river and ground- waters have been noted in the following parameters: pH, Cl, Na, K, Sr, bacteriological parameters and temperature. Site - specific studies are usually needed to determine which of these parameters is most suitable for water provenance tracer experiments (Hydrotechnica, 1988; Edmunds, Owen and Tate, 1976; Ridings et al, 1977).

3.3 -- THE HYDROGEOLOGY OF THE TERTIARY STRATA.

3.3.1 -- Introduction.

The Tertiary Strata in the Thames Basin are rarely present and seldom important in riverside settings. Nonetheless, a brief appraisal of them is warranted so that their contribution (or otherwise) in riverside settings may be adequately conceptualised.

3.3.2 -- Geology.

The Tertiary strata in the Thames Basin comprise a number of generally fine - grained clastic formations (Table 3.1). The Thanet Beds are the coarsest of the formations, being predominantly fine - grained sandstones and siltstones. The Reading Beds mainly comprise mudstones and silty sandstones, and the London Clay (within the Thames Basin at least) predominantly comprises stiff dark pyritic mudstone with calcitic nodules, although a thin (2m - 10m) silty, glauconitic, basal member is usually present (British Geological Survey, 1984).

3.3.3 -- Hydraulic Properties.

The Tertiary strata tend to act as efficient aquitards (especially the London Clay) or as leaky aquitards (eg the Thanet and Reading Beds). Lateral facies variations result in these formations being locally useful as minor aquifers, but in all the riverside sites studied, these units behave as aquitards. No specific data on their hydraulic properties within the study area appear to be available.

3.3.4 -- Geochemical Properties.

Because they are rich in clay minerals, the Tertiary strata are likely to be moderately adsorptive, and their pyrite content results in them being prone to release sulphate to oxidising groundwaters flowing through them. As mentioned above, this has led to water quality problems where the confined Chalk aquifer is recharged by leakage through the London Clay.

3.4 -- THE HYDROGEOLOGY OF THE QUATERNARY FLUVIAL SEDIMENTS.

3.4.1 -- Introduction. Quaternary fluvial sediments studied in this project comprise the Devensian valley train "gravels", which occur along the valleys of both the Thames and the Lea, and the modern streambed sediments of the Thames. Of these three, the Thames Gravels have been studied most by previous workers. Both suites of gravels lie unconformably on an irregularly eroded surface of Chalk and Tertiary beds, which is the product of a number of processes including chalk dissolution, fluvial scouring and periglacial erosion (Gibbard, 1985, pp. 100 - 102; Wakeling and Jennings, 1976; Berry, 1979).

3.4.2 -- The Middle Thames Gravel Formation.

3.4.2.1 -- Geology. Quaternary gravels flank the valley of the Thames throughout its course, so that the gravels in the Middle Thames area are representatives of a much more extensive body of deposits. This suggests that information from outside the immediate study area may shed some light on the hydrogeology of the Middle Thames gravels, and indeed this proves to be the case. For instance, the Upper Thames Gravels (ie those terrace deposits of the Thames which lie upstream of the Goring gap) are so similar geologically and hydraulically to their downstream equivalents that inferences for the Upper Thames can generally be applied further downstream. Detailed reviews of the geology of the Upper and Middle Thames Gravels have been published by Briggs et al (1985) and Gibbard (1985) respectively.

Gibbard (1985) has proposed a formal lithostratigraphic classification of the gravel deposits of the Middle Thames. In this classification, the gravels as a whole are referred to as the Middle Thames Gravel Formation. Deposition of the Middle Thames Gravel Formation occurred as part of a cycle of erosion and aggradation throughout the Quaternary:

> "... These deposits are thought to result from a progressive series of incisions into the valley floor bedrock followed by aggradation of alluvial sediment. This series of downcutting and aggradational cycles gave rise to the preservation of a sequence of progressively younger deposits down the valley side, the youngest being those immediately beneath the modern river floodplain..." (Gibbard, 1985).

The youngest members of the Middle Thames Gravel Formation are the Kempton Park Gravel, Shepperton Gravel and Staines Alluvial Members. Of the two Gravel Members, the Shepperton Gravel Member is dominant in the sites studied, although the Kempton Park Gravel Member occurs as an outlier near Bray.

The Kempton Park Gravel Member is of Middle Devensian age (ie it was deposited during the Upton Warren Interstadial, beginning 44000 years before present (ybp) and lasting until 30000 ybp). At the type section (TQ118703) the member comprises 4 m of cross - bedded sand and gravel (Gibbard, 1985), and seems to be very similar to the younger Shepperton Gravel Member (late Devensian; 30000 ybp - 13000 ybp) which forms the floodplain at most of the field sites.

The author inspected sediments of the Shepperton and Taplow Gravel Members (and their upstream equivalents in the Upper Thames Valley) at the following sites: Wraysbury (TQ 013744), Medmenham (SU 793843), Egham (TQ 043683), Taplow (SU 915821), Dix's Pit (SP 411048), Brown's Pit (SP 427035) and Hardwick Pit (SP 392058). The finest exposures of sediments of the Shepperton Gravel Member were found in the gravel pit at Wraysbury. Here, as elsewhere, the Shepperton Gravels are seen to be dominated by two groups of facies (detailed in Table 3.2):

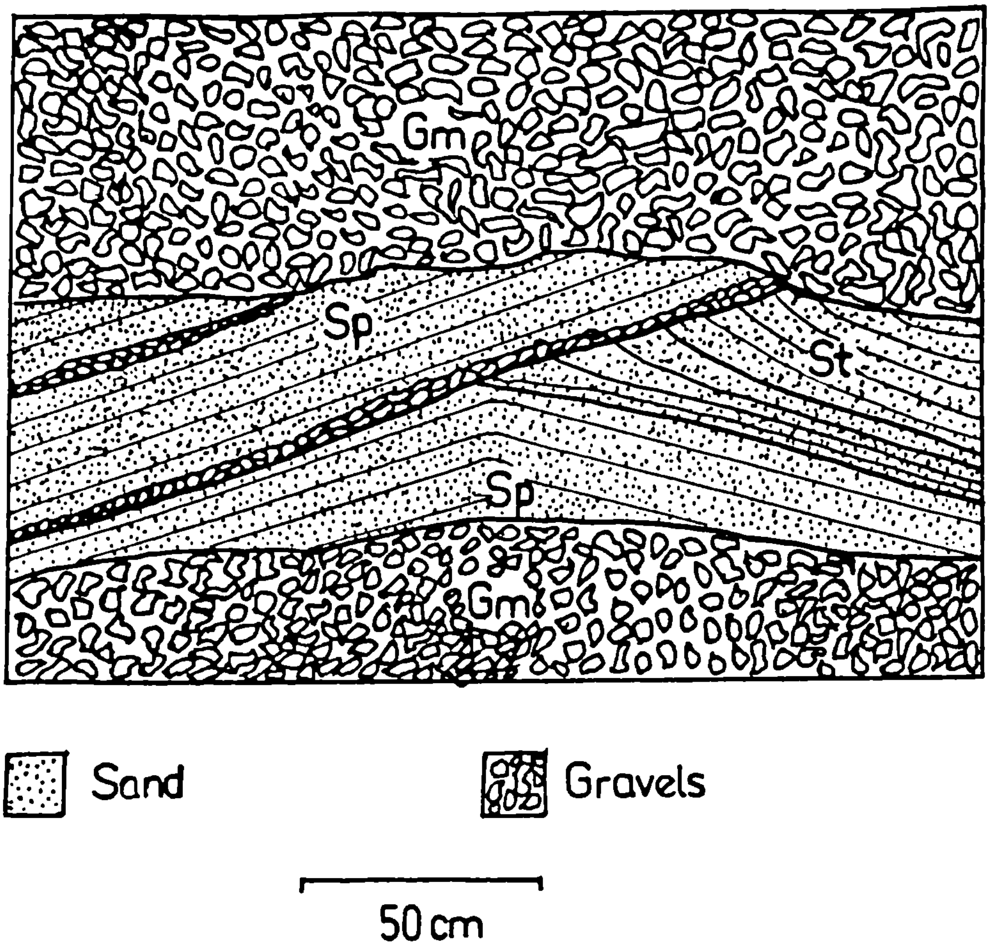
-- massive (or low - angle - cross - bedded) flint - clast (coarse sand - matrix - supported) conglomeratic gravels (facies Gm, Gt and Gp)

-- Cross - bedded, texturally mature arenite sands in channel - fills and scour - fills, embedded within Gm bodies (facies Ss, St, Sp, Sh)

At all exposures, the Shepperton Gravels (and all the other gravel members) show a striking pattern of small (generally 15m x 1.5m) sand - filled channel structures interbedded with the Gm gravel facies. A sketch of these field relations is given in Figure 3.5. The relative abundances of gravel and sand facies in these exposures have been determined by field measurements at Wraysbury, Taplow, Dix's Pit and Brown's Pit, and show remarkable consistency throughout the outcrop. All of the exposures studied return values of about 60% for the gravel facies and 40% for the sand facies. Similar results have been reported for the Upper Thames Gravels by Bryant (1983b) and Dixon (Institute of Hydrology, personal communication, 1989), and for the Lea Gravels (Section 3.4.3.1 below) by Gozzard (1981) and Hopson and Samuel (1982).

Most of the clasts in the Shepperton Member are flint, with lesser quantities of vein - quartz and quartzite. Chalk clasts are fairly rare, since chalk fragments are liable to severe physical erosion during fluvial transport. Coatings of chalk do occur on some of the larger flint clasts, however. Greater quantities of allocthonous clasts such as glauconite (Robinson, personal communication, 1987) and haematite (cf sample

Figure 3.5 -- Field Relations in the Shepperton Gravels at Wraysbury.



descriptions in Table C.1, Appendix C) occur in upstream areas, which are closer to source areas containing Cretaceous Greensands and ironstones. The Upper Thames Gravels are dominated by clasts of Jurassic limestone, which are more platy than the flints and are thus more prone to displaying sedimentary structures such as imbrication. It may be noted that peat and silt channel - fills (Fl facies) were occasionally observed interbedded with Gm in the Upper Thames Gravels, but never in the Middle Thames Gravels.

The field relations and facies distributions within the gravel members of the Middle Thames Gravel Formation conform to the well developed facies model for the braided stream depositional environment (Miall, 1977). The "Scott - Type Braided - Stream Facies" consists mainly of longitudinal bar - gravels, with sand lenses formed by the infilling of channels and scour - hollows during lower flows (Miall, 1977). Table 3.2 summarises the various sub - facies which are developed in the Middle Thames Gravels along with the interpretation of these in terms of the Scott - Type facies model. The Shepperton Gravels are known by radiocarbon dating to have been deposited during the Devensian epoch of the Quaternary (Gibbard, 1985). Abundant evidence that the Middle Thames Valley had a periglacial climate during this time is provided by the ice wedge casts and involutions which are found throughout the outcrop of the Shepperton Gravels and their upstream equivalents (Figure 3.6). The Devensian proto-Thames is thought to have had an arctic nival discharge regime dominated by spring snowmelt (Bryant, 1983b), and palaeohydrological analysis (Briggs, 1983) indicates that the <u>minimum</u> discharge (total for all the channels) of the braided proto-Thames was about 13 times the <u>maximum</u> discharge of the modern Thames. These environmental factors are discussed further in Chapter 4, where their importance for the modern permeability distribution in the Chalk is explored.

The Staines Alluvial Deposits are the youngest of the three units found in close proximity to the modern river channel. At the type section (TQ042685; Gibbard, 1985, p. 87) they comprise

Table 3.2 -- Description of Sub-Facies in the Middle Thames Gravels and their Interpretation in Terms of the Scott - Type Braided Stream Facies Model of Miall 1977).

SUB-FACIES[4]	DESCRIPTION[5]	INTERPRETATION[6]
Gm	Most common sub-facies. Massive or flat - bedded gravel (grain size; 2 - 30 cm). Generally matrix - supported, though coarser fraction may be clast - supported. Large scale planar erosion surfaces often present. Units typically 0.9 m thick by 30 m wide.	Deposited during the migration of low - amplitude longitudinal bars. Accumulation of fines in pores may obscure flat bedding.
Gp Sp	Planar x - bedded gravel and planar x - bedded sand. Gp and Sp usually interbedded in channel fills (15 m wide by 1.5 m deep) cut into Gm gravels. Basal gravel lag and fining - upwards sequences common, though seldom completed due to truncation by re - activation surfaces.	Formed by upper - flow regime *migration of sand* waves.
Gt St	*Trough x - bedded gravel* & trough x - bedded sand. Occur in channel - fills cutting earlier sediments and alternating with Gm. Channel dimensions similar to those of Gp and Sp.	*Infilling* of major channels during lateral migration. St is the product of dune and mega - ripple migration within these channels

[4]Letter designations after Gibbard (1985)

[5]cf. Gibbard (1985)

[6]cf. Miall (1977)

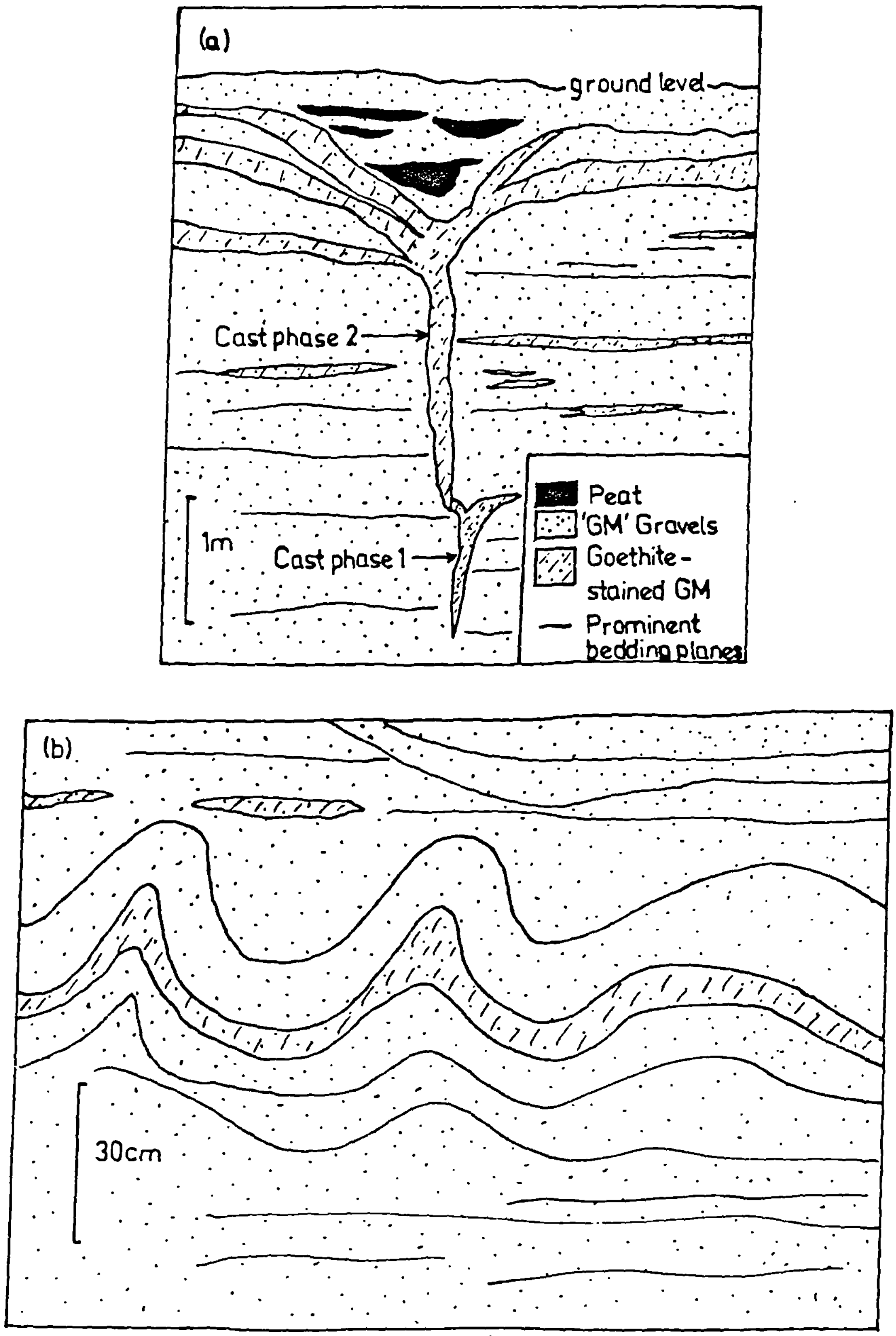
Table 3.2 (Continued).

SUB-FACIES	DESCRIPTION	INTERPRETATION
Ss	Scour - fill sands. Scours typically 50 cm deep and 1.5 m wide. Sand bedded parallel to scour boundaries. Ss common as lenses in Gm.	Shallow sand filled channels within main channel. Formed by scour associated with local eddies.
Sh	Flat bedded or massive sands (20 cm thick) in very localised spreads.	Lower flow regime flat bed formed in shallow water, or, if primary current lineations are present, under upper flow regime conditions.
Fl	Bedded fine grained deposits: Silty clay, clayey silt and fine organic matter. Typically brown or grey. Occur as channel - fills or as fills in floodplain depressions, frequently at the top of Gp and Sp fining - upwards units.	Accumulation from suspension in abandoned or partially abandoned channels, especially in the higher parts of the floodplain.
[7]Mp	Mudstones with floating pebbles of chalk and flint in tongue - shaped or wedge - shaped bodies near valley sides.	Mudflows and/or solifluction deposits of "rubble chalk" emplaced by slides from steep valley walls.

numerous channel - fills and channel - spill spreads of predominantly fine - grained sediments (brown and grey silts and clays containing abundant organic matter), with a few lenses and horizons of sand and gravel (typically stained orange by iron oxides). All dated samples of the Staines Alluvial Deposits have yielded Flandrian ages (ie post - Glacial, 13000 ybp - 0 ybp).

[7]Designated by the present author.

Figure 3.6 -- Periglacial Features in the Thames Gravels: (a) Syngenetic Ice - Wedge Cast (b) Involutions.



(Exposures in Dix's Pit)

Deposits of the Staines Alluvial Member typically flank the modern channel of the Thames for a few tens of metres on either side (they are shown on the Geological Survey maps as "Alluvium"), and it is clear that deposition would be continuing today were the Thames uncontrolled (cf Gibbard, 1985, p. 87). Squirrell (1976) has described the Staines Alluvium in the vicinity of Gatehampton as consisting "dominantly of brown silty clay". Peat occurs within the alluvium in some places; the author has observed exposures of peat up to 1m thick at Wraysbury (TQ 013744). Black and fibrous, the peat at that site is disposed in a 150m - wide trough, grading into khaki/grey, orange - streaked plastic mud on either side. The Staines Alluvium never exceeds 4m in thickness, and averages 2m (Gibbard, 1985); as such it probably forms a 'seal' on the banks of the Thames wherever it occurs, since the river is typically less than 3m deep.

<u>3.4.2.2 -- Hydraulic Properties.</u> Where the Middle Thames Gravels overlie the Chalk, data on their own hydraulic properties are somewhat limited. This is because the Gravels are generally hydraulically connected to the Chalk and the Thames, rendering hydraulic analysis of pumping tests by usual analytical methods impossible. Where the Gravels overlie the London Clay they function as an aquifer in their own right, and hence there are more data on their hydraulic properties from this setting. For example Naylor (1974) studied the groundwater resources of the Middle Thames Gravels where they overlie the London Clay. The values for transmissivity (T) and specific yield (Sy) which he quotes are given in Table 3.3, along with those published by other authors. Despite the fact that the granular nature of the Middle Thames Gravels would readily lend itself to standard Darcy - based aquifer analysis, most of the available data for the Formation is based on the estimation of hydraulic conductivity from grain size analyses using empirical equations such as Hazen's Rule. This must account for some of the variations in reported values (Table 3.3). Other causes are the textural heterogeneity of the Formation (cf Table 3.2) and variations in thickness from 1 to 13 m. Data for the hydraulic conductivity of

TABLE 3.3 -- Aquifer Properties of the Middle Thames Gravels

AUTHOR	(T) (m^2/d)		K (m/d)		Sy
	Range	Mean	Range	Mean	
[8]Naylor (1974)	10 - 7000	850	14 - 2000	280	0.2
[9]Morgan - Jones et al (1984)	21 - 79200	-	21 - 7200	1200	0.08
[9]Ridings et al (1977)	- - - -	9000	- - - -	1500	0.08

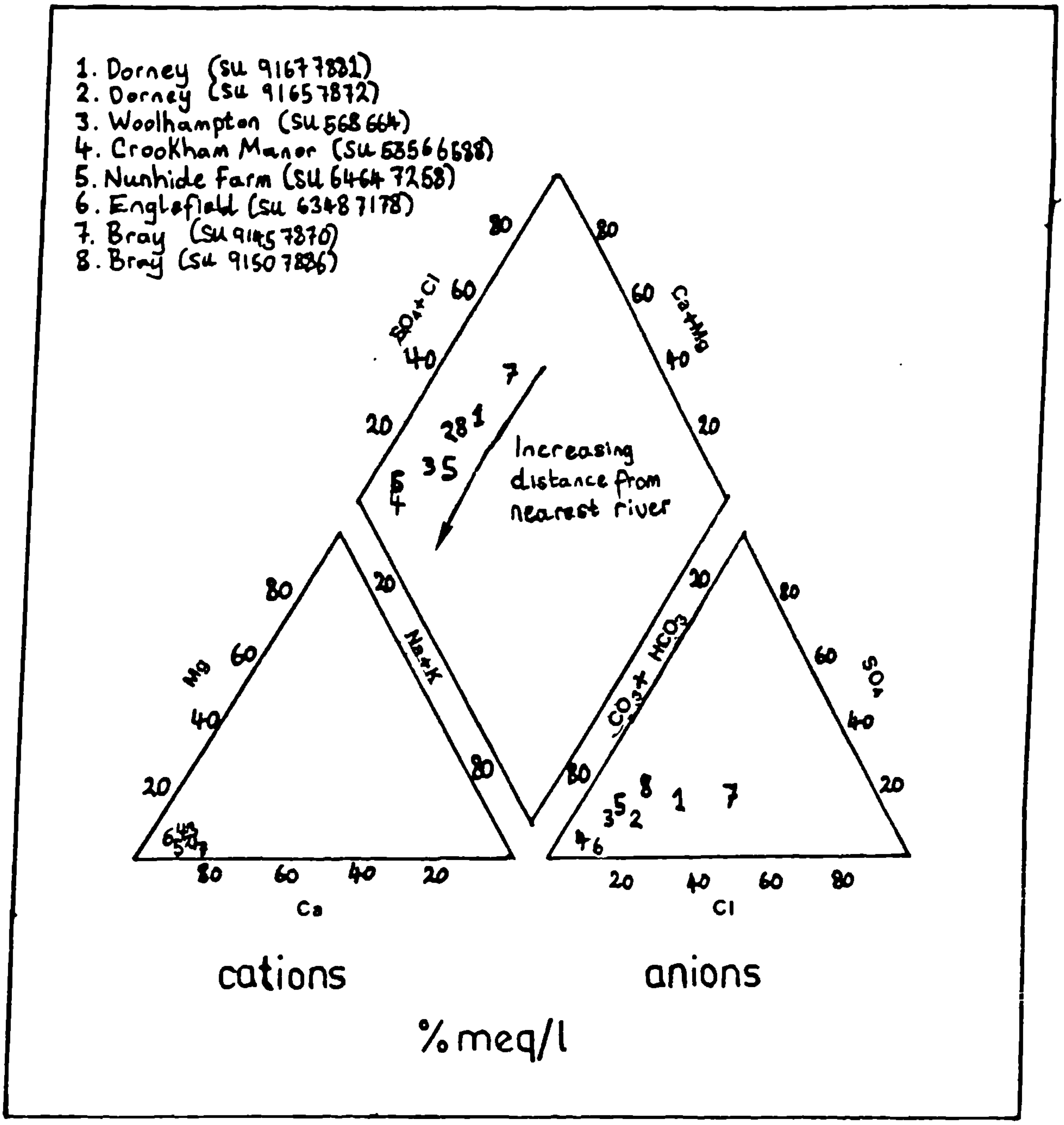
the Upper Thames Gravels are in broad agreement with the values quoted in Table 3.3; viz 1500 m/d for the Gm facies (Dixon, personal communication, 1989) and 100 to 1000 m/d for all the sand and gravel facies together (Dixon et al, 1989). There are no data on the hydraulic properties of the Staines Alluvium, but in view of its predominantly fine - grained nature, it seems fair to assume that it has very low permeability and storage capacity.

3.4.2.3 -- Geochemical Properties. Processes of adsorption (including ion exchange) and redox transformations are known to occur in the Shepperton Gravels and the Staines Alluvium from natural water chemistry. Eight chemical analyses of water samples taken from wells in the Middle Thames Gravels are plotted in terms of major ions on a Piper Diagram (Figure 3.7). It is clear that the waters in the Middle Thames Gravels are of Ca - HCO_3 type, and as such they are very similar in composition to unconfined Chalk water (cf Figure 3.4). Similarities are also seen in the range of total dissolved solids (TDS) values; the range of 299 - 806 mg/l closely follows that of Chalk waters. The obvious relationship with Chalk groundwater quality requires

[8] Values from yield - drawdown estimations and grain - size analyses.

[9] Values from induced infiltration aquifer tests.

Figure 3.7 -- Piper Plot of Shepperton Gravels Groundwaters.



no explanation where groundwater discharges from the Chalk into the Middle Thames Gravels en route for the Thames. Where no such direct link is possible (eg at sites overlying the London Clay), other explanations may be:
(i) the dissolution of Chalk which coats many of the flint clasts
(ii) recharge of Chalk - like river water (which originated as Chalk baseflow upstream). If this is the case, higher Cl values (due to anthropogenic influences on river quality) may be seen (eg samples 1, 2, 7 and 8 on Figure 3.7, which are from the induced infiltration sites at Dorney and Bray).

The ratio of [Na + K]/Mg is generally greater in Middle Thames Gravel waters than in Chalk waters, and Ridings et al (1977) note that the Mg/Ca ratio is lower in the Middle Thames Gravels than in the Chalk. These differences presumably reflect the fact that more ion exchange occurs in the Gravels than in the Chalk.

Morgan - Jones et al (1984) have discussed a redox mechanism for iron transport and deposition in the Middle Thames Gravels. Where recharge to the Gravels moves through clayey soil or peaty alluvium, dissolved O_2 is reduced and anoxic conditions, favourable to the mobilisation of iron, are established. When this reduced, iron - bearing, groundwater comes into contact with an oxygenated unsaturated zone, iron oxide is precipitated as horizons of hard, lowly permeable, fused ironstone concretions. Ironstone of this type was examined and collected by the author in the Shepperton Gravels near Egham (TQ 043683), where the ironstone forms a distinct horizon about 30cm thick at the level of the modern water table (ie the water level in a flooded gravel pit). Goethite is the main iron mineral present at this location, with minor amounts of haematite coating the flint clasts. The distinctive rusty colour of goethite has also been observed by the author at numerous seepage faces in gravel pits in the Upper Thames Valley (in particular, in Brown's Pit and Dix's Pit), suggesting that this redox mechanism is widespread in the Thames Gravels.

Pollution of the Middle Thames Gravels by landfill leachate has been described by Naylor (1974, pp. 26 - 29) and by Morgan - Jones et al (1984). At Thorpe, near Chertsey, the TDS of groundwater in the Gravels rose from 500 to 5000 mg/l as a result of leaching from a domestic waste landfill. Filtration of bacteria during flow through the Gravels was shown to be very effective, and dilution effects caused a 90% reduction in Cl concentration within three kilometres of the landfill. Morgan - Jones et al (1984) noted that the steepening of hydraulic gradient caused by the dewatering of gravel pits can exacerbate pollution problems by inducing flows of polluted water to previously clean stretches of the aquifer.

3.4.3 -- The Lea Gravels.

3.4.3.1 -- Geology. The floodplain gravels of the River Lea have not been studied as extensively as their counterparts in the Middle Thames Valley. In part this may be due to the greater difficulty in obtaining permission to visit working pits in this area, which the author encountered during this study. In fact, no operators granted permission within a reasonable time frame to allow field study of the gravels. From fleeting glimpses over boundary fences, however, the Lea Gravels appear to closely resemble the Middle Thames Gravels in lithology, facies and colour.

Whitaker (1889) noted that the Lea is the only tributary of the Thames to have an extensive spread of floodplain gravels. His descriptions of the alluvium and gravels are brief, but are reminiscent of the Fl and Gm sub-facies of the braided stream Facies Model (Miall, 1977; and cf Table 3.2). As in the Middle Thames Gravel Formation, flint clasts predominate.

Thames Water Authority (1978) have described the Lea Gravels at Rye Meads Sewage Works as poorly sorted, medium to coarse, flint - clast gravels, with cobbly horizons and variable quantities of sand (25 - 40%). These are overlain by 0.5 - 4m of peaty alluvium.

Gozzard (1981) described a borehole section through the Lea

Valley Floodplain Gravels at Cheshunt (TL 34820055). The Gravels here comprised 2.7m of sand (37%; quartzite clasts) and gravel (57%; flint clasts), with angular to sub - rounded clasts. These were overlain by 2.2m of "brickearth" alluvium (soft brown silty clay).

Hopson and Samuel (1982) described the Lea Valley Floodplain Gravels as 29% sand and 66% gravel, with the sand fraction comprising subangular to rounded flint and quartz and the gravel fraction predominantly flint. At Rye Meads the gravel was seen to be planar - bedded sand and gravel (cf. Gm, Gp / Sp ?, Table 3.2). The alluvium overlying these deposits was described as 4.8m of silty, fine sandy clay with local gravel stringers and accumulations of organic matter.

2 - 3m of silty clay and peat overlying 1m of yellow - brown sand (?Ss) and 6m of medium to coarse gravel have been described from several boreholes in the Lea Valley near Ware (Hall and Constantine, 1987).

<u>3.4.3.2 -- Aquifer Properties.</u> Very few data exist on the hydraulic properties of the Lea Floodplain Gravels.

The Thames Water Authority (1978) quote the following hydraulic conductivity values based on bail - recovery tests at Rye Meads: 8.1, 10.5, 25.2, 2.5, 12.2 (m/d). Mean Value = 14 m/d. These values are considerably lower than the accepted values for the Middle Thames Gravels, despite the geological similarity of the two suites of deposits noted above. It is therefore suspected that well construction methods may have affected these results.

Hydrotechnica (1988) have observed delayed vertical leakage from the Lea Gravels into the underlying Chalk when the piezometric surface of the latter is lowered by pumping. This may be due to the presence of undetected 'putty chalk', as described above from the Middle Thames Valley.

3.4.3.3 -- Hydrochemistry. Again, very few data are available. Only the studies by the Thames Water Authority (1978) and Hydrotechnica (1988) give details of any hydrochemical analyses of waters from the Lea Gravels, and since the former was concerned with grossly polluted groundwater, only the Hydrotechnica (1988) analyses reveal anything about indigenous Gravel groundwater chemistry.

The chemistry of Lea Gravel groundwaters is very variable. Where Chalk groundwater discharges into the Gravels, the Gravel waters are obviously akin to those of the Chalk (i.e. Ca - HCO_3 Type). Local occurrences of peaty alluvium (e.g. at Broadmeads, gravel piezometers BM 1 - 7; Hydrotechnica, 1988) lead to the establishment of reducing conditions, shown by the reduction of NO_3 to N_2 and the mobilisation of Mn and Fe. This accords well with the redox processes in the Middle and Upper Thames Gravels mentioned above (Section 3.4.2.3).

3.4.4 -- The Modern Streambed Sediments.

3.4.4.1 -- Introduction. The modern streambed sediments are the least studied of all the sedimentary deposits in the Thames Basin. This is due to a number of factors, not least their inaccessibility, and their limited significance to most geologists and engineers. Nonetheless, it is anticipated that they may be the most important of all units in controlling the movement of contaminants from rivers to aquifers. This is because they are fine-grained sediments, which are likely to contain far higher proportions of sorbent materials (eg clays, amorphous hydroxides and disseminated organic matter) than coarse sediments such as the Shepperton Gravels.

During normal groundwater flow through a mixed system of coarse and fine layers, advection will predominantly occur in the coarse layers, and thus little of the water will come into contact with the sorbents in the fine layers, other than through limited exchange by molecular diffusion (as postulated by Goltz and Roberts, 1988, among others). Where the water is obliged by the head distribution to flow through the fine sediment, as in stream - aquifer settings, all of the water in the system will come into contact with the sorbents. It is for this reason that most pollutant attenuation in stream - aquifer systems may be expected to occur within the streambed sediment (cf the review of relevant literature in Section 2.3 above).

By way of illustration, a news item from the ITN Television News programme on 12-3-1989 may be quoted. Aldrin (a chlorinated aromatic pesticide) has been used by farmers and market gardeners in the Newlyn Valley, Cornwall, for many years. Prior to 1989, no environmental problems were associated with the use of Aldrin in this area, although it is illegal to use aldrin in the USA on the grounds that it is a carcinogen. In late 1988, mass fatalities amongst eels and other fish were observed in the River Newlyn. These fatalities were found to be caused by dieldrin (another chlorinated aromatic pesticide) which had accumulated in the streambed sediments which are grazed by the fish. Investigations into the provenance of the dieldrin revealed that it was formed by degradation of aldrin in the subsurface, and had been adsorbed by the streambed sediment during baseflow discharge. Had the streambed sediment been absent, the dilution of contaminated baseflow by surface runoff would certainly have reduced the dieldrin to negligible concentrations (especially in view of the low solubilities of aldrin and dieldrin); the high sorption capacity of the streambed sediment ensured that the dieldrin became a sediment quality hazard instead.

Quite apart from these geochemical considerations, however, the effects of the rate of leakage of water from the stream to the aquifer must be considered. If the streambed is highly permeable, much more water can pass across it in a given time than if it is lowly permeable. Hence for a high - permeability streambed, the amount of stream water mixing with 'native' groundwater will be high, and the concentration of a stream pollutant in the well water will be high also. Where the streambed is lowly permeable, the proportion of stream - derived water to groundwater will be much lower, and mixing will result in a much lower concentration of any stream pollutant in the well water. This effect is well illustrated by a pollution incident at Bray, described by Flavin (1986). In this case, the quality of water in wells close to the badly polluted Cut deteriorated dramatically when the bed sediment of the Cut was dredged away for navigational purposes. In the words of Flavin (1986), "It therefore appears that the dredging operation increased the rate of flow of river water through the bed of the Cut thus increasing the proportion of Cut water reaching [the] boreholes".

While these properties of the streambed sediment illustrate its importance to this study, there is a general dearth of information in the literature on the hydrogeology and geochemistry of modern streambed sediments. Environmental scientists occasionally study such deposits as part of wider investigations of water quality and/or ecology (eg Golterman et al, 1983; Day and Zumpe, 1986), but none of the papers in this genre studied by the author give details of any relevance to the present investigations. Surprisingly, even the detailed study of stream - aquifer interactions by Gay and Frimpter (1985), which was reviewed in Section 2.3, does not contain such details. On the few occasions that hydrogeological investigators have referred to the streambed sediment in the Thames Basin, they have not studied it directly but have invoked its inferred presence to help explain poorly understood water balances during induced infiltration (eg Edmunds Owen and Tate, 1976, pp. 7 - 10; Ridings et al, 1977, pp. 11 - 12; Robinson et al, 1987). The most recent study of the Thames streambed sediment was by the freshwater biology unit at Thames Water, who described sediment from the vicinity of Maidenhead as being 'laminated compacted silt' (Robinson, personal communication, 1989), but gave no further details of relevance to the present study.

Given the general lack of knowledge about the nature and properties of the streambed sediment, and the postulated impact of these on solute transport in stream-aquifer systems, a modest programme of sampling and characterisation was undertaken as part of the present study. The methods and results of this study are given in Appendix C, while the geological, hydraulic and geochemical implications of these results are discussed in the following sections.

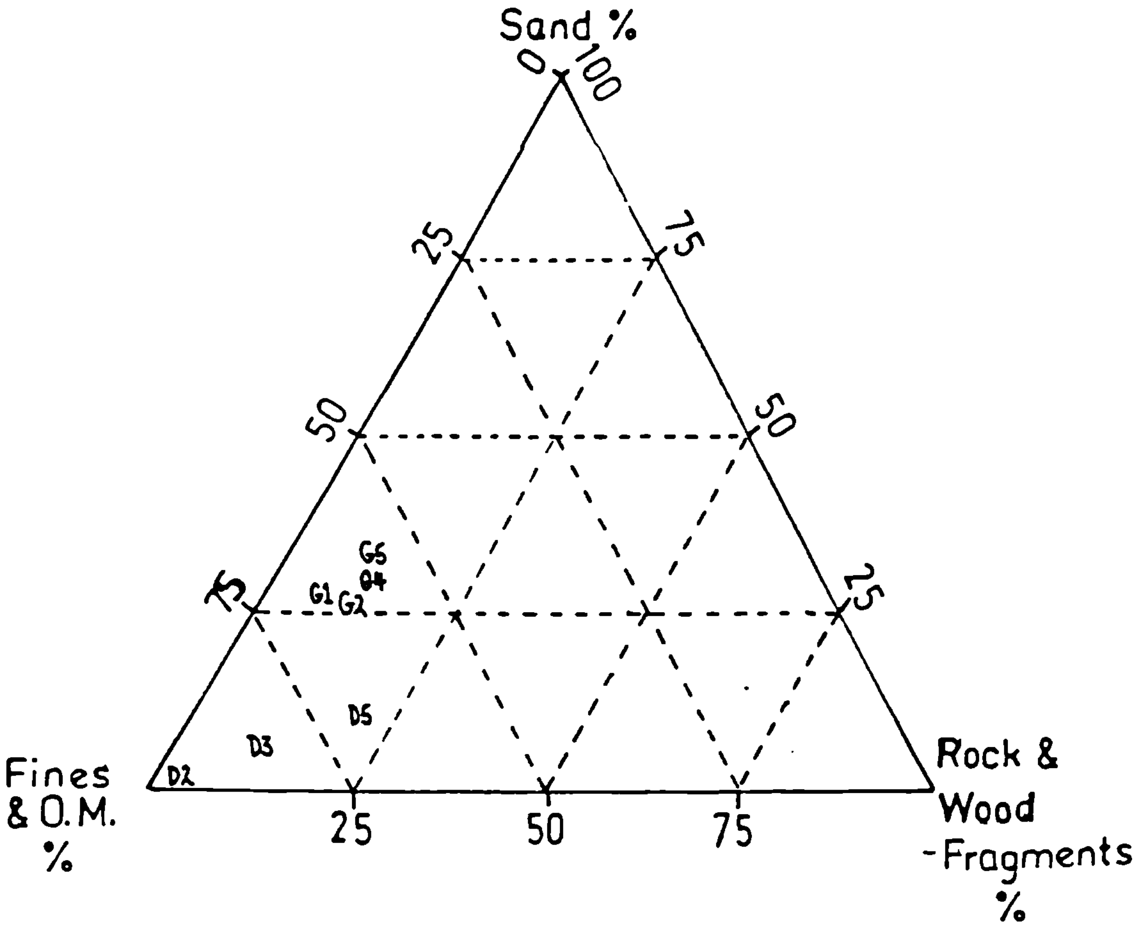
3.4.4.2 -- Geological Features.

Thickness The streambed sediment probably attains a thickness of about 0.5m to 1.0m at most sites in the Middle Thames Valley, judging from the spatially variable sedimentation rate (0.0 m/yr to 1.5 m/yr) and the variable frequency of dredging operations (once a decade to once a year) reported by Mr Chris Sellwood (Thames Water Authority, Rivers Division, personal communication, 1989).

Sedimentology As shown in ternary diagram (Figure 3.8) the streambed sediments of the Middle Thames are predominantly fine grained. Within the fine fraction, most of the sediment falls into the silt category, although the downstream samples have a higher mud content. Calcareous mud ('marl') comprises about half of the silt fraction at Gatehampton, but this proportion decreases downstream. The clay mineralogy of the sediments (a palygorskite - montmorillonite assemblage) is consistent with the obvious postulate that they are derived from the Thames Gravels and the Chalk, since montmorillonite dominates the clay mineralogy of both formations, and palygorskite has been identified in eight samples of Upper Chalk from Fair Cross, Berkshire (Chartres, 1981; Morgan - Jones, 1977).

In terms of the coarser fraction, the sediments show classic provenance control. The Gatehampton samples contain glauconite, limestone fragments, marl and iron oxide minerals, all of which are typical weathering products of the Jurassic and Lower Cretaceous (Greensand) sequences exposed upstream. The burnt coal fragments, which appear to be coke - like cinders, are found only in the Gatehampton samples, and probably come from the stacks of Didcot power station to the north-west. The high proportion of marl in the Gatehampton sediments is probably due

Figure 3.8 -- The Composition of the Thames Streambed Sediment.



to continuing erosion of Chalk in the Goring Gap, although abrasion of modern shell fragments and accumulation of microfaunal tests may also yield some fine grained carbonate. When the sediments near Dorney are examined, a downstream decrease in all these components is revealed, together with a skewing of the grain - size distribution even further towards the fine fraction. This accords well with the basic sedimentological principle that the finest sediments are transported the furthest, although the high clay content of the Dorney samples may reflect a provenance control (weathering of the Lower London Tertiaries) as well as a depositional control.

The change in the dominant iron species from oxides to pyrite as the sediments are traced downstream indicates that in the finer-grained, more organic rich Dorney/Bray sediments, reducing conditions have been established which allow precipitation of fresh pyrite (or preservation of detrital pyrite), whereas at Gatehampton the redox conditions in the streambed allow detrital and diagenetic oxides to remain intact.

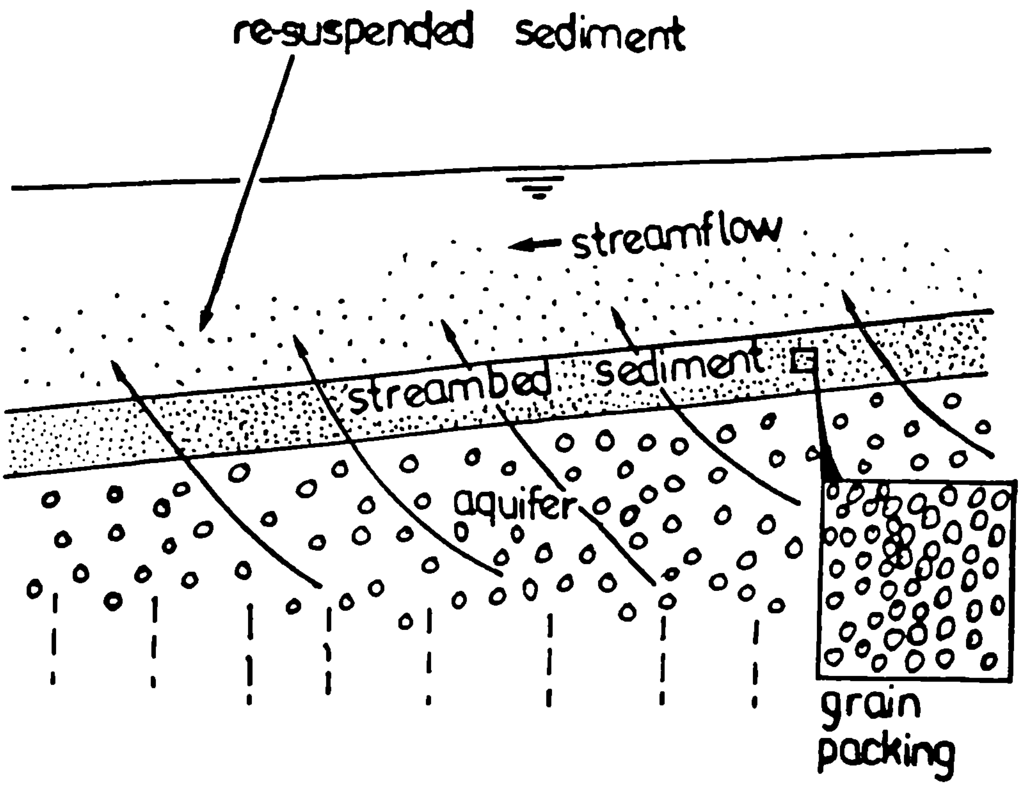
Two samples (G3 and G6) have large clasts of flint supported by a matrix of silt. Given the rarity of the deposits with large clasts, and the fact that their matrices are identical to the main body of surrounding sediment, some explanation for their genesis is warranted. Since the sampling point for G3 was closer to the bank than those for the other samples, it is likely that the large clasts are locally introduced into the streambed environment by collapse of the stream bank, which is cut into flint - rich Shepperton Gravels. This would explain the local occurrence of such coarse clasts in a quiescent sedimentary regime which is depositing silt.

The lamination observed in the sediment from Maidenhead (Robinson, personal communication, 1989) probably reflects steady accumulation of silt by settling from suspension under low flow conditions.

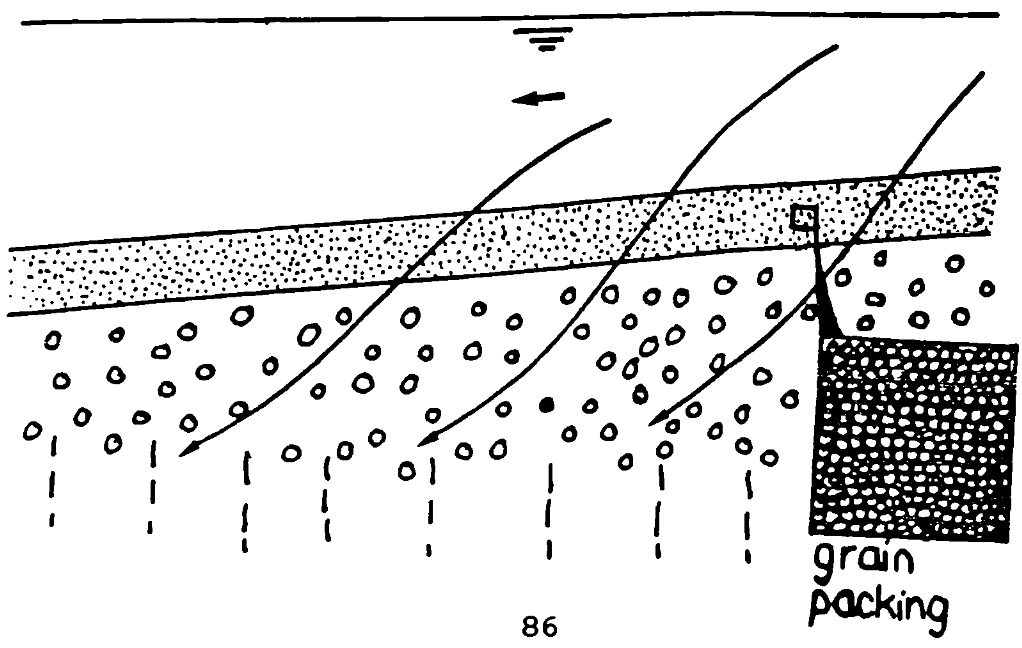
One further sedimentological feature of the streambed sediment

Figure 3.9 -- Stream - Aquifer Flows and Sediment Erosion.

(a) Baseflow Causing Uplift



(b) Compaction During Induced Infiltration.



which has not as yet been identified in field studies may nonetheless be of some importance. This concerns the effects of groundwater flow on the compaction of the sediment (Figure 3.9). When a stream is gaining, the net force exerted on the sediment by groundwater will be upwards, such that the grains are pushed apart in a manner analogous to the quicksand effect. This will clearly lead to looser packing, higher permeability, and an increase in the erodibility of the sediment (Figure 3.9a). During induced infiltration, or *when the stream is naturally* losing, the net force of the groundwater flow will be downwards, in the same direction as the hydrostatic and gravitational forces which lead to compaction. The net effect is to favour closer packing of grains and thus lower permeabilities (Figure 3.9b). In this manner, the stream - aquifer system has a built - in defence mechanism against induced infiltration, while natural baseflow has a tendency to make itself more efficient. While the mechanisms outlined above are based only on theory (rather than direct observation), there is a small amount of evidence in the literature to support the proposal of this theory. This is presented by Harrison and Clayton (1970), who describe differences in erodibility by a factor of 500 between adjacent gaining and losing reaches of a river in Alaska (which were identical in terms of velocity regime, bank sediment and channel slope). In the gaining reach, pebbles of a few inches diameter were transported at the same velocities that would only entrain silt in the losing reaches. Laboratory flume experiments reproduced the enhanced deposition and compaction of silt and mud under 'losing' conditions.

<u>3.4.4.3 -- Hydraulic Properties.</u> Data on the hydraulic properties of the modern streambed sediments are restricted to measurements and estimates of hydraulic conductivity. No information on storage parameters is available; however, as release of water from storage in the streambed sediments can never be by de-watering under normal field conditions, and since specific retention is in any case high in fine grained sediments, the storage coefficient for the sediments is likely to be very low (say around 5×10^{-5}; cf. Todd, 1980, p.45).

Apart from the measurements made during this study (Appendix C), information on the hydraulic conductivity of the streambed sediments is restricted to estimates from analytical modelling of an aquifer test at Dorney (Ridings et al, 1977). Values in the range of 0.1 to 1.0 m/d are quoted by these authors. Given the fine grained, locally laminated, nature of the sediments, these values are perfectly reasonable.

The data obtained for reconstituted samples using a falling head permeameter (Appendix C) yielded much lower values of about 0.002 m/d, although this is still well within the range of values normally associated with unconsolidated silt (cf Freeze and Cherry, 1979, p. 29). One of the samples with large clasts was tested in the permeameter. Since the resulting hydraulic conductivity is similar to those from samples without large clasts, it would appear that the matrix - support fabric of the sediment results in the matrix hydraulic conductivity dominating the overall hydraulic conductivity of the sample. Hence the appearance of large clasts in the sediment does not herald an increase in hydraulic conductivity.

The discrepancy between the 'field' values of Ridings et al (1977) and the new lab values illustrates the passionate debate about the usefulness of laboratory measurements in site investigations (see Rushton, 1989). The discrepancy in this case almost certainly arises from sampling size differences. The field values are 'averages' for a reach of the Thames extending several hundred metres, while the lab values only relate to the permeability of dense sediment. In the field, macropores such as root holes, faunal burrows and syneresis cracks are all likely to provide 'fast channels' through which water may preferentially flow. Hence it is no surprise that the average field values are higher than the lab values.

Because of the different effects of upward and downward moving seepage forces on the compaction of sediments (as discussed in Section 3.4.4.2 above), it is likely that hydraulic conductivity and storativity will be lower when the river is losing than they are when it is gaining.

<u>3.4.4.4 -- Geochemical Properties.</u> The most important geochemical property of the streambed sediment is its sorptive capacity, which is a function of the mineralogy and organic matter content of the sediment.

The results in Appendix C indicate that the clay fraction of the streambed sediment includes palygorskite and montmorillonite. Clay assemblages which include montmorillonite are characterised by the highest cation - exchange capacities of any clay mineral suites (ie 80 to 150 meq/100g dry weight; *Fenwick and Knapp*, 1982, p. 43). Thus even in the absence of organic matter, the streambed sediment could be expected to be highly sorptive.

The effect of organic matter on sorption is so strong that where the organic content of a sediment exceeds 1% by weight, the contribution of mineral surfaces to the total sorption in the sediment is negligible (McCarty et al, 1981; Karickhoff, 1984, p. 711). Thus the high organic content of the streambed sediment (1.6% to 57.4%) indicates an extremely high sorptive capacity.

While adsorption is likely to be the primary attenuation process operating in the streambed sediments, it is important to realise that this process has many side - effects on overall pollutant attenuation. To quote Karickhoff (1984):

> " . . . In addition to an obvious effect on physical transport, sorption can be involved directly or indirectly in pollutant degradation. The chemical reactivity of a pollutant in a sorbed state may differ significantly from that in aqueous solution, both in extent and chemical pathway. Moreover, natural sorbents may indirectly mediate solution phase processes by altering the solution phase concentration or by controlling pollutant release into the aqueous phase and thereby potentially rate-limiting solution phase reaction. In addition, natural sorbents

> "introduce" into solution a "buffered" suite of inorganic and organic species that can significantly affect pollutant reactivity in the aqueous phase . . ."

Furthermore, the high organic content of the sediment is both symptom and cause of a high rate of biological activity. Thus biodegradation of one sort or another is likely to be very important in these deposits.

One complex phenomenon associated with high organic contents is non-equilibrium sorption. Two types of nonequilibrium are distinguished; chemical nonequilibrium (where the rate of adsorption is limited by the rate coefficient for the reaction at the solid - liquid interface) and physical nonequilibrium (where the rate of adsorption is limited by the slow rate of diffusion through immobile solvent prior to relatively rapid adsorption at the solid - liquid interface). Where a sediment has a high organic content, physical nonequilibrium can result from the slow diffusion of solutes within the organic carbon matrix (Bouchard et al, 1988). Hence the streambed sediment may not only be highly sorptive, but may be apt to promote sorption nonequilibrium. This factor may be borne in mind when interpreting any field data which is obtained in the future.

Notice should be taken of the geological evidence discussed above which suggests that reducing conditions exist in the Dorney sediments, while an oxidising environment characterises the Gatehampton sediments. Reducing conditions are a mixed blessing from the point of view of groundwater contamination. On the one hand, they favour the mobility of iron, manganese and various heavy metal pollutants. On the other hand, recent field and laboratory studies by Wyer and Kay (1989) demonstrated the removal of nitrates from stream water during percolation through reduced streambed sediments in the Afon Teifi, Wales. Under the anaerobic conditions, which are themselves a function of high biological activity in the Afon Teifi, the nitrates were used as a source of oxygen by the microbes which reduced them biochemically.

3.5 -- HYDROGEOLOGICAL CONFIGURATIONS OF STREAM - AQUIFER SYSTEMS IN THE THAMES BASIN.

3.5.1 -- General Description.

In this section, a general description of the field configurations of stream - aquifer systems in the valleys of the Lea (between Ware and Turnford) and the Thames (between the Goring Gap and Chertsey) will be given. Two specific sites are described in Section 3.5.2, to exemplify the present general discussion. This discussion is based on information from the literature, on unpublished records of the Thames Water Authority, on field work by the author and on recent site investigations (by the Thames Water Authority and Hydrotechnica Ltd), in which the author participated on several occasions.

In terms of the main classificational language of hydrology (introduced in Chapters One and Two), the River Lea and the River Thames are partially penetrating streams, which are gaining in the study area under usual natural conditions[1], although hydraulic connection with the saturated zone is generally impeded to some extent by the presence of a layer of lowly permeable silty streambed sediment.

The Lea Stream - Aquifer Systems. As shown in Figure 3.1, the River Lea flows over Devensian floodplain gravels throughout its course in the study area. North of Hoddesdon, these gravels are underlain by Chalk, while the Lower London Tertiaries underlie the gravels south of Hoddesdon. Eight wells, originally constructed in the 19th Century, pump water from the Chalk at distances of 175m to 550m from the River Lea. The two most southerly of these wells (Broxbourne and Turnford) are screened in confined Chalk below the Tertiary deposits. Recent pumping tests at these two sites (Hydrotechnica, 1988) have confirmed that

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1. Save that the Thames is known to have been losing in the study area during the 1975 - 76 drought; Price, 1985, p. 103 - 4)

the Tertiaries are efficient confining horizons. Large drawdowns of the confined piezometric surface of the Chalk have no effect on piezometric levels in the gravels above the London Clay, but the Thanet Sands (which lie between the London Clay and the Chalk) do react to Chalk pumping in a subdued manner, and act as the source for some leakage to the Chalk. Clearly, the Lea valley wells tapping Chalk confined beneath Tertiary cover do not qualify as induced infiltration sites.

It might be anticipated that the sites further north, where the gravels are underlain by essentially unconfined Chalk, would show more sign of interaction with the river. Prior to a detailed analysis of this possibility by Hydrotechnica (1988), a preliminary investigation was made by the author. The purpose of this study was to calculate the maximum river contribution to the wells, using the least conservative assumptions possible. Water samples were collected from pumping wells at Amwell End, Amwell Marsh, and Rye Common, and from two sites on the River Lea, during an eight - hour period on a rain - free sunny day (19/5/87). These samples were sent for trace element analysis on the NERC Inductively Coupled Plasma Mass Spectrometer (ICPMS) at Egham, Surrey. The chemical results are given in Appendix D. In common with the results obtained by Ridings et al (1977) and Edmunds, Owen and Tate (1976) for Middle Thames sites, Na, K and P were found at slightly higher concentrations in the river than in the groundwater, and Sr showed the opposite relation. However, the differences between river and aquifer concentrations are very slight. To determine the proportion of river derived water in a riverside well pumping at a steady rate the following equations are commonly applied (Pettyjohn, 1985a):

$$Qw = Qa + Qr \quad \ldots\ldots \quad (3.1)$$

$$CwQw = CaQa + CrQr \quad \ldots\ldots\ldots \quad (3.2)$$

where Q = discharge

C = concentration of water

and the subscripts w, a and r refer to well, aquifer and river water respectively.

These equations were applied to the data showing the greatest distinctions in sodium concentration between

(i) the River Lea

(ii) regional chalk groundwater (using new data which have since been presented by Hydrotechnica, 1988), and

(iii) water produced from Amwell End pumping station (which is known to be too far north to be affected by swallow hole water from North Mimms; Harold, 1937).

The results obtained indicated that, assuming there is no sodium exchange in the streambed sediments or the gravels (which is probably not the case; see Sections 3.4.2.3 and 3.4.4.4), the maximum possible river contribution to Amwell End equals 23% of the total well discharge. Under conservative assumptions, such as assuming Na - Ca ion exchange in the streambed sediments and the gravels, the maximum river contribution would be far less than this. Even 23% is a very low contribution when compared with the range of 40% to 100% for wells by the Thames near Maidenhead (Edmunds, Owen and Tate 1976; Ridings et al, 1977). Upon completion of the main study, moreover, Hydrotechnica (1988) concluded that the mass of hydrochemical evidence rules out a significant component of river water in any of the well discharges.

Three geological features can be invoked in an attempt to explain these unexpected results:

(i) Water from the North Mimms swallow hole complex is known to account for up to 40% of the discharge of all wells south of Amwell End (Hydrotechnica, 1988), to which it moves at velocities up to 5.5 km/d (Harold, 1937). Thus the karstified parts of the Chalk represent a large resource of readily available water.

(ii) Water level measurements for many of the sites indicate partial breach of hydraulic connection between the gravels and the Chalk. The reasons for this are not clear, but the existence of a confining layer of putty chalk, as observed in the Middle Thames Valley, may be postulated. If such a layer exists, it will tend to make the river water (which must flow through the gravels before it reaches the Chalk) less accessible to the wells.

(iii) The Lea is known to have silty streambed sediment (Day and Zumpe, 1986), and it is in all probability lowly permeable, like its lateral equivalent in the Middle Thames Valley (see section 3.4.4 above). Therefore, the energy required to attract water from the river to the wells will be much higher than that needed to attract water from the caverns and fissures of the North Mimms complex.

Since induced infiltration is now thought to be negligible in the Lea Valley, the risk of well contamination from a river pollution event must also be negligible. For this reason, efforts during the later parts of the study were concentrated on more 'promising' sites in the Middle Thames Valley.

<u>The Middle Thames Stream - Aquifer Systems.</u> The basic geology of the Middle Thames Valley resembles that of the Lea Valley, inasmuch as the Thames flows over Devensian gravels throughout the valley, with Chalk beneath the gravels in the upper reaches of the valley, and the Lower London Tertiaries beneath them downstream of Taplow. Hydrogeologically, however, the Middle Thames is rather different, since a number of studies have demonstrated a significant river - derived component in some well discharges (Ridings et al, 1977; Edmunds, Owen and Tate; 1976). Furthermore, unlike the Lea sites studied, many wells downstream of the Cretaceous / Tertiary boundary are screened in the unconfined gravels, rather than in confined Chalk. Thus independent information is available on the stream - aquifer behaviour of the gravels, which is

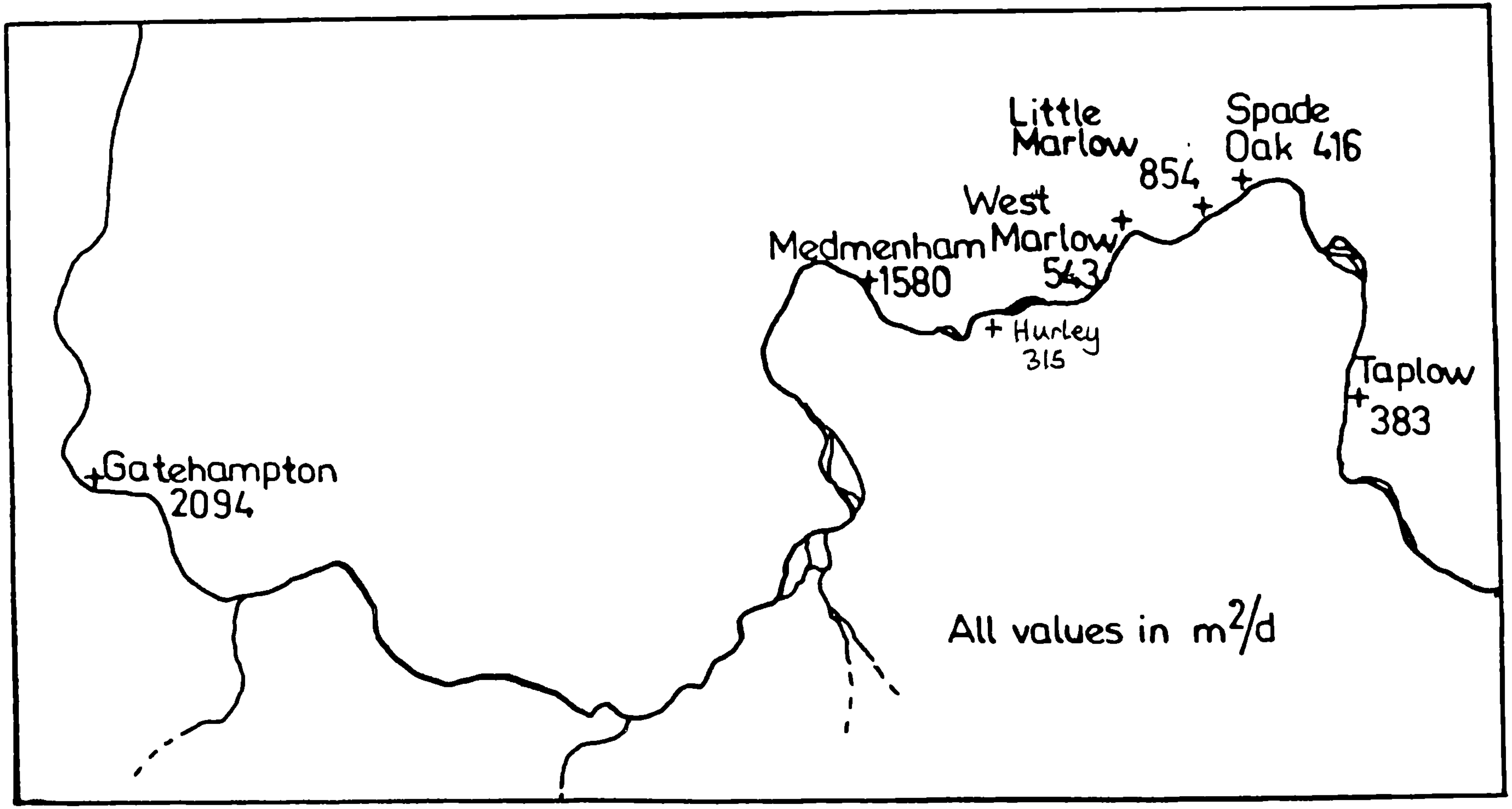


Figure 3.10 -- Mean Specific Capacities for Wellfields in the Middle Thames Valley.

often confounded with information on the behaviour of the Chalk where the latter underlies the gravels.

At all sites studied, the streambed sediments appear to play an important role in restricting exchange between the Thames and the gravels, except at localities where scouring keeps the bed free of silt, as in the tail pools of weirs.

Figure 3.10 shows the mean specific capacities for riverside wells in the Middle Thames Valley, which were calculated from previously unpublished yield - drawdown data from the Thames Water Authority. It emerges that while all yields are generally good by normal British standards, they are exceptionally good at some sites (eg Medmenham and Gatehampton) but surprisingly poor at others (eg Hurley and West Marlow). During the course of this study, it has been increasingly recognised that the hydraulic connection between the gravels and the Chalk is locally breached at these low yield sites by a layer of 'putty chalk' at the gravel - chalk interface. An understanding of the distribution of such zones of confined and lowly permeable Chalk in stream - aquifer systems has obvious importance for resource management as well as for scientific curiosity. Therefore a detailed geological model was developed to describe the origin and distribution of this putty chalk (Chapter 4).

Earlier studies of stream - aquifer interactions in the Middle Thames Valley include the classic Taplow investigation (Edmunds, Owen and Tate, 1976) in which geophysical logging of temperature distributions, analytical modelling of pumping test data, and hydrochemical methods were all used in an attempt to determine the component of river - derived water in a number of boreholes. Measurements of groundwater temperature at various times during pumping provided striking qualitative evidence of induced infiltration. Quantification of the river component in well waters was accomplished by a 2 - year monitoring programme for selected natural tracers. Eventually, a graph was obtained which related the proportion of river water entering the boreholes to the concentrations of K^+, Sr and HPO_4 in the pumped water. At steady state production rates, up to 70% of the well abstractions were found to be river - derived.

Since the two detailed site descriptions in Section 3.5.2 concern Middle Thames Sites, no more examples will be given here. In summary, however, it may be stated that a significant (though variable) component of river - derived water has been detected in many riverside well sites in the Middle Thames Valley, and it therefore appears that, unlike the Lea Valley wells, those Middle Thames sources unprotected by putty chalk are at some risk of contamination if a major pollution spill were to enter the Thames. The modelling efforts described in Chapters 5 through 8 represent the first steps towards assessing this risk.

3.5.2 -- Detailed Examples.

3.5.2.1 -- Gatehampton. Gatehampton lies at a bend in the Thames immediately south of Goring, in the heart of the prominent breach in the Chalk escarpment known as the Goring Gap (Figure 3.11). The geology of the site is quite straightforward (Figure 3.12); up to 13m of Shepperton Gravels and Staines Alluvium overlying eroded, strongly fissured, highly permeable, gently dipping ($<5^o$ to the southeast) Middle and Lower Chalk. The Chalk and Gravels are known to be in hydraulic continuity (Robinson, 1984), and no putty chalk has been found in any of the boreholes on this site. Fluid flowmeter logging in pumping boreholes revealed a non-linear decrease in hydraulic conductivity with depth, and below depths of about 50 - 60m the Lower Chalk is effectively 'tight' and serves as a base to the Chalk aquifer. As the land rises in the valley walls (ie the slopes of the Chilterns and the Berkshire Downs which bound the Goring Gap to the north and south

Figure 3.11 -- Location of the Gatehampton Wellfield.

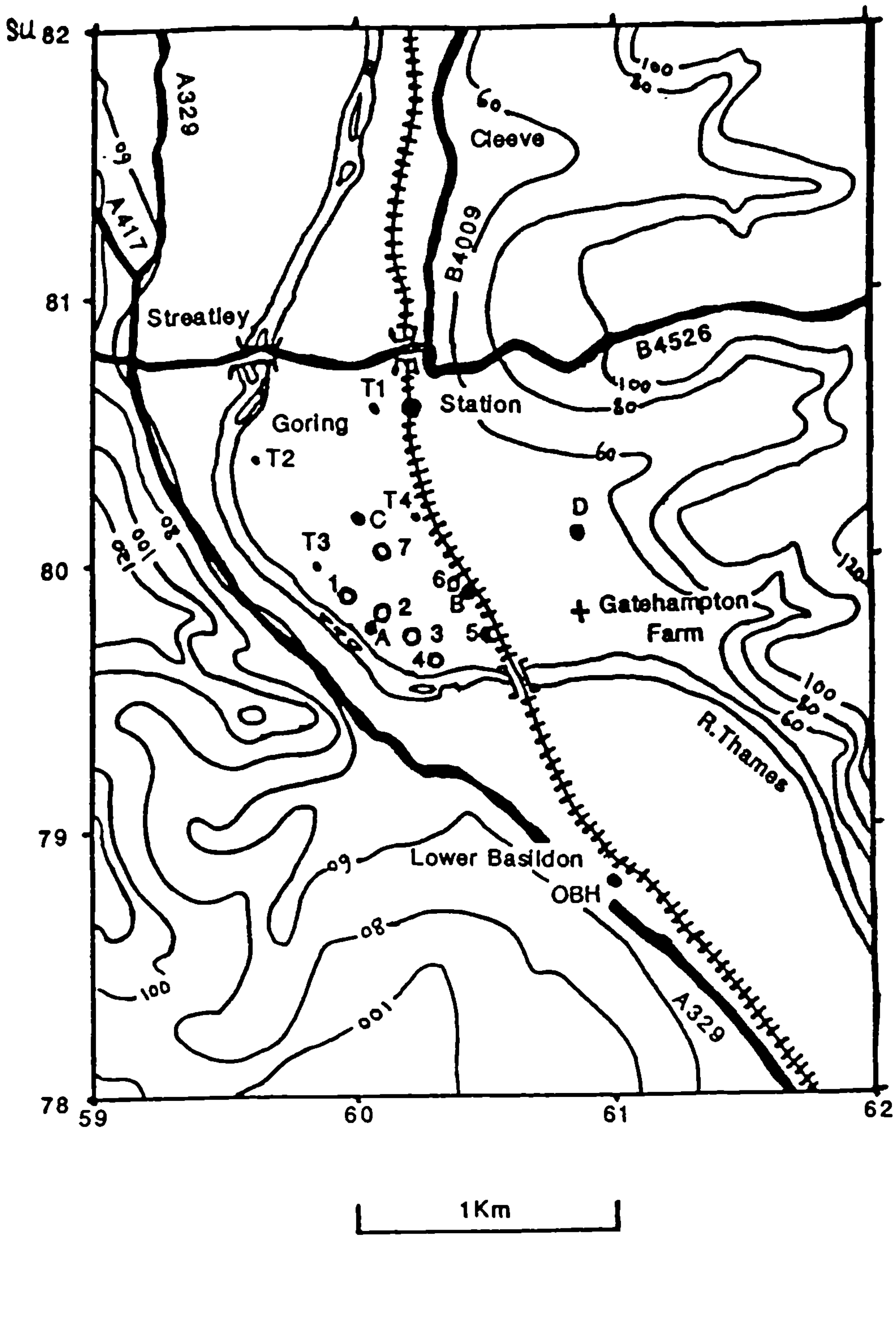
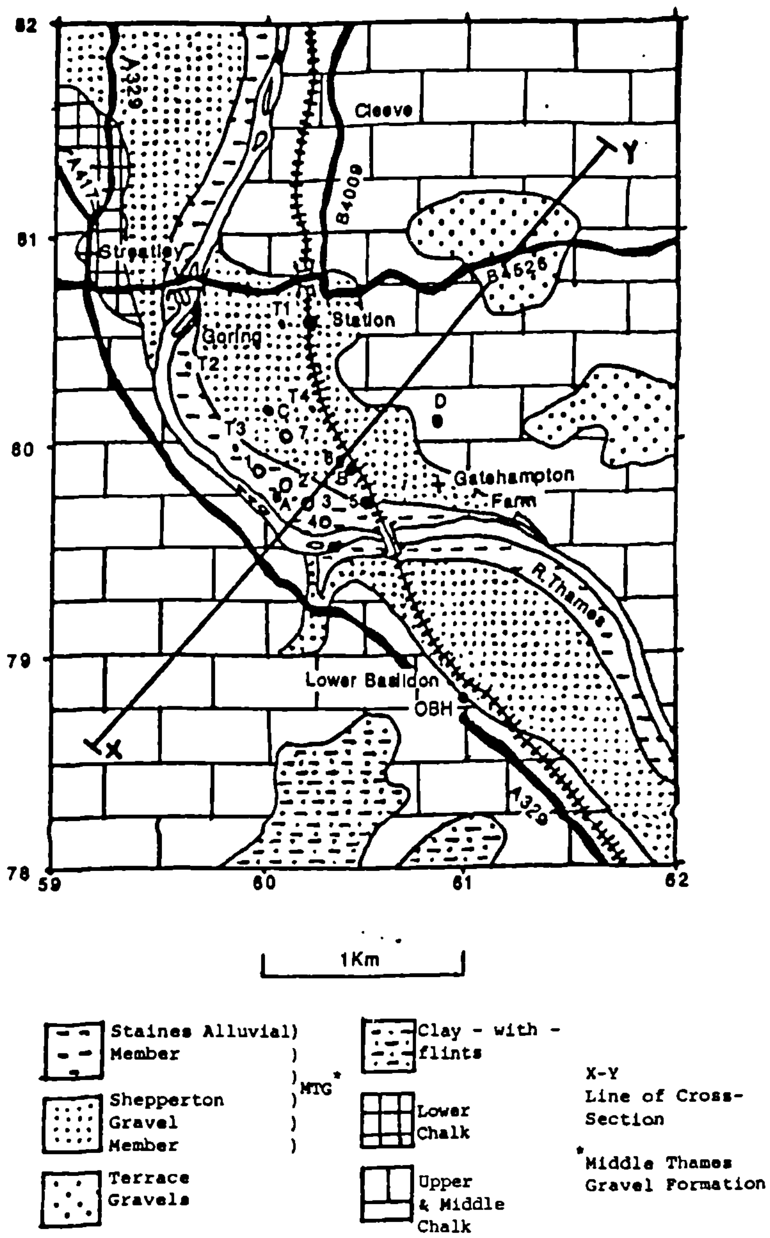
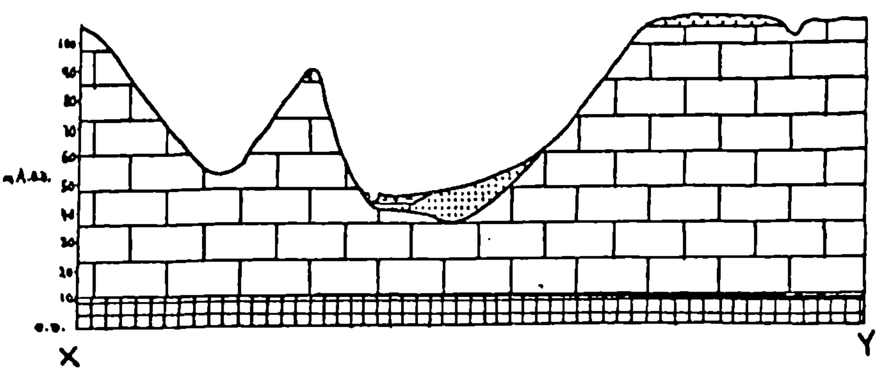


Figure 3.12 -- Geology of the Gatehampton Area.





Vertical Exaggeration 13.25

respectively), beyond the outcrop of the Shepperton Gravels, Chalk permeability decreases quite markedly.

Anticipated population growth in the Didcot area prompted the Thames Water Authority to explore for new resources in the Goring - Wallingford area. In 1984, the eleven existing groundwater sources in the area supplied about 67 TCMD (thousand cubic metres per day), though this fell to 37 TCMD during the 1976 drought. Demand in 1984 was about 46 TCMD (average) and 62 TCMD (peak). Projected demands for the area by the year 2011 are 56 TCMD (average) and 80 TCMD (peak). The investigation of the Gatehampton site revealed the existence of a resource far in excess of aspirations, with a sustainable average daily abstraction rate of 70 TCMD and a peak abstraction rate of 100 TCMD. These latter two figures were entered on the licence for the Gatehampton site, and work is currently underway on a pipeline link to Didcot.

A long and detailed programme of test pumping was undertaken during the development of the site. These tests were carried out in two phases; firstly, three abstraction boreholes (750mm diameter), two observation wells (200mm diameter) and ten tubewells were emplaced and tested during 1984 (Robinson, 1984); secondly, a further four abstraction boreholes (730mm to 750mm diameter), two 200mm observation boreholes and seventeen tubewells were added in 1986 and tested in various combinations between September 1986 and February 1987 (Robinson et al, 1987). The pumping revealed excellent yield - drawdown characteristics for the abstraction boreholes, with ABH 4, for example, showing only 3.45m of steady drawdown when pumped at 15,100 m^3/d for a week. While the complex nature of the river boundary and the structured variation in hydraulic conductivity with depth introduce great uncertainties into the determination of aquifer parameters using standard analytical models, Robinson (1984) used Theis, Jacob and Hantush methods (all described in Freeze and Cherry, 1979) to estimate transmissivities and specific yields at Gatehampton. Assuming a saturated thickness of 60m, the values obtained imply hydraulic conductivities in the range 150 - 400m/d, and specific yields in the range 0.0003 - 0.01. These values are consistent with the general observation that the Chalk is 'a high permeability - low storage aquifer' (Foster and Milton, 1974).

During the 1986 - 87 test the cone of depression produced by the pumping eventually extended beneath the river to cause small drawdowns on the opposite bank (Robinson et al, 1987). Hydraulic connection between the river and the saturated zone does not appear to have been breached, however. This drawdown behaviour suggests that the bed of the Thames is of lower hydraulic conductivity than the Middle Thames Gravels, and that it thus impedes induced infiltration to some extent.

The influence of low - permeability Chalk in the valley wall appears to account for increased drawdown rates in the abstraction boreholes which appeared on November 14th/15th 1986 (ie two months after the start of group pumping). These increased drawdown rates were attributed by Robinson et al (1987, p.11) to 'barrier boundary effects' on the part of the valley wall Chalk.

Another feature of the Gatehampton site is worthy of record. This concerns loading effects of British Rail passenger trains which frequently pass on the embankment which bounds the site to the east. For example, during a site visit on 3-12-1986, the author observed a rise of about 1cm in the water level in observation hole B (which was fitted with a continuous chart recorder) each time a train passed by. As the trains receded into the distance, the water level would subside again. These effects provide a vivid illustration of the compressibility of the gravels and the Chalk.

When the 1986 - 87 pumping tests were first planned, it was proposed that intensive chemical monitoring of the wells and the river water be carried out. In the event, the team in charge of river water monitoring failed to sample the river during the test, thus severely hampering hydrochemical interpretations with respect to induced infiltration. Tentative assessments (based upon routinely collected river samples from upstream and downstream of the site) failed to yield any conclusive evidence of river water ingress, although Cl concentrations and values of the K/Na ratio do suggest that river water entered abstraction boreholes 1 and 4 (Robinson et al, 1987). However, Morgan-Jones (in Robinson et al, 1987) summarises the situation by saying that induced infiltration 'cannot be quantified (on the basis of existing chemical data) and if existing can only be verified by evaluation in the long term under an established pumping regime'.

At the time of writing, construction work on a pipeline to carry water from Gatehampton to Didcot is still under way, and no further pumping or chemical sampling of the Gatehampton wells has been undertaken.

3.5.2.2 -- Dorney. The riverside well site at Dorney (Figure 3.13) lies about 4 km southeast of Maidenhead, on a wide expanse of Middle Thames Gravels which form an impressive flood plain between the Chalk hills at Taplow and the dominating landmark of Windsor Castle, which sits on an anticlinal inlier of Chalk some 6km downstream from the wells. The geology of the site (Figure 3.14) is even simpler than at Gatehampton, with the modern ground surface being developed solely on Shepperton Gravels, which are about 6 or 7m thick in this vicinity. Beneath the gravels lie the London Clay and the Reading Beds, with their gently dipping contact subcropping beneath the gravels as shown in Figure 3.14. Hydrogeological studies in this area have demonstrated that these Tertiary beds behave as efficient aquitards, thus forming an effective

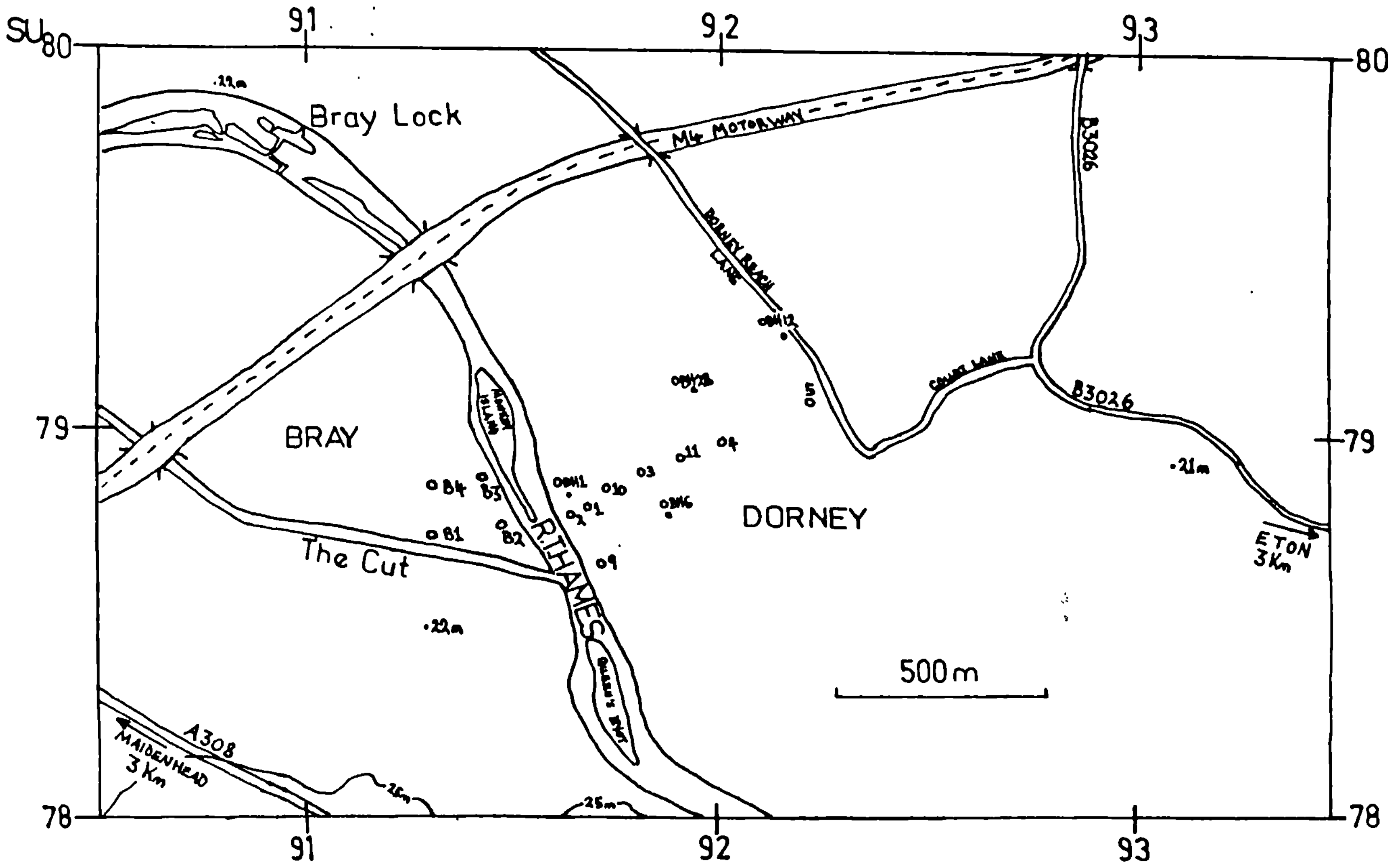


Figure 3.13 -- Location of the Dorney Wellfield.

base to the gravel aquifer. With the nearest gravel feather - edge lying about 2 km to the south-west (beyond the limits of the site), the Dorney wells are situated in the midst of one of the most laterally extensive alluvial aquifers in England. At present the aggregated licensed abstraction rate for the eight Dorney abstraction wells is 27.276 TCMD.

The Dorney wells were emplaced in three phases (Ridings et al, 1977):

(1) July 1970 to September 1971. Two abstraction boreholes (ABHs) and thirteen observation boreholes (OBHs) were constructed and test pumped.

(2) June through July 1973. Five boreholes and a number of tube wells were constructed and test pumped. During the test, one of the pumping boreholes collapsed. The four remaining boreholes were used as OBHs during subsequent operations.

(3) 1975 - 1976. Six new ABHs were constructed, and test-pumped along with the two existing ABHs (which had been constructed in the 1970 - 71 season). All ABHs have diameters of 915mm, which is typical of the large diameters used in wells elsewhere in the gravels. At the same time, four new 915mm ABHs were constructed on the opposite bank of the Thames at Bray. The Bray boreholes are operated by the Mid - Southern Water Company. A number of OBHs were also constructed at this time, including two nested groups designed to investigate hydraulic relationships between the gravels, the Reading Beds and the Chalk. OBHs 15 and 19 were cased through the gravels and screened at about 18m depth, within the Reading Beds, while OBHs 14 and 20 were cased through both the Reading Beds and the gravels and screened in the Chalk at about 35m depth.

Test pumping was carried out from April through October

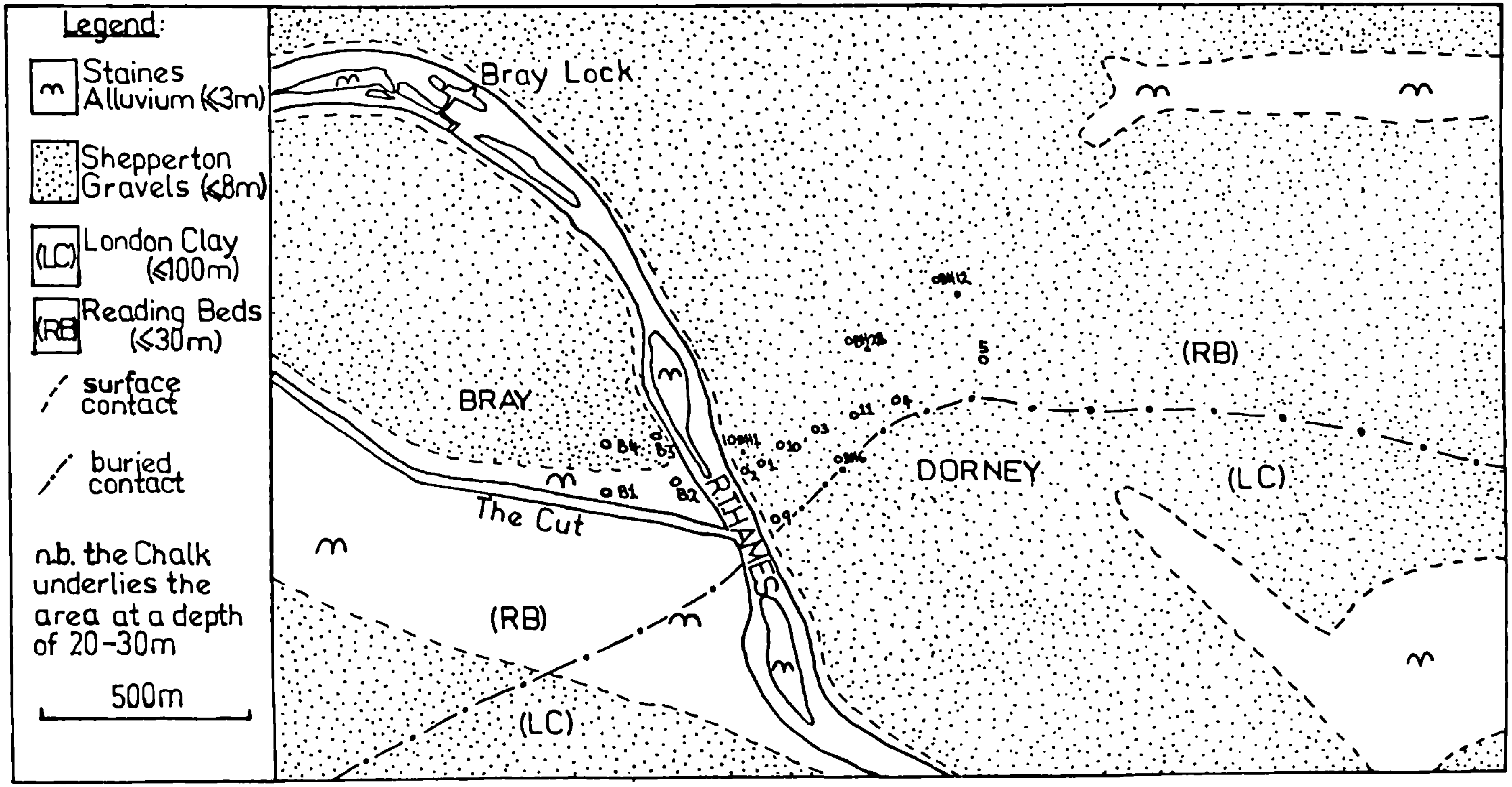


Figure 3.14 -- Geology of the Dorney Area.

(Adopted from various BGS and TWA data)

1976. Individual step - tests of ABHs provided no data of use in evaluating well losses. When the group tests of Dorney and Bray were performed, however, repeated power failures and pump breakdowns badly hindered progress. Nonetheless, some attempt was made to determine aquifer parameters using Theis and Jacob methods (Ridings et al, 1977). Borehole yields were varied during the course of the test, but had settled at around 2 to 3.5 TCMD per hole by mid-July. These yields were obtained with steady drawdowns of less than 4.5m (and only 1.4m at ABH 4). During this test - pumping, hydrochemical monitoring was carried out by the Institute of Geological Sciences (Edmunds, Giddings and El Agib, 1976) with the intention of discovering and quantifying the provenance of the water produced from the abstraction boreholes (using an approach like that described in Section 3.5.1 above, involving equations 3.1 and 3.2).

The results of these various investigations provided much insight into the hydrogeology of the site. The main points are summarised below:

(1) The monitoring of both water chemistry and water levels from OBHs 14, 15, 19 and 20 indicated that the lower portions of the Reading Beds act as a very efficient confining layer, isolating the Chalk from the gravel aquifer.

(2) The geometry of the wellfield is significantly different from the idealised geometry on which standard pumping test analysis methods are based (ie infinite extent, constant saturated thickness, confined conditions; Freeze and Cherry, 1979). In particular, the aquifer at Dorney is markedly finite, being so close to the partially penetrating Thames. Because of this, results of Theis, Jacob and image well analyses of Dorney pumping - test data are subject to considerable uncertainty. Nonetheless, the figures obtained do give some indication of the orders of

magnitude of hydraulic parameters. The mean values quoted by Ridings et al (1977) are:

Hydraulic Conductivity = 1500 m/d

Transmissivity = 9000 m^2/d

Specific Yield = 0.08

These values are consistent with other data for the Thames Gravels (cf Table 3.3 and Dixon et al, 1989).

(3) The results of the hydrochemical studies (Edmunds, Giddings and El Agib, 1976) suggested that, at approximate equilibrium in July 1976, the two ABHs nearest the river (2 and 9) were producing water which was 100% river - derived, while the next nearest wells (1 and 10) had 40% river contributions. The remaining four wells showed no evidence of river contributions at all. On the basis of these calculations, the total amount of water entering the aquifer from the river was estimated at 8.2 TCMD, or about 36% of the site yield. The accuracy of these estimates is stated to be plus or minus 10%. For the sake of comparison, baseflow prior to pumping (April 1976) in the reach of the Thames *falling within the final* radius of influence of the Dorney wells (in July 1976) has been estimated at about 0.85 TCMD (Cathy Glenny, Thames Water, personal communication, 1989).

At present, 13 years after the installation of the Dorney ABHs, some yield problems have developed at the site (Connorton, personal communication, 1989), though details are as yet unavailable.

Although the Bray wells were not studied in any great detail during this project, it is worth mentioning that the licensed abstraction rate at Bray is the same as that at Dorney, although at Bray the yield is obtained from only four ABHs. Water quality problems have affected the Bray wells, however, with polluted water flowing in from the Cut (Flavin, 1986). This situation, which was reviewed in Section 3.4.4.1 above, has led to the Mid - Southern Water

Company installing and testing six new boreholes about 1 km to the northwest of the existing site (Banks, 1989). These boreholes have yield - drawdown characteristics similar to those of the older Bray wells, and Banks (1989) proposed a combined yield of 14 TCMD from the three best boreholes. This study has revealed more pronounced lateral variations in gravel permeability than have previously been recorded, with lowest permeabilities occurring in the vicinity of the modern river. Deposition of fine sediment from the modern streambed within gravel interstices may account for the reduction in permeability close to the river.

CHAPTER FOUR

A NEW MODEL FOR THE DEVELOPMENT OF CHALK PERMEABILITY IN STREAM - AQUIFER SYSTEMS OF THE MIDDLE THAMES VALLEY.

4.1 -- INTRODUCTION.

The broad features of the areal distribution of permeability in the Chalk were described in Section 3.2.3, where it was noted that the permeability is usually highest beneath river valleys and dry valleys, and lowest in the interfluve areas between these valleys (Ineson, 1962; Owen et al, 1977; British Geological Survey, 1984). It was also noted that recent investigations in the Middle Thames Valley have revealed the localised presence of soft, lowly permeable 'putty chalk' at the gravel / chalk interface, where it functions as an efficient confining layer. Modest bulk permeabilities have been noted in the main mass of Chalk beneath these 'putty chalk' zones. Because these discoveries are so clearly at odds with the generally accepted views of Chalk permeability distribution, it was considered worthwhile investigating the factors controlling the distribution and origin of these putty chalk zones. The results of this investigation prompted the development of a new geological model for the distribution of permeability in the Chalk, which has important implications for the conceptual and mathematical models of the Middle Thames stream - aquifer systems developed in Chapters Five and Six. This Chapter is dedicated to describing this new geological model.

4.2 -- DESCRIPTION OF THE PROBLEM.

Robinson and Ridings (1978) were the first to describe the hydrogeological effects of putty chalk at a gravel / Chalk interface. They recorded up to 48 metres of 'soft to very soft Chalk putty and slurry' acting as a leaky confining layer between 'normal' Chalk and the Shepperton Gravels at Little Marlow (SU 877870). When modelled analytically, this putty chalk was estimated to have a hydraulic conductivity in the range 0.2 - 2.0 m/d. The Chalk at this site is devoid of regular widened fissures.

When Robinson and Ridings (1978) first recorded these features of the Little Marlow site, the occurrence of putty chalk was thought to be a unique local anomaly which could be largely ignored. However, subsequent site investigations at Spade Oak (SU 883873) nearby revealed a similar hydrogeological configuration (Rylands and Robinson, 1983). Putty chalk was again found between the Gravels and the Chalk and Rylands and Robinson (1983) reported that "pumping the Chalk had no effect on groundwater levels in the gravels" and vice versa. Hence the putty chalk is an even more efficient confining layer at Spade Oak than it is at Little Marlow.

Most recently, during the installation of riverside wells at West Marlow, Bucks (SU 845857), 'soft, sticky "putty" chalk was reported to have been found at the base of the drift deposits' in two of the three abstraction boreholes and in one of the four observation boreholes (Banks and May, 1988). When the site was test - pumped, the hydraulic response indicated that the Gravels were not in full hydraulic continuity with the Chalk across the site, probably due to the effects of the putty chalk. Furthermore, borehole fluid flowmeter logs showed that the distribution of major flow horizons in the Chalk has no consistent relationship with depth at this site. Maximum sustainable yields for individual wells were estimated to vary from 4 to 6 Ml/d.

At Hurley (SU 832843) very low yields have been obtained from the Chalk beneath the Gravels in wells operated by the Mid-Southern Water Company (Banks and May, 1988). In an attempt to salvage something from the site development, satellite boreholes were constructed to tap gravel water. Yields have never exceeded 23.6 Ml/d from the five boreholes and their satellites (Robinson, Personal Communication, 1989), which represents about one-quarter of the yield obtained at Gatehampton. Although Banks and May (1988) do not mention putty chalk at Hurley, inspection of the driller's logs for the site in the BGS archive at Wallingford (Record SU 88/76 a - b) revealed a sequence of '7m of gravel overlying putty chalk'.

Hence it is clear that the normally high permeability of the Chalk in the river valleys is locally replaced by lower permeabilities, associated with poor fissure development, and that the normally excellent hydraulic connection between the Gravels and the Chalk is broken at some sites by a layer of putty chalk between the two formations.

4.3 -- COMPLEMENTARY INFORMATION.

4.3.1 -- Other Occurrences of Putty Chalk.

Williams (1987) studied the distribution of weathering mantles on the Chalk throughout its English outcrop, and has observed that putty chalk frequently occurs as a coating on the upper surface of the Chalk in elevated interfluve areas. By analogy with modern weathering mantles forming in periglacial regions, it is thought that this putty chalk was formed by repeated freezing and thawing of the Chalk in an 'active zone' above the perennial permafrost table (Williams, 1987; see Washburn, 1979, for a review of periglaciological terminology).

Putty chalk has been observed by the author at several sites in the Middle Thames Valley. In an interfluve setting, it occurs as a mantle on the sub-soil surface of the Upper Chalk, where it occasionally forms the source material for gelifluction lobes, as described in Section 3.2.2 (and shown in Figure 3.3).

In a valley floor setting, the author found putty chalk at the interface between the Taplow Member of the Middle Thames Gravel Formation and the Chalk in the quarry at

Berry Hill (SU 912815). This putty chalk was a very soft, pasty, brilliant white, plastic, carbonate mud, completely devoid of the fractures found elsewhere in the Chalk. It is interesting to note the occurrence of 'chalky paste' in the same stratigraphic position some 700m to the east (SU 919816), as recounted by Gibbard (1985, p.44).

Consultation of borehole records in the BGS collection at Wallingford revealed a further occurrence of putty chalk at the gravel - chalk interface beneath the modern floodplain at Wargrave (SU 785779; BGS Record SU 77/1 a - c). Here, 3m of gravel are recorded overlying 'clayey chalk' and 'rubble chalk with putty chalk and flints'.

As was noted in Section 3.4.2.1, deposition of the Shepperton Gravels occurred under periglacial conditions during the Devensian. It is therefore obvious that the gravel / chalk disconformity can be dated to the same period. When postulating a mechanism for development of putty chalk at the gravel / chalk interface, therefore, Devensian environmental conditions must be taken into account. Any proposed mechanism must also take account of the field relations which strongly suggest that the putty chalk formed in situ by weathering of underlying chalk (Banks and Robinson, personal communication, 1989). The importance of this point may be gauged by the following example: It could be argued that the putty chalk beneath the gravels was emplaced by gelifluction from adjacent Chalk slopes prior to deposition of the gravels. After all, the existence of geliflucted putty chalk at Hindhay was noted above. Nonetheless, the apparent absence of any gelifluction fabrics in the putty chalk at the well sites (and in the exposures at Taplow) precludes this notion. Furthermore, the distances between putty chalk patches and the nearest suitable source areas for gelifluction lobes are too great to admit of such an explanation. Indeed, in the narrowest reaches of the valley (eg at Gatehampton and Medmenham; see Section 4.3.2 below), where gelifluction -

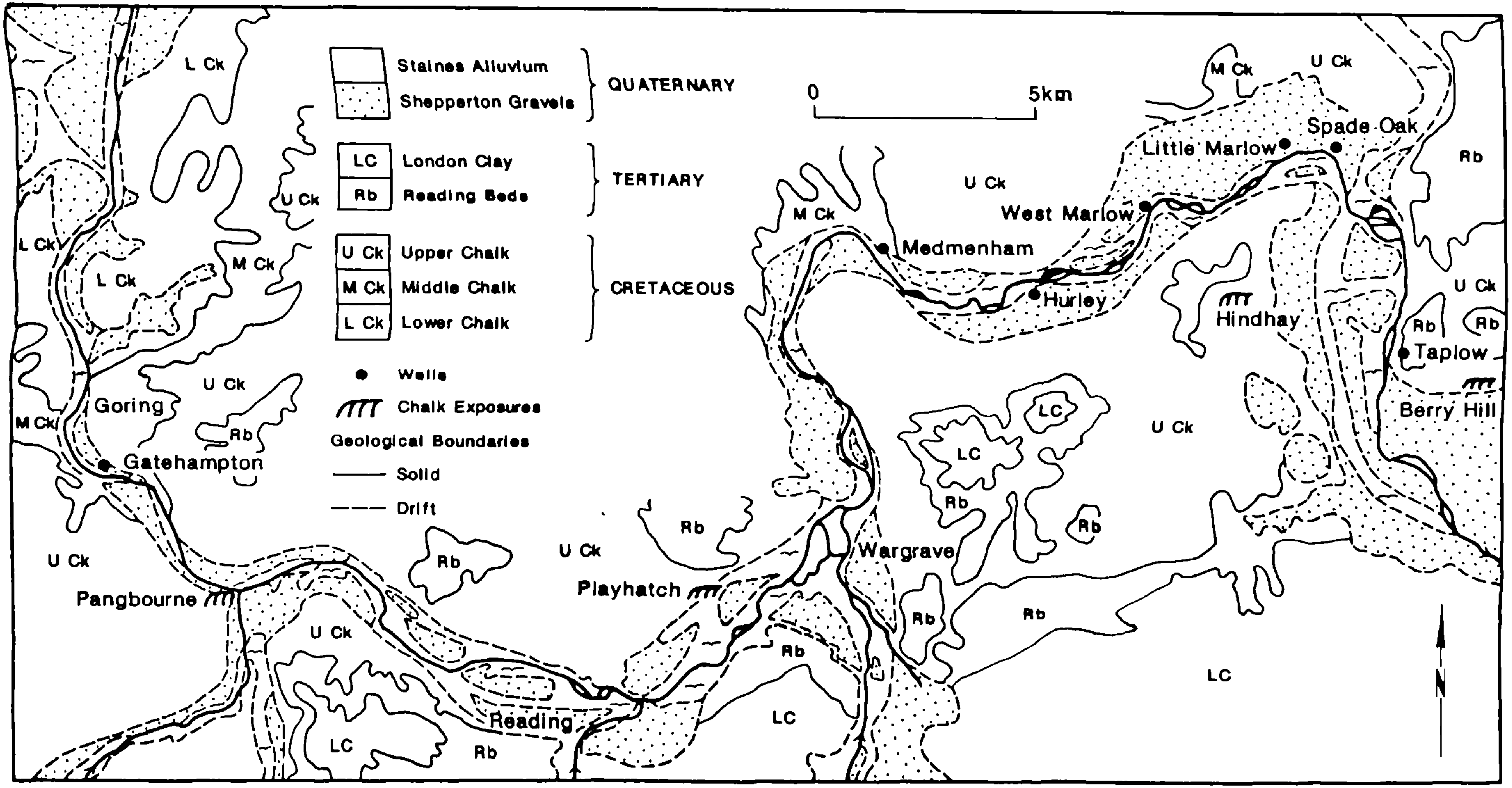


Figure 4.1 -- Location map showing sites mentioned in the text, with simplified geology (based upon field observations and the map by the Institute of Geological Sciences and the Thames Water Authority, 1978).

prone Chalk slopes are nearest to valley floor sites, putty chalk is conspicuous by its absence. The mechanism for putty chalk formation proffered in Section 4.4.2 below was formulated with these factors in mind.

4.3.2 -- Geometric Characteristics of Different Sites.

Visits to the sites shown on Figure 4.1, and inspection of published topographic and geological maps of the area (OS Landranger Sheet 175; BGS 1:50,000 Sheets 254, 255 and 268), has revealed that the sites where putty chalk occurs beneath the Shepperton Gravels (Spade Oak, Little Marlow, West Marlow, Hurley, Wargrave) are in places where the Middle Thames Valley is widest, whereas Gatehampton and Medmenham (the two "mega-yield" sites, to borrow a term from Banks and May, 1988) are located in narrow sections of the valley (Figure 4.1; Table 4.1). Attention is drawn to the constriction of the valley at Medmenham by fans of chalk-rich flint gravel (marked as Younger Coombe Deposits on BGS Sheet 254), which are 'derived from the series of narrow dry valleys that dissect the northern valley side above the river' (Gibbard, 1985, p.77). These have considerable palaeo-environmental significance, as will be seen below. More subtly, borehole data show that the putty chalk well sites are characterised by a smaller thickness of gravels than are the "mega-yield" sites (Table 4.1). The ratio [valley width (km) / maximum gravel thickness (m)] seems to give a discriminatory criterion; putty chalk sites have ratio values greater than 0.10, while ratios lower than 0.10 were obtained for the two mega-yield sites. Obviously this criterion is based on too few samples to have any real statistical significance, but it does serve to illustrate the distinction in valley width and gravel thickness between the two types of site.

4.3.3 -- Form and Process in Modern Periglacial Braided River / Aquifer Systems. Modern braided rivers in periglacial environments include the Scott (Alaska) and the Donjek (Canada) (Miall, 1977; Rust, 1972), both of

Table 4.1 -- Geometry of Middle Thames Valley - Floor Sites With and Without Putty Chalk

(a) Sites With Putty Chalk.

Site Name	Valley Width (km)	Thickness of Shepperton Gravels (m) Max.	Mean	Ratio of Width to Max. Depth
Wargrave[1]	1.7	3	-	0.57
Hurley	1.3	7	5.5	0.18
West Marlow	1.5	7	4.6	0.21
Little Marlow	1.7	8.3	6.7	0.20
Spade Oak	1.3	7.5	-	0.17
(Berry Hill[2]	4.6	8.0	-	0.57)

(b) Sites Without Putty Chalk.

Site Name	Valley Width (km)	Thickness of Shepperton Gravels (m) Max.	Mean	Ratio of Width to Max. Depth
Gatehampton	0.8	13.5	6.7	0.06
Medmenham	0.5	8.2	7.4	0.06

Notes: Gravel thickness data from BGS records at Wallingford and from the Thames Water Internal Reports cited. Information on valley width pertains to the depositional valley width for the Shepperton Gravel Member, obtained by measurement of outcrop width on BGS maps. Footnotes: 1. Wargrave is not a well site, data BGS record mentioned in text. 2. Berry Hill is in the Taplow Terrace, the terrace immediately below the Shepperton Gravels stratigraphically, and immediately above them topographically. The gravel thickness information is from the site visit described in the text, with the valley width being a minimum width for the old Taplow valley of Wolstonian times, surmised from the current outcrop pattern.

which have sediment assemblages similar to those described from the Shepperton Gravels (Gibbard, 1985, p. 99). Detailed mapping of the Donjek River by Rust (1972) has revealed spatial variations in channel morphology which correlate with the width of the river valley. In reaches where the valley is narrow (less than 1km wide), the river flows as one deep single channel (with internal braid bars), whereas the river assumes an anastomosing form in the wider reaches of the valley, with two or three shallower internally braided anabranch channels (cf Figure 2 in Rust, 1972). The Donjek valley is narrowed considerably where outwash fans (similar to those described from Medmenham in Section 3.2.2) descend from tributary valleys. The discharge regime of these rivers is characterised by one major flood event each year, when the accumulated snow fall of the winter melts at the onset of spring. At other times of the year, flows may be very low except where sustained glacier melting provides water after the seasonal snow has been removed (Bryant, 1983a).

Williams (1970) has described groundwater conditions in the periglacial areas through which such modern braided rivers flow. Below a thin 'active zone' of seasonal freezing and thawing, permafrost is usually continuous in interfluve areas. The permafrost functions as an aquitard, impeding recharge and confining those deep groundwaters which remain unfrozen beneath the permafrost. In the river valleys, however, beneath the major river channels, perennial taliks (unfrozen zones) occur as a result of the warming effect of the flowing surface water. These perennial taliks may pierce the permafrost completely if the river channel is sufficiently substantial. In this case, the deep, confined sub-permafrost groundwaters will flow up through the talik to discharge as baseflow into the river channel. Beneath smaller river channels, the taliks are seasonal, being present as slight depressions in the permafrost table during the summer. Most taliks beneath smaller channels extend at least 3m below the river bed, and often much further (10m or more). Small channels freeze to the bottom in winter, so that the seasonal talik beneath them disappears and the river ice becomes continuous with the permafrost below (Klimentov, 1983, p. 216). When the total river discharge rises sharply at the spring melting flood event, the ice in these small channels will be broken up and melted. Thus an annual freeze - thaw cycle affects the sediments and rocks in seasonal taliks.

4.4 -- DISCUSSION.

4.4.1 -- Previous Models for the Areal Variation in the Permeability of the Chalk.

Previous models for the areal variation in the permeability of the Chalk were proffered before the existence of 'putty chalk' zones in the river valleys was known, and thus they are all weakened by the fact that they cannot explain the appearance of lowly permeable Chalk in the river valleys.

Woodland (1946) first documented the association of high Chalk permeabilities with river valleys, and Ineson (1962) proposed an explanation for this phenomenon which assumes that fracture frequency increases in the valley areas. Ineson (1962) used this supposition to contend that the rivers follow zones of structural or lithological weakness in the Chalk, and/or that erosional removal of Chalk from the valleys caused fracturing upon release of overburden pressure. In this model, therefore, carbonate dissolution is regarded as an enhancement on a basically tectonic development of permeability.

It is shown in Appendix B that there is no evidence that fracture frequency in the Chalk increases towards the river valleys. Hence it seems that the increased permeability is due to solutional enlargement of the same fracture system which occurs in the interfluves. Even were this not the case, fundamental objections to the theory of pressure-release fracturing in the Chalk would still remain (Williams, 1987; p. 131). Pressure - release fracturing (otherwise known as sheeting) is widely held to be restricted to igneous and metamorphic rocks which have been buried to great depths. It is, for example, frequently invoked to explain the development of permeability in many granites (see Trainer, 1988). In a review of permeability development in all the major carbonate aquifers in North America, sheeting is not mentioned (Brahana et al, 1988). In the face of this evidence, it seems unlikely that sheeting effects can have made a major contribution to the opening of bedding plane fissures in the Chalk, although the possibility of a modest contribution cannot be ruled out.

While Connorton (1976) and Robinson (1976) did not reject Ineson's (1962) assertion that the river valleys are 'zones of structural weakness', they clearly did not regard it as crucial in explaining the development of fissure permeability in the Chalk. Rather, their model centres on the spatial variability in carbonate equilibria in Chalk groundwater. Connorton (1976) argues that if it is assumed that the partial pressure of carbon dioxide (pCO_2) in Chalk groundwater decays at a constant rate as it infiltrates through the unsaturated zone, then the thicker the unsaturated zone is at a given site, the lower will be the ability of the water to dissolve calcite by the time it reaches the water table. The net effect is that dissolution beneath the water table will be negligible in the interfluves, but considerably higher in the river valleys, where the pCO_2 of local recharge and the total through - put of groundwater will be highest. This model therefore explains neatly why permeability should be lower in interfluve areas (where the unsaturated zone is thick) than in the river valleys, (where the unsaturated zone is thin). Furthermore, it also explains observed fissuring in the unsaturated zone of the interfluves. Indeed the appeal of this model is enhanced when it is realised that Morel's (1979) negative criticisms of the model are largely invalid. For instance, Morel (1979) claims the Connorton

(1976) model is invalid because 'the residence time of water in the major fissures of the unsaturated zone is only a few days', ie the long residence time in the unsaturated zone (needed for the model to work) will not occur. However, Morel himself cites evidence which contradicts this statement (see Morel, 1979, pp. 85 and 120), including the isotope studies (reviewed recently by Geake and Foster, 1989) which indicate that most flow in the Chalk unsaturated zone occurs in microfissures and in the larger intergranular pores of the matrix blocks, with downward flow in the larger fractures only occurring when rainfall intensity exceeds the infiltration rate of the matrix blocks. Thus Morel's (1979) criticisms seem to be groundless.

A more fundamental criticism of the Connorton - Robinson model is that it is implicitly based upon the assumption that the groundwater regime has been free from permafrost throughout the time the dissolution has been occurring. Serious questions arise as to whether this mechanism is sufficiently rapid that it alone could have produced the present permeability distribution in the Chalk during the last 10000 years (ie since the end of the Devensian) (Price, 1987; and see discussion below). Even if it is argued that the solution mechanism was effective prior to the Devensian, the problem remains that the zones of highest permeability in the Thames Valley are coincident with a channel that was cut in late Devensian times. Therefore any pre-Devensian operation of the Connorton-Robinson mechanism would have produced high sub-river permeabilities beneath older gravel trains.

Morel (1979) rejected the Connorton (1976) and Robinson (1976) model, and threw his support behind the theory of Ineson (1962), which was reviewed above. Morel (1979) used the supposed continuation of the river valley permeability association below Tertiary cover as the basis for insisting that the areal variation in Chalk permeability developed during the late Cretaceous and Tertiary periods, with no real Quaternary contribution. The theory is that pre-Quaternary rivers followed the same line as the modern rivers of the Thames Basin and East Anglia, encouraged by the never - proven 'zones of structural weakness'. While rivers often follow lines of weakness initially, structural controls on the lines of rivers need not dominate their behaviour ever after. For example, it is circumstantially obvious that the present course of the Thames is controlled by the valley which was cut by the braided palaeo-Thames during the early Devensian, while pre-Devensian sediments show the that the palaeo-Thames once flowed much further to the north. Moreover, field evidence presented by Morel (1979, p.89) himself contradicts the supposed continuation of the river valley permeability association beneath Tertiary cover. Indeed the original evidence for this phenomenon (the maps presented by Ineson, 1962) does not really stand up to scrutiny. For example, some of the 'extensions' of the river valley association shown by Ineson (1962) include those at Bray on the Thames (SU 914787), Fordstreet on the Stour (TL 920270), Ipswich (TM 160445) and Bramford (TM 125465) on the Orwell, Sible Hedingham on the East Anglian Colne (TL 784342), and two points on the Stour near Wormingford (TL 940335) and Bures (TL 896365). Of these sites, the first three have a stratigraphy such that the river valley is cut into sandy sediments (local varieties of the Lower London Tertiaries, and a local lower sandy member of the London Clay; Ellison and Lake, 1986, pp. 7-13) which are likely to be hydraulically connected to Chalk, while at the last four the Chalk outcrops in the river bed (in the first two cases as parts of the main outcrop, in the latter two as inliers; see BGS 1:50,000 Sheets 223 and 207). Clearly it is not satisfactory to maintain that these sites are completely confined from the modern river valleys by the Tertiary deposits (Price, 1987, p. 151, makes this same point in a slightly different context). Indeed where the East Anglian Chalk is overlain by considerable thicknesses of London Clay (eg around Chelmsford in Essex), transmissivity is uniformly low, since the Chalk is 'not subject to secondary weathering processes' (Bristow, 1985, p. 94). Moreover, while the highest permeabilities within the deeply confined Chalk of the London Basin do show an association with structural features (such as faults and anticlinal axes), none of these features show any more than local coincidental alignment with modern rivers. Hence the main burden of Morel's (1979) argument can be neglected.

Price (1987), working without access to the model of Connorton (1976) and Robinson (1976), produced a model for the development of Chalk permeability which closely resembles that of the two earlier authors. Basing his discussion on theoretical work by Rhoades and Sinacori (1941), Price (1987) argued that the permeability patterns seen in the Chalk today could have been produced by the combined effects of:

(a) the concentration of flow near river channels, and

(b) the lower calcite saturation of water recharged near the rivers.

Apart from a slight difference in emphasis, these arguments are indistinguishable from those given in support of the Connorton - Robinson model.

However, like Ineson (1962), Morel (1979), Connorton (1976) and Robinson (1976) before him, Price (1987) steered clear of seriously considering the possible impact of periglaciation on the Chalk permeability distribution. In a discussion of the rate at which the mechanisms he proposes would operate, Price (1987) suggests that 16000 years would be required for the development of the present distribution, given a constant recharge throughout that period equal to the modern average rate. These figures will apply just as well to the Connorton - Robinson model. Since 16000 ybp falls in the late Devensian (it is the approximate date at which the periglacial palaeo-Thames was switching from net down-cutting to net aggradation), this time interval is clearly too long to allow neglect of the Devensian with impunity. Even though Price (1987) suggests that the high early Flandrian recharge rates (ie higher than the present rate) could have speeded up the process, it is just as likely that lower mid - Flandrian rates would have slowed it down.

Most recently, Williams (1987) broke with tradition by considering periglacial influences on Chalk permeability development. He briefly suggested that the high permeability of the Chalk in the main river valleys may be due to deep mechanical weathering by repeated formation and melting of permafrost, since field evidence indicates that this is responsible for brecciation of the Chalk to depths of 20 m or more in the floor of some dry valleys. However, borehole evidence shows that brecciated chalk is not normally found within the main body of the Chalk beneath the main river valleys, although it may occur amongst the lowest units of the Shepperton Gravels as a localised fluvial 'rip-up' breccia. In modern Arctic river valleys, the main river channels flow perennially, while lesser channels and tributaries are prone to drying out in the summer, or freezing to the bottom in the winter (Bryant, 1983a). Hence it is quite credible that annual variations in talik thickness beneath the tributary valleys (which are now the dry valleys) led to brecciation, whereas the more or less permanent talik beneath the main river valleys prevented this from occurring.

4.4.2 -- A New Model.

There is clearly a need for a new model for the areal variation in Chalk permeability which avoids the short-comings of the earlier models reviewed above. Such a model is proposed below.

It was argued above that the fissure permeability of the Chalk is highest in valleys because of increased dissolution of the aquifer there, leading to wider fracture apertures. The rival theories of increased tectonic fracturing, or an association with pre-Quaternary river valleys, were shown to be incompatible with the field evidence. Because of the close areal association with the Gravels, it is assumed in this model that most of the solutional widening of fissure apertures occurred during the Devensian, when the Middle Thames Valley was subject to periglaciation.

By analogy with modern periglacial braided river systems (described in Section 4.3.3 above), the geometry of the river - aquifer - permafrost system in the Middle Thames area during the Devensian is likely to have exhibited considerable spatial variation. It was noted that in the Donjek River Valley, Yukon Territory, there is a single deep (internally braided) river channel in narrow parts of the valley, and a number of shallower anabranch channels where the valley is wider. A schematic diagram shows how this configuration would look in the Middle Thames Valley (Figure 4.2). It is clear that the high - yielding sites occur in single channel areas, while the valley-floor putty chalk sites all fall in multi-channel reaches (cf Table 4.1).

Schematised cross - sections across the narrow and wide reaches (Figure 4.3) show the probable configuration of taliks and permafrost in these two different zones. In the interfluve areas of both zones, all shallow groundwater circulation would be prevented below the perennial permafrost table. This quite simply explains the low permeabilities in modern interfluve areas. As outlined above, in the active zone above the perennial permafrost table frost weathering of the Chalk would be intense in winter (leading to putty chalk formation), and the ground would be largely saturated in summer (leading to gelifluction). Dissolution above the perennial permafrost table during the summer would lead to some fissure

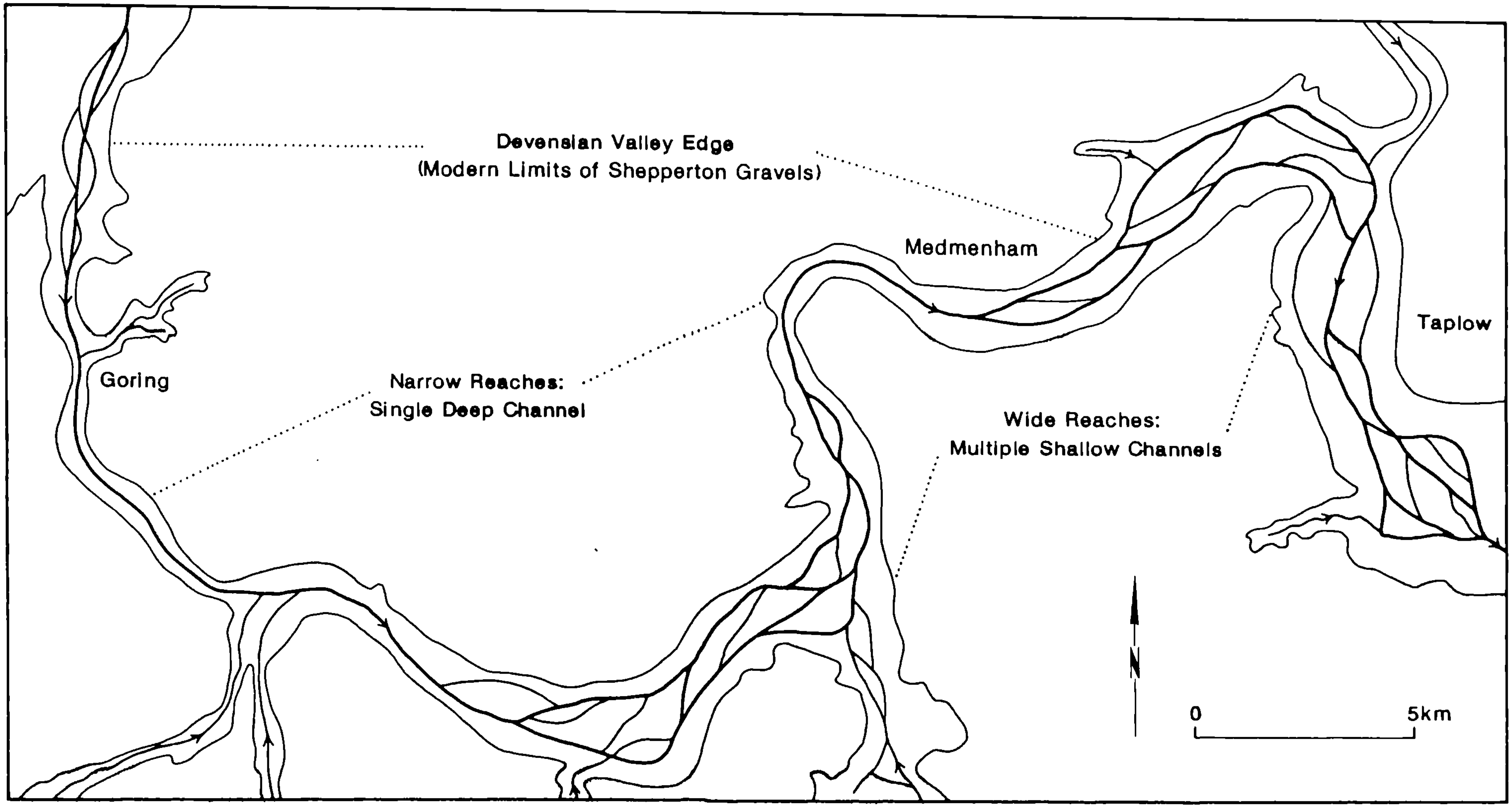


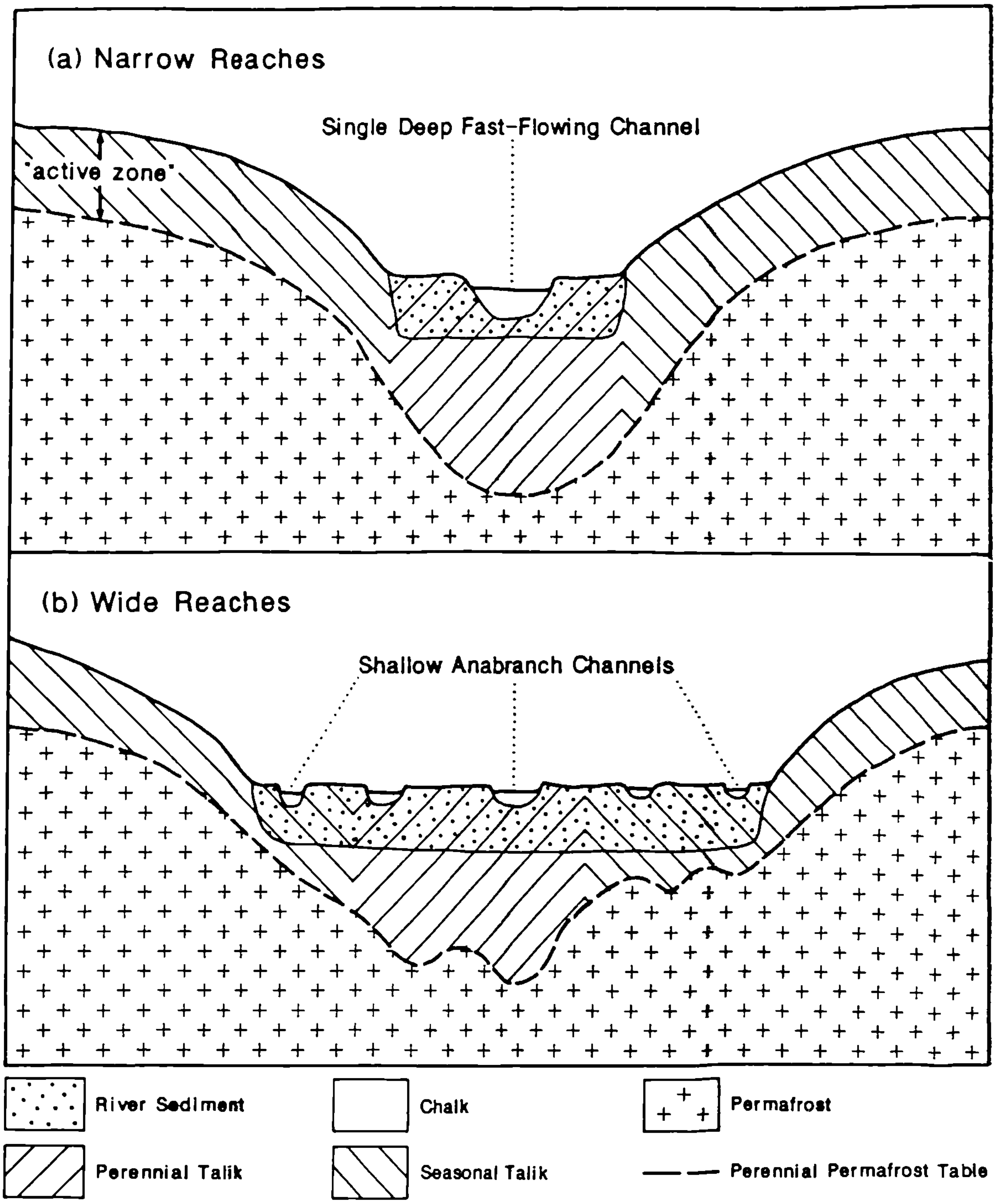
Figure 4.2 -- Schematic representation of probable channel configuration for the braided palaeo-Thames River in Devensian times.

enlargement beneath the interfluves, above the position of the modern water table. This would explain the occurrence of cavities in such a position in the Berkshire and Marlborough Downs, as mentioned in Appendix B.

Beneath the single deep channel in the narrow valley reach (Figure 4.3(a)), a perennial talik would be well developed, and would probably span the width of the valley. Interaction of river water and groundwater (which may locally include a component of deep cool Chalk water, rising from beneath confinement by the interfluve permafrost) in this perennial talik would lead to dissolution of the Chalk lining the major fractures. Side valleys (which are now dry valleys), being narrow, would have been occupied by deep fast flowing rivers during the spring meltout events, and would thus have experienced ephemeral talik dissolution. During the winter, however, deep freezing would lead to cryoturbation of the Chalk.

With lower velocities and shallower flows, the perennial taliks beneath the wider valley reaches (Figure 4.3 (b)) would be less well developed, and thus less of the Chalk would be subject to dissolution. Moreover, the smaller channels would be susceptible to complete freezing during the winter, so that the seasonal talik beneath them would fuse with the underlying permafrost, as described from the modern Arctic (Williams, 1970; Klimentov, 1983). The sediments beneath these minor channels would therefore be exposed to an annual freeze - thaw cycle. As mentioned above (Section 4.3.1), Williams (1987) has presented evidence which shows that putty chalk in the interfluve areas developed by pulverisation of the Chalk in the active zone (seasonal talik) due to seasonal freezing and thawing. Thus it seems obvious to conclude that the putty chalk described from the Middle Thames well sites developed in seasonal freeze - thaw zones which penetrated to the gravel / Chalk interface beneath minor channels. This process would clearly only occur beneath the lesser anabranch

Figure 4.3 -- Schematic cross-sections (not to scale) showing the likely periglacial configurations of (a) narrow reaches and (b) wide reaches of the palaeo-Thames during Devensian times.



channels, but this very fact explains the lateral impersistence of the putty chalk confining layers observed in the field.

It is important to assess whether the putty chalk formation mechanism proposed here is compatible with the probable configuration of the late Devensian river - aquifer-permafrost system in the Middle Thames Valley (Figures 4.2 and 4.3(b)). With regard to the depth at which putty chalk could have formed, a minimum for the river valley setting can be estimated by reference to the prevailing conditions in the interfluves. In the interfluve active zones, summer thawing (due mostly to insolation) would be less substantial than in the river valleys, where channel talik extensions would work in tandem with insolation. The depth to which active zone freeze - thaw processes penetrated in Chalk interfluve areas during the Devensian is difficult to assess, but estimates (based on the depth to which Chalk is clearly brecciated (Williams, 1987; Catt and Hodgson, 1976), and the depths of bases of involutions in unconsolidated sediments (Williams, 1975)) tend to fall in the range 1m to 5m, with a mean close to 3m. These estimates accord well with measured active zone thicknesses of 3 - 5m reported by Klimentov (1983, p. 205) from the USSR, and give a minimum depth of penetration for sub-river active zone depths in the Thames Valley of around 5m. Of course actual late Devensian sub-river penetrations cannot be independently estimated, but comparison of this estimated minimum with the 3 - 10m penetrations quoted for taliks beneath minor channels in the modern Arctic (Williams, 1970; and see Section 4.3.3 above) lends credence to the estimate. Assuming that the thicknesses of gravels beneath the palaeo-channels were no greater than the thicknesses of individual facies units (eg $\sim$3m for St facies; Gibbard, 1985, p. 97), such depths of penetration seem comfortably sufficient to ensure freeze - thaw in the upper zones of the Chalk beneath the gravels. Even if it is conservatively assumed that the sub-channel thicknesses during deposition were more akin to the thicknesses of preserved sequences (Table 4.1), the depths of penetration are still within feasible bounds.

The model described above accounts for all of the details of the areal variation in Chalk permeability described in Section 3.2.3 above, as well as for the new information on putty chalk presented in this Chapter. None of the earlier models reviewed above can explain all of these features. Nonetheless, the model of Connorton (1976), Robinson (1976) and Price (1987) may be seen as a description of how the Devensian permeability distribution has been preserved and enhanced during the last 10,000 years. Indeed, in one sense the new model can be viewed as an explanation of how the dissolution mechanisms identified by that model were intensified and rendered extremely effective during the Devensian. During warmer periods of the Quaternary, as today, the dissolution mechanisms identified by Connorton (1976), Robinson (1976) and Price (1987) would have dominated. Study of sites where gravel accumulation occurred during interstadials (eg Harpsden, SU 769802, on the Kempton Park Terrace) may yield insight into this.

4.5 -- IMPLICATIONS OF THE NEW MODEL.

On the basis of the new model, it may be anticipated that enlarged fissures and/or putty chalk should be found beneath older members of the Middle Thames Gravel Formation, and indeed an occurrence of putty chalk from the base of the Taplow Member was described in Section 4.4.1. Gibbard (1985, pp. 100 - 102) mentions collapse structures in the Chalk beneath older members, which he suggests are related to Chalk dissolution in sub-river taliks. Similar observations have been made by Robinson and Banks (personal communication, 1989). Taken together with the model proposed above, these field relations suggest that many 'fossilised' periglacial stream - aquifer systems flank the valley of the Thames, above the level of the modern water table. Such an inference has important implications for Chalk recharge studies.

Extension of this model to other areas depends on their Quaternary history. The shallow highly permeable zone in the Chalk in Hampshire described by Headworth et al (1982) appears to be explicable in terms of intense dissolution in a thin perennial talik associated with the Devensian predecessor of the Candover Stream. Given the depths of penetration of perennial river valley taliks in the modern Arctic (Williams, 1970), it is possible that talik-controlled dissolution may have occurred in the East Anglian river valley sites listed in Section 4.4.1 above, but more detailed study would be needed to confirm this. A more certain site for extension of the model appears to be the valley of the Baughurst Stream, a tributary of the River Enborne near Newbury, where recent studies by the Thames Water Authority show a pronounced increase in Chalk permeability along a valley which is shown to be underlain by considerable thickness of Tertiary strata on the Geological Survey Maps. However, evidence of extreme cryoturbation associated with a river talik is furnished by a remarkable pinnacle of rubbly chalk, which pierces Tertiary cover to touch Devensian river sediments (Hawkins, 1952; Hill, 1985). The mode of origin of this pinnacle is uncertain, but it is definitely of periglacial origin, and may have been associated with large scale pingo development (Hill, 1985). The circumstantial evidence is thus compatible with the notion that the high Chalk permeability in this supposedly 'confined' valley aquifer may be attributed to deep talik - controlled dissolution and associated periglacial phenomena.

Further afield, other associations between river valley axes and high permeability in carbonate aquifers may be explicable in terms of the present model. For instance, dramatic solution cavities beneath river beds in the Tennessee Valley, USA, (Moneymaker, 1941) occur in an area which probably underwent Devensian (Wisconsinian) periglaciation (cf. Washburn, 1979, p. 305). Further research on such problems may well prove fruitful.

4.6 -- SUMMARY AND CONCLUSIONS.

The new model for the development of spatially variable permeability in the Chalk of southeast England may be summarised as follows:

(i) During the Devensian, when the Shepperton Gravels were accumulating in a braided river system, periglacial conditions obtained in the Middle Thames Valley.

(ii) By analogy with modern periglacial stream - aquifer systems, it is clear that permafrost would have restricted most groundwater flow in the interfluve areas, but that beneath major river channels, substantial flows would have occurred in taliks (unfrozen zones). Enlargement of fissures by carbonate dissolution would therefore have been negligible in interfluve areas, but reasonably vigorous in the cold groundwater systems of the sub-river taliks.

(iii) Comparison with modern braided rivers suggests that in narrow areas of the valley, such as the Goring Gap and the northwestern bend of the Henley Loop, the flow in the braided palaeo-Thames would have been concentrated into a few deep fast - flowing channels, which would have flowed perennially and sustained a deep perennial sub-river talik. Uninterrupted dissolution of Chalk in these perennial taliks would account for the zones of very high permeability found in the narrow parts of the Middle Thames Valley.

(iv) In wider reaches of the valley, the palaeo-Thames would have assumed a more highly anastomosing form, with many shallower anabranch channels. These smaller channels probably froze to the bottom in winter, so that the taliks beneath them disappeared as surface ice fused with the perennial permafrost ice below. Not only would this prevent groundwater circulation for a large part of each year, thereby restricting dissolution, but the annual cycle of freeze - thaw would cause pulverisation of the Chalk below the minor channels, leading to the development of putty chalk at the gravel / Chalk interface. This would explain the occurrence of confining layers of putty chalk, and of bodies of Chalk with comparatively low permeabilities, at sites such as West Marlow and Spade Oak.

The association between valley width and putty chalk development identified in the new model has obvious importance for those concerned with exploration for new groundwater sources in the Middle Thames Valley and elsewhere, since it allows prediction of sites where more intensive geological sampling might be warranted before money is committed to sinking an abstraction borehole and conducting a pumping test.

From the point of view of mathematical modelling, the new model implies that the highest permeabilities in the Chalk are likely to be coincident with the subcrop of the Chalk beneath the gravels. This provides a control on data estimation and model formulation.

CHAPTER FIVE
THE CONCEPTUAL STREAM - AQUIFER MODEL.

5.1 -- INTRODUCTION.

The term 'conceptual model' has been defined by Bear and Verruijt, (1987) as the set of assumptions that represent our simplified perception of the real system which is to be mathematically modelled. In this chapter, a conceptual model for stream - aquifer systems of the Thames Basin is developed. The conceptualisations given here are of general application to the stream - aquifer systems described in Chapters 3 and 4, with some site - specific assumptions being presented for the two sites which were studied most closely in this project (Gatehampton and Dorney).

Conceptual modelling is a necessary prerequisite for the development of a mathematical model (see Chapters Six and Seven). However, the process of conceptualisation has an intrinsic value independent of any mathematical utility. In any kind of scientific study, or indeed in many other spheres, the methods of conceptual modelling are widely used to simplify, summarise and generalise information about complex processes and events. In everyday life, the only way most people can hold complex information in their memories is by reducing it to a few simple generalisations which are readily retained. This is the sort of approach that hydrogeologists grace with the name 'conceptual modelling'.

In the sections which follow, the flow and solute transport components of the general conceptual model are described in turn. In both cases, the assumptions to be made about the properties of the three porous media involved are first proffered and then justified. In a final section, the conceptual model is summarised, and some concluding statements are given concerning the implementation of the model. It is important to realise that the conceptual model presented below was developed by trial and error over a considerable period of time. Some of the assumptions were adopted or modified in the light of early mathematical modelling results. The mathematical model was then updated in the light of the latest version of the conceptual model. Thus the model presented here is a final manifestation of the interaction between theory and practice which took place throughout the duration of this project.

5.2 -- THE FLOW COMPONENT OF THE MODEL

5.2.1 -- General Assumptions.

Assumptions:

(1) It is assumed that the depletion of river flow by induced infiltration is so small compared to the total discharge of the river that external coupling of river flow and groundwater flow solutions may be used.

(2) It is assumed that all groundwater flow is laminar, so that Darcy's Law is a valid description of flow.

Justifications:

(1) During the site investigations at Gatehampton (Section 3.5.2.1), which is the highest - yielding riverside source in the Thames Basin, river stage and groundwater heads were continuously monitored. While groundwater heads did prove fairly sensitive to fluctuations in river stage, river stage showed no sensitivity to variations in groundwater head. It is not difficult to see why this should be: Even if all of the water coming from the Gatehampton wells were river - derived (which is manifestly not the case), this would still amount to only 8% of the total river discharge. In reality, much less river depletion is likely, so that

the first of the above assumptions seems wholly reasonable.

(2) The assumption of laminar flow is the most commonly-made assumption in groundwater modelling, and it is normally valid except in karstified terrain. It is possible to test the validity of this assumption by calculating the Reynolds Number for a porous medium, using the groundwater velocity for the domain of interest (Freeze and Cherry, 1979, p. 72). Since the velocities for the field sites are not known a priori, it is desirable to subject modelled velocities to this test to ensure that they do not imply turbulent flow. For further discussion on this point, see Section 8.2.1.2.

A single exception to this assumption is made in the evaluation of well losses for abstraction boreholes, where turbulent flow in the well bore and gravel pack can lead to drawdowns in excess of those that would develop if all flow was laminar (see Section 7.2.3).

5.2.2 -- The Chalk

Assumptions:

(1) The Chalk aquifer is isotropic in the (x,y) plane, but shows anisotropy with regard to vertical hydraulic conductivity (i.e. $Kh = Kx = Ky$, $Kh \neq Kz$).

(2) The Chalk shows trending heterogeneity of hydraulic conductivity, such that it is highest where it underlies the modern floodplain gravels (Shepperton Member), but decreases towards the interfluves. Structured variation in hydraulic conductivity with depth is assumed to occur only where the Chalk underlies the gravels.

(3) Advection occurs only in the fissure system, and is generally laminar so that Darcy's Law applies. Water in the matrix blocks is assumed to be stagnant.

(4) The fissure system may be treated as a continuum, so that there is no need to model flow in individual fissures.

(5) Where the Chalk is overlain by saturated Gravels, it tends to have the storage characteristics of a confined aquifer. Where the water table lies wholly within the Chalk (whether or not there are Gravels on top of the Chalk) then the storage characteristics can be described in terms of a specific yield.

Justifications:

(1) The assumption of (x,y) isotropy is consistent with the isotropic geometry of the horizontal fracture system in the Middle Thames Valley (Appendix B), and with the observed hydraulic behaviour of the Chalk in the Thames valley. Since mean fracture frequencies differ between the horizontal and vertical fracture systems, however, the ratio of vertical to horizontal hydraulic conductivity will be less than unity. For instance, if the mean frequencies for bedding - plane parallel (BPP) and bedding - plane normal (BPN) fracture sets in the Thames - Cambridge Province are used (9.4 and 6.3 fractures/m; Appendix B), and it is conservatively assumed that the BPP set have the same aperture as the BPN set, then the ratio of vertical to horizontal hydraulic conductivity will be about 0.67. In reality, BPP apertures are usually greater than BPN apertures, so that the ratio will generally be substantially less than 0.67.

(2) The trend in Chalk K from high values in the centre of river valleys to low values on the interfluves is well documented, and is discussed in some detail in Chapters 3 and 4, and in Appendix B. The geological model proposed in Chapter 4 strongly suggests that the highest permeabilities will be associated with the subcrop of the Chalk beneath the Shepperton Gravels, where periglacial talik dissolution would have been most intense. As a corollary,

geomorphological considerations strongly suggest that the rapid decline in hydraulic conductivity away from the Gravels will be simply correlated with the height of the present ground surface, since the higher a piece of ground is, the less likely it is to have been subject to talik dissolution in the past. Thus a simple relationship between topography and hydraulic conductivity can be used to provide initial estimates for modelling purposes (see Section 7.2.1 and equation 7.3).

(3) The assumption that advection occurs in the fissures alone is common in Chalk studies, and the arguments surrounding this notion are reviewed in Section 3.2.3 (see also Downing et al, 1979).

(4) The continuum assumption implies that an effective hydraulic conductivity can be defined for the Chalk based on flow in the fissures alone. This in turn implies that the mean spacing of fissures is small enough that it will always be considerably less than the scale over which fissure-derived hydraulic conductivity is averaged (equivalent to grid spacings in finite difference modelling). The finest discretisation used in this study was 10 metres (Chapter 7), and the fissure frequency assumed was about 9 fissures per metre. This gives about 90 fissures per finite difference block (or 450 fissures in 50m of saturated thickness in all blocks), which is taken to be sufficiently large that assumption (4) is valid. This judgement is necessarily subjective since quantitative methods for objectively assessing the validity of this assumption are not yet established (cf Huyakorn and Pinder, 1983, p.274). Nonetheless, confidence in this assumption is bolstered by comparison with successful earlier studies in which the number of fissures per block was similar (Müller, 1987).

(5) All aquifer storage has two components; specific yield and storativity. The former refers to that amount of

storage which is accounted for by drainage of pore space, while the latter refers to water stored due to compression of the water under pressure and elastic expansion of the pore space on account of this. In a confined aquifer, specific yield is zero, and storativity accounts for all the storage changes. In an unconfined aquifer, on the other hand, specific yield dominates the total storage in the aquifer, although at depth within the aquifer, removal of water from storage may still occur by expansion of water and compaction of the aquifer material. Storage contributions from deeper portions of the aquifer are therefore small by comparison with those from the zone of water table fluctuation, but they still exist. This is the basis for assumption (5) as stated above. It has important implications for data assignment in the numerical model, since assignment of specific yield values to sub - gravel Chalk of low storativity would lead to erroneous results.

5.2.3 -- The Gravels

Assumptions:

(1) It is assumed that the Shepperton Gravels can be regarded as a homogeneous, highly permeable, unconfined aquifer.

(2) It is assumed that the Shepperton Gravels are effectively isotropic in the horizontal (x,y) plane, but that substantial differences may exist between hydraulic properties in the horizontal and vertical (z) directions. Hydraulic conductivity is further assumed to show no variation with depth.

(3) The Staines Alluvium behaves as an aquitard which forms a seal to the river banks wherever it occurs, but which has no other significant impact on the stream - aquifer flow regime.

Justifications:

(1) As was described in Section 3.4.2, the most striking feature of the lithostratigraphy of the Shepperton Gravels is the ubiquitous pattern of small (generally 15m x 1.5m) sand - filled channel structures interbedded with the gravel facies (dominated by Gm). The relative abundance of the gravel and sand facies (60% gravel to 40% sand) also shows remarkable consistency throughout the outcrop. Both of these facies are highly permeable. It is therefore clear that while the Shepperton *Gravels* are heterogeneous, they are heterogeneous in a predictable and regular manner. Furthermore, the heterogeneity of the gravels only results in relatively minor variations in a very high hydraulic conductivity.

It would theoretically be possible to determine values of hydraulic conductivity associated with these two sub-facies, and then create Monte Carlo realisations of the distribution of hydraulic conductivity using the statistics obtained from the field and laboratory studies. Indeed, work of this sort is under consideration or under development for a number of other aquifers, for example in Switzerland (Jussel, 1989), and in southern England (Dixon, Institute of Hydrology, personal communication, 1989). Since geostatistics is beyond the scope of the present study, however, a simpler approach is called for. The regular percentage distribution of the subfacies, and the fact that both subfacies are highly permeable, holds out the possibility that the calculation of prevailing hydraulic conductivities for the Shepperton Gravels as a whole may be possible. The following formula (Raudkivi and Callander, 1976) is generally used to calculate the prevailing hydraulic conductivity of aquifers comprising a number of layers of different permeability:

$$K_b = [K_1 b_1 + K_2 b_2 + \ldots K_n b_n] / [b_1 + b_2 + \ldots b_n] \quad \ldots\ldots (5.1)$$

where

K_b = bulk K value

K_1, K_2, ... K_n = K values of the layers 1, 2 to n

b_1, b_2, ... b_n = thicknesses of layers 1, 2 to n

Given the relative abundances of the sand and gravel in the Shepperton Gravels, Equation (5.1) reduces to:

$$K_b = 0.6K_g + 0.4K_s \quad \ldots\ldots\ldots\ldots \quad (5.2)$$

where K_g = K value for the gravel subfacies

K_s = K value for the sand subfacies

Assuming that the gravel facies (Gm) has a hydraulic conductivity of the order of magnitude of 2000 m/d (equal to the highest values quoted from field and laboratory analysis of Shepperton Gravel samples by Naylor, 1974), and that the sand facies has a hydraulic conductivity of about 300 m/d (which is the mean for sand samples analysed by Naylor, 1974), then application of (5.2) yields a prevailing hydraulic conductivity of 1320 m/d. This corresponds well with the mean pumping test values of 1200 m/d and 1500 m/d quoted by Ridings et al (1977) and Morgan - Jones et al (1984) respectively (see Table 3.3, Chapter 3). It therefore seems that calculation of a prevailing hydraulic conductivity in this simple manner may be a useful simplification.

It seems obvious to extend the above approach to the determination of an 'effective' specific yield for the gravels. During a trip to Dix's Pit, near Stanton Harcourt, the author participated in the collection of samples from the different facies units of the Gravels. These samples were then subjected to column drainage experiments at the Institute of Hydrology, yielding the following values for specific yield (Dixon, written communication, 1989):

'Openwork' (matrix - free) gravels: 33%

Sand lenses (Sp, St, Sh): 26%

Massive gravel with sandy matrix (Gm): 19%

With 60% Gm and 40% sand facies, the effective specific yield obtained by substituting the above values into equation 5.2 is 21.8%. This agrees closely with the average value of 20% quoted by Naylor (1974).

(2) The arguments for assumption (1), concerning the regular distribution of sand and gravel facies in the Shepperton Gravel Member, are also cogent arguments in support of the assumption of isotropy in the (x,y) - plane. The layered, bedded and channelised nature *of the* Gravels, however, suggests that vertical hydraulic conductivity (Kz) is likely to be lower than horizontal hydraulic conductivity (Kh). As may be anticipated, no measurements of Kz in the Shepperton Gravels have been published; indeed there is very little information in the literature on the anisotropy of K in fluvial sediments in general. One detailed study, quoted by Freeze and Cherry (1979) found that Kh exceeded Kv by factors of 2 to 10 in bedded unconsolidated clastic sediments. Thus assuming a value of 0.5 for the ratio of Kv/Kh is *probably reasonably* conservative.

(3) The Staines Alluvium never exceeds 4m in thickness, and averages 2m (Gibbard, 1985); since the underlying Shepperton Gravels are usually about 8m in thickness, and the river is generally less than 3m deep, it is assumed that flow in the alluvium can be neglected, and that most induced recharge occurs through the streambed sediment straight into the Shepperton Gravels. Locally, the Staines Alluvium may confine the Gravels, but this is not held to be important during induced infiltration, where the gravels are rapidly rendered unconfined, or even dewatered (cf Robinson et al, 1987). This ties in with the end of assumption (1), namely that the Gravels are unconfined.

5.2.4 -- The Streambed Sediment

Assumptions:

(1) The streambed sediment is assumed to be homogeneous, isotropic and lowly permeable.

(2) It is assumed that all flow in the streambed sediment is one - dimensional, and takes place in the vertical direction.

(3) It is assumed that the streambed sediment is permanently saturated, and that it has very low storage.

Justifications:

(1) Although the streambed sediment was found to vary somewhat geologically (from silts to peats locally), all varieties are fine - grained and reasonably massive (see Appendix C and Section 3.4.4). Thus assumption (1) is compatible with the available field data.

(2) The effect of the Staines Alluvium in restricting or preventing flow through the river banks was mentioned above. This, combined with the large hydraulic gradients developed between the stream and the aquifer, strongly suggests that flow in the streambed sediment will be predominantly vertical.

(3) None of the field investigations of induced infiltration in the Thames Basin have ever shown a cessation of flow in the river due to pumping, or any other kind of dewatering of the streambed sediment. In the absence of drainage of pore space, therefore, elastic storage is the only possible contribution to storage in the streambed sediment. The storage coefficient value adopted for the streambed sediment must be very small, therefore, since it is essentially equivalent to a confined

storativity.

5.3 -- SOLUTE TRANSPORT COMPONENT OF THE MODEL

5.3.1 -- Introduction.

Conceptualisation of flow in a given system is largely a problem of classification, whereby hydrostratigraphic units are classified as 'unconfined', 'isotropic' etc. In developing a conceptual model for solute transport, however, the decisions which need to be made are less concerned with classification than with prioritisation. For instance, a given process may occur in all the media in a system, but for various reasons the relative importance of this process will differ radically between these different media. Mineralogy, organic matter content, depth of burial, diagenesis and weathering history are all major controls on the development of the geochemical properties and behaviour of a given geological deposit.

Nonetheless, present hydrogeological conditions allow certain assumptions to be made which apply to solute transport in all three porous media. These include:

(1) Water temperature does not differ significantly from one medium to another. This assumption has implications for flow modelling as well as for chemical reactions.

(2) Salinity is never high enough to influence fluid density (and therefore to influence flow), so that solute transport calculations can be performed in isolation from flow calculations.

(3) Precipitation and dissolution, redox transformations and biodegradation are negligible for the solutes concerned, and therefore need not be modelled.

With regard to the first of the above assumptions, it is worth recalling the observations of Kazmann (1948), who noted that yields of induced infiltration sources adjacent to the Ohio River decreased markedly during cold periods in the winter, due to changes in viscosity of the infiltrating river water. This effect is neglected here since all pumping tests modelled occurred in the Summer or Autumn. Nonetheless, it is a factor worthy of greater consideration.

The third assumption is a matter of fact; those species selected for simulations in this study are either highly conservative (chloride) or have a hydrochemistry which is far more strongly controlled by sorption phenomena than by equilibration with an isochemical solid phase, redox or biodegradation (lindane).

To be consistent with the external coupling which is assumed to be a valid description of stream - aquifer flows (5.2.1 above), it is assumed that a mass balance representation of solute movement from the river to the streambed sediment can also be made. This assumption is explored in greater detail in Section 6.3.4.2.

5.3.2 -- Hydrogeochemistry of the Chalk.

Assumptions:

(1) The main process of geochemical significance in the Chalk is matrix diffusion.

(2) Adsorption is negligible in the Chalk.

(3) Dispersion in the fissure system is dominated by mechanical mixing, and molecular diffusion is assumed to be negligible (save insofar as it contributes to matrix diffusion).

Justifications:

(1) Field observations and modelling studies alike have repeatedly shown that the movement of solutes in and out of matrix blocks by molecular diffusion can play a critical role in retarding pollutants during flow in the Chalk (see Sections 3.2.3 and 3.2.4, and the papers by Edmunds et al, 1973; Foster, 1975; Downing et al, 1979; Foster and Smith-Carington, 1980; Wellings and Bell, 1980; Bath and Edmunds, 1981; Bibby, 1981; Black and Kipp, 1983). Thus it is important that the possible effects of this process during induced infiltration be considered.

(2) Organic matter, clay minerals and hydroxides of iron and manganese are the most important adsorbents in hydrogeological systems. It was noted in Section 3.2.2 that the Chalk is exceedingly pure in composition (>96% $CaCO_3$). While the Chalk does contain some iron hydroxides (in the form of oxidised pyrite nodule pseudomorphs), and manganese hydroxides (as localised dendritic growths on joint faces), the patchy distribution and low percentage contents of these minerals must render their effects very slight. Clay minerals are only present in any amount in the Lower Chalk, which occurs at considerable depth in the study sites (depths at which the Chalk has very little permeability; cf Appendix B). Fixed organic matter is virtually absent from the Chalk (Hancock, 1975). It thus seems reasonable to assume that negligible adsorption occurs in the Chalk.

(3) While matrix diffusion is, in a sense, a component of dispersion (Lever et al, 1983), the modeller's dispersion coefficent for bulk flow in the Chalk is really a measure of dispersion in the fissures, in which (at the high prevailing velocities; Chapter 7) mechanical mixing is bound to be far more important than molecular diffusion.

5.3.3 -- Hydrogeochemistry of the Gravels.

Assumptions:

(1) The most significant geochemical process in the gravels is adsorption, and this is only moderately important.

(2) Dispersion is dominated by mechanical mixing.

Justifications:

(1) Since the Middle Thames Gravels are mainly composed of flint and quartz, they are generally chemically inert. The local presence of clayey horizons and organic matter (generally rare in the Shepperton Gravels) means that they will adsorb various pollutant species. Possibly more important are those horizons in discharge areas where iron oxides and hydroxides have been precipitated as a strong cement in the Gravels (see Section 3.4.2.3 and also Morgan - Jones et al, 1984). Given the importance of iron oxides in the adsorption of heavy metals (Hounslow, 1983) it is important that the contribution of these oxides to the overall adsorptive capacity of the Gravels is remembered, particularly since they are known to occur preferentially in riverside settings.

(2) In earlier studies of dispersion in unconsolidated clastic aquifers, it has been postulated that a significant amount of dispersion arises from an exchange of solutes between fine and coarse sediment bodies by molecular diffusion (Goltz and Roberts, 1988). However, the shortage of lenses of fine material in the Shepperton Gravels (Section 3.4.2.1) appears to preclude this possibility in the present case. Again, the high velocities in the gravels (Chapters 7 and 8) suggest that mechanical mixing will tend to dominate dispersion.

5.3.4 -- Hydrogeochemistry of the Streambed Sediment.

Assumptions:

(1) Adsorption is extremely efficient in the streambed sediments, and dominates all other geochemical processes.

(2) Dispersion is dominated by molecular diffusion.

Justifications:

(1) The composition of the streambed sediments could hardly be more typical of a highly sorptive porous medium (Section 3.4.4.4). There is no doubt whatsoever that the sorption capacity of the streambed sediment is extremely high. While the possibility of non-equilibrium sorption occurring in the sediment was raised in Section 3.4.4.4, there is no field data to support this hypothesis and it is therefore felt that an attempt to model this process would be unjustified.

(2) In fine - grained sediment, where velocities are low, mechanical dispersion is likely to be negligible, and total dispersion is likely to be dominated by molecular diffusion (see Section 6.3.2). Under the prevailing streambed velocities (Chapters 7 and 8), molecular diffusion is likely to dominate dispersion.

5.4 -- CONCLUSION.

The conceptual model outlined above effectively summarises much of the information presented in previous Chapters and paves the way for the description of the mathematical model which is given in subsequent Chapters. To aid reference to the conceptual model during a reading of Chapters 6, 7 and 8, summaries of the main assumptions which comprise the model are given in Figure 5.1 and in Table 5.1 below.

Table 5.1 -- Summary of Conceptual Model of Stream - Aquifer Systems in the Thames Basin.

(a) Flow Model

UNIT	AQUIFER PROPERTIES	MODELLED AS ...
The Middle Thames Gravels		
(i) Alluvium	Impermeable	"Seal" on river banks, where present
(ii) Shepperton Gravels	Isotropic (x,y), anisotropic (x,z), homogeneous.	Unconfined aquifer
Chalk	Isotropic (x,y), anisotropic (x,z)	"Leaky" aquifer if overlain by Gravels, otherwise unconfined.
Streambed Sediment	Isotropic, homogeneous.	Low K layer, which nonetheless will transmit considerable quantities of water at low velocities.

(b) Solute Transport Model

UNIT	IMPORTANT PROCESSES FOR INCLUSION IN TRANSPORT MODEL
Middle Thames Gravels	Advection, mechanically - dominated dispersion, some adsorption by disseminated clays, organic matter and iron oxides.
Chalk	Advection, dispersion including effects of hydrodynamic dispersion in fracture network and diffusion into the fine - grained rock matrix.
Streambed Sediment	Slow advection, dispersion mostly by molecular diffusion, strong adsorption.

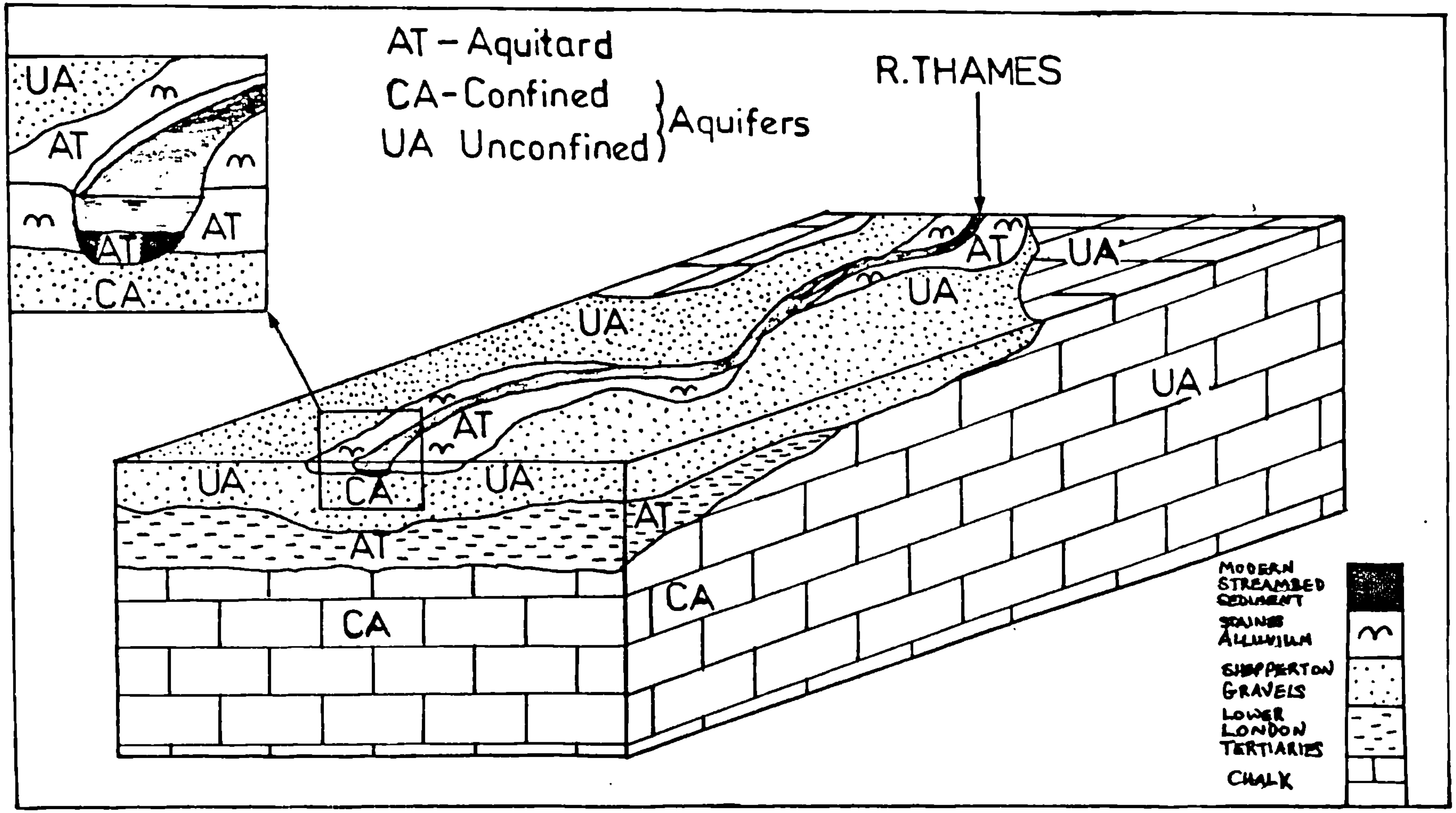


Figure 5.1 -- Block Diagram Showing the Hydrostratigraphic Units Identified in the Conceptual Model for Flow.

CHAPTER SIX
THE MATHEMATICAL AND NUMERICAL STREAM - AQUIFER MODELS

6.1 -- INTRODUCTION

This Chapter describes the mathematical and numerical formulations which were used to turn the conceptual model of Chapter Five into a useful computer code. The FORTRAN-77 routines which enshrine these formulations are referred to collectively by the acronym UNCLESAM (University of NewCastLE Stream - Aquifer Model). Description of the flow module of UNCLESAM (ie US-FLOW) is given in Section 6.2, while Section 6.3 contains a description of the solute transport module (which comprises two codes; US-VEL and US-TRACK).

6.2 -- FLOW MODEL FORMULATION: THE US-FLOW MODULE OF UNCLESAM.

6.2.1 -- Flow Equations and Boundary Conditions.

6.2.1.1 -- Introduction. Because external coupling of streamflow and groundwater flow is assumed (Section 5.2.1), it is not necessary to solve any equations describing streamflow; specification of stage in the stream as a function of space and time is all that is required, and this information is available from field records. In this Section, therefore, it is only necessary to derive specific formulations of the groundwater flow equation for the three media in the model. This is accomplished by considerations of mass continuity with reference to the particular sets of boundary conditions which obtain in stream - aquifer systems.

6.2.1.2 -- The General Equation. In order to define the groundwater flow equation for specific media in a one- to three -layer stream - aquifer system, it is desirable to define a general form of the equation, from which specific versions may be subsequently developed. The starting point for the derivation of the general equation is the equation for continuity of mass in flow through porous media, which can be expressed:

$$- \text{div} \,.\, q = Ss \partial \Phi / \partial t \quad \ldots\ldots \quad (6.1)$$

where: div = the divergence operator ($\equiv \partial/\partial x, \partial/\partial y, \partial/\partial z$)

q = the specific discharge vector ($\equiv q_x, q_y, q_z$)

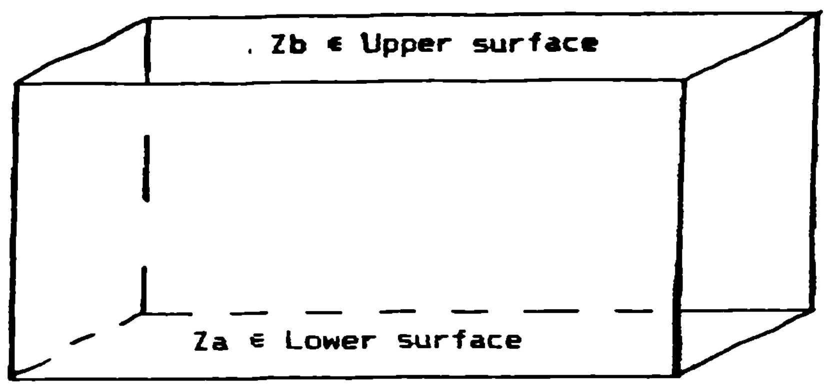
Ss = the specific storage parameter

Φ = groundwater potential

t = time.

The derivation of equation (6.1), which involves consideration of the balance of flows through an elementary volume, is widely available in standard groundwater texts (e.g. Bear and Verruijt, 1987) and is therefore not reproduced here.

Figure 6.1 -- Domain of Integration for Equation (6.1)



To expedite the representation of the three media in a stream - aquifer system, it is desirable to reduce the dimensionality of the problem from three dimensions to two, which requires integration of the continuity equation in space. For the upper and lower aquifer layers, the aquifer (Figure 6.1) is more laterally extensive than vertically extensive, and the lateral extension is approximately in the horizontal (x,y) plane (so that the z - axis coincides with the plane of gravity). Under these conditions, the general integration of the LHS of (6.1) between a point on the lower boundary Za and a point on the upper boundary Zb (Figure 6.1) is:

$$\int_{Za}^{Zb} - \operatorname{div} . q \, \partial z = -\int_{Za}^{Zb}\left[\frac{\partial(q_x)}{\partial x} + \frac{\partial(q_y)}{\partial y}\right]\partial z - \int_{Za}^{Zb} \frac{\partial(q_z)}{\partial z}\,\partial z \quad \ldots\ldots\ldots\ldots (6.2)$$

and the integral for the RHS of equation (6.1) for transient conditions is:

$$\int_{Za}^{Zb} Ss\,\frac{\partial\Phi}{\partial t}\,\partial z \quad \ldots\ldots\ldots\ldots (6.3)$$

In the discussion below, the RHS is neglected for the sake of clarity. The various manipulations and simplifications of the LHS are such that no changes in the RHS are implied until the final step (final removal of the integral signs). Continuing from expression (6.2) then, the integral of the derivative of q with respect to z yields:

$$\int_{Za}^{Zb} \frac{\partial}{\partial z}(q)\,\partial z = q_z\Big|_{Za}^{Zb} \quad \ldots\ldots\ldots\ldots (6.4)$$

Substituting (6.4) into the right - hand side of (6.2) yields:

$$\int_{Za}^{Zb} - \operatorname{div} . q \, \partial z = -\int_{Za}^{Zb}\left[\frac{\partial}{\partial x}(q_x) + \frac{\partial}{\partial y}(q_y)\right]\partial z - q_z\Big|_{Zb} + q_z\Big|_{Za}$$

$$\ldots\ldots (6.5)$$

Differentiation beneath an integral sign can be performed according to Leibnitz's Rule (Huyakorn and Pinder, 1983, p.100), which, in a form appropriate to our problem, states:

$$\int_a^b \mathrm{div}_{xy}\, F\, \partial z = \mathrm{div}_{xy}\left[\int_a^b F\, \partial z\right] - F\Big|_b .\mathrm{div}_{xy}.Z2 + F\Big|_a .\mathrm{div}_{xy}.Z1 \qquad \ldots\ldots\ldots (6.6)$$

where:

$F(x,y)$ is the function concerned (in our case, $\equiv q(x,y)$)

div_{xy} = divergence (i.e. $\partial/\partial x$, $\partial/\partial y$)

a, b = the lower and upper limits in the z - direction.

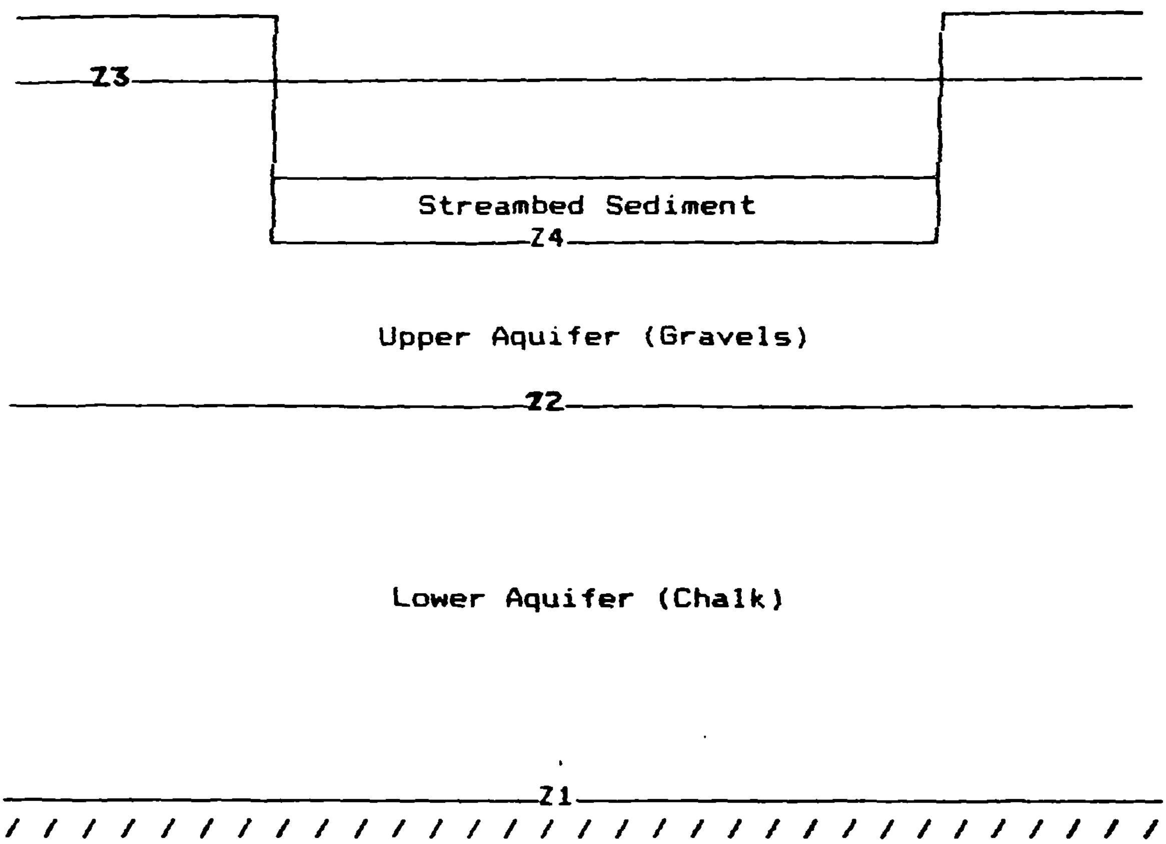
Applying this to the first term on the RHS of equation (6.5) yields:

$$\int_{Za}^{Zb} - \mathrm{div}\ .\ q\ \partial z = -\frac{\partial}{\partial x}\left[\int_{Za}^{Zb} q_x\ \partial z\right] + q_x\Big|_{Zb} . \frac{\partial Zb}{\partial x} - q_x\Big|_{Za} . \frac{\partial Za}{\partial x} -$$

$$\frac{\partial}{\partial y}\left[\int_{Za}^{Zb} q_y\ \partial z\right] + q_y\Big|_{Zb} . \frac{\partial Zb}{\partial y} - q_y\Big|_{Za} . \frac{\partial Za}{\partial y} - q_z\Big|_{Zb} + q_z\Big|_{Za} \qquad \ldots\ldots\ldots (6.7)$$

Equation (6.7) is thus the fully expanded version of the general two - dimensional groundwater flow equation. The two terms involving square brackets describe the x and y flow components throughout the flow domain, and all the other terms are evaluated at the upper and lower boundaries. Note in particular that no assumptions (such as neglect of flow in the z - direction for instance) have been introduced during the derivation of (6.7) from (6.2)

Figure 6.2 -- Boundaries in the Layered Stream - Aquifer System.



Key: Z1 -- Base of Lower Aquifer; Z2 -- Upper/Lower Aquifer Contact; Z3 -- Water Table; Z4 -- Base of Streambed Sediment

(cf Connorton, 1985, p.284). All that has taken place is the integration of the continuity equation with respect to the vertical dimension. The vertical components of the specific discharge vector q have been 'placed' on the upper and lower boundaries by this process. The other terms (ie those in $\partial Za/\partial x$, $\partial Za/\partial y$, $\partial Zb/\partial x$ and $\partial Zb/\partial y$) concern x and y components of q evaluated at the boundaries (Za and Zb; Figure 6.1) and include the effects of boundary topography on these specific discharges. It is in the treatment of these boundary conditions for the various combinations of the three media (streambed sediment, upper and lower aquifer layers) that approximations and simplifying assumptions are introduced.

6.2.1.3 -- Specific Equations. To facilitate discussion, a number of surface datum points are now introduced (Figure 6.2). These will eventually substitute for Za and Zb in equation (6.7) as the boundary conditions for the various layers are considered. Each layer in the system sketched above will now be considered in turn.

The Lower Aquifer Layer. For the specific instance in this project, the lower aquifer layer is usually Chalk, but the derivation which follows is general and could be applied to a clastic regional formation underlying localised alluvium without modification. In order to stress the general nature of this formulation, the terms 'lower and upper aquifer layers' will be used here.

For the lower layer, then, the integration to be performed is from the aquifer base (Z1) to the Lower/Upper (Gravel/Chalk) aquifer interface (Z2). The general equation for this integration (substituting these boundaries in (6.7)) is:

$$\int_{Z1}^{Z2} - \mathrm{div} \, . \, q \, \partial z = \frac{-\partial}{\partial x}\left[\int_{Z1}^{Z2} q_x \, \partial z\right] + q_x\Big|_{Z2} . \frac{\partial Z2}{\partial x} - q_x\Big|_{Z1} . \frac{\partial Z1}{\partial x} -$$

$$\frac{\partial}{\partial y}\left[\int_{Z1}^{Z2} q_y \, \partial z\right] + q_y\Big|_{Z2} . \frac{\partial Z2}{\partial y} - q_y\Big|_{Z1} . \frac{\partial Z1}{\partial y} - q_z\Big|_{Z2} + q_z\Big|_{Z1} \quad \ldots\ldots\ldots (6.8)$$

Consider boundary Z1. This is the base of the aquifer, and it is assumed impermeable, ie:

$$q \, . \, n = 0 \quad \ldots\ldots\ldots (6.9)$$

where n is a unit vector perpendicular to the boundary.

Because q is the specific discharge vector, all flows across Z1 (ie all terms in equation (6.8) which are evaluated at Z1) must sum to zero for (6.9) to be satisfied.

With regard to the upper boundary, it is clear that q_z evaluated at Z2 is not equal to zero, but is some function of the head difference between the two layers. Hence the term for q_z evaluated at Z2 must be retained. Evaluation of this term will be discussed below. While it is true that $\partial Z2/\partial x$ and $\partial Z2/\partial y$ are not equal to zero in the case of most alluvial aquifers (and certainly as regards the Middle Thames Gravels, which can have irregular contacts with the Chalk; see Section 3.4.2 and Chapter Four) it is felt that the errors introduced by neglecting these terms are not very important. This is because the vertical component of flow between the two layers is likely to considerably exceed the horizontal components. Hence it is assumed here that $\partial Z2/\partial x$ and $\partial Z2/\partial y$ are negligible, and that all terms in them may be neglected. Using the foregoing assumptions, then, (6.8) now becomes:

$$\int_{Z1}^{Z2} -\operatorname{div} . q \, \partial z = -\frac{\partial}{\partial x}\left[\int_{Z1}^{Z2} q_x \, \partial z\right] - \frac{\partial}{\partial y}\left[\int_{Z1}^{Z2} q_y \, \partial z\right] - q_z\Big|_{Z2}$$

. . . . . . (6.10)

It is now convenient to reconsider (6.3), which describes changes in aquifer storage. Unless information on the variation in storage properties with depth is available (which is not usually the case), then it is customary to assume that the specific storage (Ss) is constant with depth. Employing this assumption, (6.3) can be freed of its integral sign. Since

$$Ss = \rho_w g(\alpha + n\beta) \quad . . . . . (6.11)$$

where ρ_w = density of the water

g = acceleration due to gravity

α = aquifer compressibility

β = compressibility of water

n = porosity of the aquifer

(Freeze and Cherry, 1979, p. 59), the assumption that Ss is constant with depth implcitly suggests that aquifer and water properties which control it are also constant with depth. Multiplication of (6.3) by (Z2 - Z1) completes the integration so that:

$$\int_{Z1}^{Z2} Ss \frac{\partial \Phi}{\partial t} \partial z = S \frac{\partial h}{\partial t} \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \quad (6.12)$$

where S = storativity = $Ss.(Z2 - Z1)$

and **h** is the average potential with depth, defined by:

$$h = (1/b) \int_{Z1}^{Z2} \Phi \, \partial z \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; . \quad (6.13)$$

(cf Huyakorn and Pinder, 1983, p. 102).

Combination of equations (6.10) and (6.12) leads to the definition of the final equation for transient flow in the lower aquifer layer:

$$-\frac{\partial}{\partial x}\left[\int_{Z1}^{Z2} q_x \, \partial z\right] - \frac{\partial}{\partial y}\left[\int_{Z1}^{Z2} q_y \, \partial z\right] - q_z\Big|_{Z2} = S \frac{\partial h}{\partial t} \quad . \; . \; . \; . \; . \quad (6.14)$$

A note on the evaluation of q_z at Z2, on which the solution of (6.14) depends is given in the following section.

<u>The Upper Aquifer Layer.</u> There are two cases to consider

here (Figure 6.2), namely where the upper boundary is the base of the streambed sediment (Z4), and where the upper boundary is the water table (Z3).

(a) Upper Boundary = Z4. In this instance the required integration (between the limits Z2 and Z4) closely resembles that for the lower layer, since the upper boundary in both cases is constant with time. Boundary conditions are slightly different however, so that the form of the final equation differs somewhat from that of equation (6.14). The basic equation is (cf equation (6.7):

$$\int_{Z2}^{Z4} - \text{div} \cdot q \; \partial z = \frac{-\partial}{\partial x}\left[\int_{Z2}^{Z4} q_x \; \partial z\right] + q_x\Big|_{Z4} \cdot \frac{\partial Z4}{\partial x} - q_x\Big|_{Z2} \cdot \frac{\partial Z2}{\partial x} -$$

$$\frac{\partial}{\partial y}\left[\int_{Z2}^{Z4} q_y \; \partial z\right] + q_y\Big|_{Z4} \cdot \frac{\partial Z4}{\partial y} - q_y\Big|_{Z2} \cdot \frac{\partial Z2}{\partial y} - q_z\Big|_{Z4} + q_z\Big|_{Z2}$$

. . . . (6.15)

The lower boundary in this case (Z2) must be assigned properties which agree with its formulation as the upper boundary for the lower layer. Thus all terms in Z2, except for q_Z evaluated at Z2, are neglected. The upper boundary resembles the lower boundary in every respect, and the terms in Z4 (except for the evaluation of q_Z at Z4) are also neglected. The case for doing so in this instance is strengthened by the fact that the base of the streambed sediment is more likely to be level than the Z2 surface simply because the evolution of the base of the streambed sediment under recent conditions has been characterised by a much gentler river regime (hardly capable of deep bedrock scour) than that which obtained during the cutting of the base of the Gravels during the Devensian (see Sections

3.4.2 and 3.4.4).

In the case of the Gravels the variation of horizontal flow with depth is not known in the way that it is for the Chalk. In lieu of such information, it is assumed to be constant with depth (Chapter Five). Therefore, a further step in the derivation is now performed, which simplifies equation (6.15) by assuming that:

$$\int_{Z1}^{Z2} q_x = q_{xm}(Z2 - Z1) \quad \ldots\ldots \quad (6.16)$$

and

$$\int_{Z1}^{Z2} q_y = q_{ym}(Z2 - Z1) \quad \ldots\ldots \quad (6.17)$$

where q_xm and q_ym are mean values (cf Huyakorn and Pinder, 1983, pp. 102 - 103). Under these conditions equation (6.15) reduces to:

$$\frac{\partial(q_{xm})b}{\partial x} + \frac{\partial(q_{ym})b}{\partial y} + q_z\Big|_{Z2} + q_z\Big|_{Z4} = S\frac{\partial h}{\partial t} \quad \ldots \quad (6.18)$$

with b = Z4 - Z2 in this case.

However, if information is available on the structure of flow with depth, then valuable information is lost by taking the step shown in (6.16) through (6.18), information which is of critical importance in solute transport modelling.

Comment on how to obtain approximations for q_z at Z4 is reserved until the equation for the streambed sediment has been obtained.

To define q_z at Z2, it is necessary to find an expression which represents the exchange as a function of the head differences and the differences in thickness and hydraulic properties between the two layers. Where no aquitard separates two aquifer layers, the exchange between them is resisted only by the thickness and hydraulic conductivity of the two layers themselves. It is therefore proposed that flow between these layers can be represented by the product of

(i) the harmonic mean of the hydraulic conductivity of the layers (weighted according to the relative thicknesses of these layers) and

(ii) the head difference between the layers, divided by half the sum of the thicknesses of both layers.

In mathematical terminology, this may be written:

$$q_z\Big|_{z2} = \left[\frac{-[(Ku.Kl)(bu + bl)]}{[(Ku.bl) + (Kl.bu)]}\right] \frac{(hu - hl)}{(bu + bl)/2} \qquad \ldots\ldots\ldots (6.19)$$

hu, hl = depth - averaged groundwater heads in the upper and lower aquifers respectively

Ku = hydraulic conductivity of the upper aquifer

Kl = hydraulic conductivity of the lower aquifer

bu = thickness of the upper aquifer

bl = thickness of the lower aquifer

Equation (6.19) is in fact Darcy's Law, formulated for flow between two superposed layers. This particular formulation has been previously derived from first principles by a number of authors. For instance, McDonald and Harbaugh (1984) use it to describe z - direction inter-cell flows in their widely used 3-D finite difference flow model, and it has recently been adopted and applied with success in a quasi - 3-D finite element flow model by WRC (1988). In view of its pedigree, therefore, no further discussion of (6.19) will be pursued here.

Since both equations (6.14) and equation (6.18) require a value for q_z at Z2 for their solution, and the definition of (6.19) includes the values for head in both layers, solutions of (6.14) and (6.18) may be coupled, and readily obtained by iteration.

(b) Upper Boundary = Z3. In this case, the upper boundary is not constant with time, and so the definition of the specific flow equation becomes more difficult. With the integration this time from Z2 to Z3 the basic equation is:

$$\int_{Z2}^{Z3} -\,\mathrm{div}\cdot q\,\partial z = -\frac{\partial}{\partial x}\left[\int_{Z2}^{Z3} q_x\,\partial z\right] + q_x\Big|_{Z3}\cdot\frac{\partial Z3}{\partial x} - q_x\Big|_{Z2}\cdot\frac{\partial Z2}{\partial x} -$$

$$\frac{\partial}{\partial y}\left[\int_{Z2}^{Z3} q_y\,\partial z\right] + q_y\Big|_{Z3}\cdot\frac{\partial Z3}{\partial y} - q_y\Big|_{Z2}\cdot\frac{\partial Z2}{\partial y} - q_z\Big|_{Z3} + q_z\Big|_{Z2} \qquad \ldots\ldots\ldots (6.20)$$

Now the terms in Z2 are dealt with in the same way as they were for case (a) above, because the boundary conditions remain the same. It is the three terms in Z3 that require special treatment. i.e.:

$$q_y\Big|_{Z3}\cdot\frac{\partial Z3}{\partial y} + q_x\Big|_{Z3}\cdot\frac{\partial Z3}{\partial x} - q_z\Big|_{Z3}$$

In this case, Z3 is the water table, where two boundary conditions must be satisfied (Marsily, 1986); namely
(i) the depth - averaged head (h; introduced in equation (6.13)) must equal the elevation of the water table (Z3 in this case), and
(ii) the specific discharge normal to the boundary (equation (6.9)) must equal qr, where qr is the rate of

recharge (L/T).

So the three boundary terms may be written as:

$$q_y\Big|_{Z3} \cdot \frac{\partial h}{\partial y} + q_x\Big|_{Z3} \cdot \frac{\partial h}{\partial x} - q_z\Big|_{Z3} = qr \; . \; . \; . \; . \; . \; (6.21)$$

If it is assumed that all recharge takes place in a vertical direction, then, in a manner similar to the other boundaries, the first two terms in (6.21) disappear and we are left with the simple identity:

$$- q_z\Big|_{Z3} = qr \; . \; . \; . \; . \; . \; (6.22)$$

We can now proceed to write the full equation for this case by analogy with equation (6.18) as:

$$\frac{\partial (q_x m) b}{\partial x} + \frac{\partial (q_y m) b}{\partial y} + q_z\Big|_{Z2} + qr = Sy \frac{\partial h}{\partial t} \; . \; . \; . \; . \; (6.23)$$

Where b = (Z3 - Z2), and Sy is the familiar specific yield, which is the ratio of the volume of water which will drain from the aquifer under gravity to the total aquifer volume (per unit surface area of aquifer, and per unit decline in head; Freeze and Cherry, 1979). This replaces the storativity (see equation (6.12)) for the case where drainage of pore space dominates storage effects (ie under water table conditions).

Conclusion for Lower and Upper Aquifer Layers. For equations (6.14), (6.18) and (6.23), one more step is required before a numerical solution may be sought. This is to express q in terms of Darcy's Law, so that the equation is obtained in terms of the depth - averaged head. Now in simplified form, Darcy's Law may be written:

$$\left.\begin{aligned} q_x &= K \, \partial h/\partial x \\ q_y &= K \, \partial h/\partial y \end{aligned}\right\} \; . \; . \; . \; . \; . \; . \; (6.24)$$

Therefore the identities in (6.24) can be substituted into all three equations to render them in a form suitable for solution, i.e.:

$$-\frac{\partial}{\partial x}\left[\int_{Z1}^{Z2}(K\partial h/\partial x)\partial z\right] - \frac{\partial}{\partial y}\left[\int_{Z1}^{Z2}(K\partial h/\partial y)\partial z\right] - q_z\Big|_{Z2} = S\frac{\partial h}{\partial t} \quad \ldots\ldots (6.25)$$

(equivalent to (6.14))

$$\frac{\partial (K\partial h/\partial x)b}{\partial x} + \frac{\partial (K\partial h/\partial y)b}{\partial y} + q_z\Big|_{Z2} + q_z\Big|_{Z4} = S\frac{\partial h}{\partial t} \quad \ldots (6.26)$$

(equivalent to (6.18))

$$\frac{\partial (K\partial h/\partial x)b}{\partial x} + \frac{\partial (K\partial h/\partial y)b}{\partial y} + q_z\Big|_{Z2} + qr = Sy\frac{\partial h}{\partial t} \quad \ldots (6.27)$$

(equivalent to (6.23))

Some clarification is needed on the definition of b (the saturated thickness). In all cases it equals the top boundary elevation minus the bottom boundary elevation. However in equation (6.27) this definition is complicated by the fact that the elevation of Z3 is not constant with time. Hence (6.27) is intrinsically non-linear.

Since information is available to describe the variation of Chalk permeability with depth where it underlies the gravels (see Chapters 3, 4, and 5, and Appendix B), the integrals of $K\partial h/\partial x$ and $K\partial h/\partial y$ are retained in equation (6.25). While this makes the equation appear more formidable than the other equations, the retention of the integral poses no particular computational problem. The Chalk saturated thickness is merely divided into intervals of known permeability, and numerical integration is performed using the trapezoidal rule.

For the sake of completeness, equations must be given for the cases where (a) the lower aquifer layer emerges from confinement to become a single-layer unconfined aquifer, and (b) where a single layer only underlies the streambed sediment. In this case, the Z2 surface in Figure 6.2 disappears and only Z1, Z3 and Z4 are considered. For case (a), by analogy with (6.27) and (6.25), the following equation can be written:

$$\frac{\partial}{\partial x}(Kb\partial h/\partial x) + \frac{\partial}{\partial y}(Kb\partial h/\partial y) + qr = Sy\frac{\partial h}{\partial t}. \quad . \quad . \quad (6.28)$$

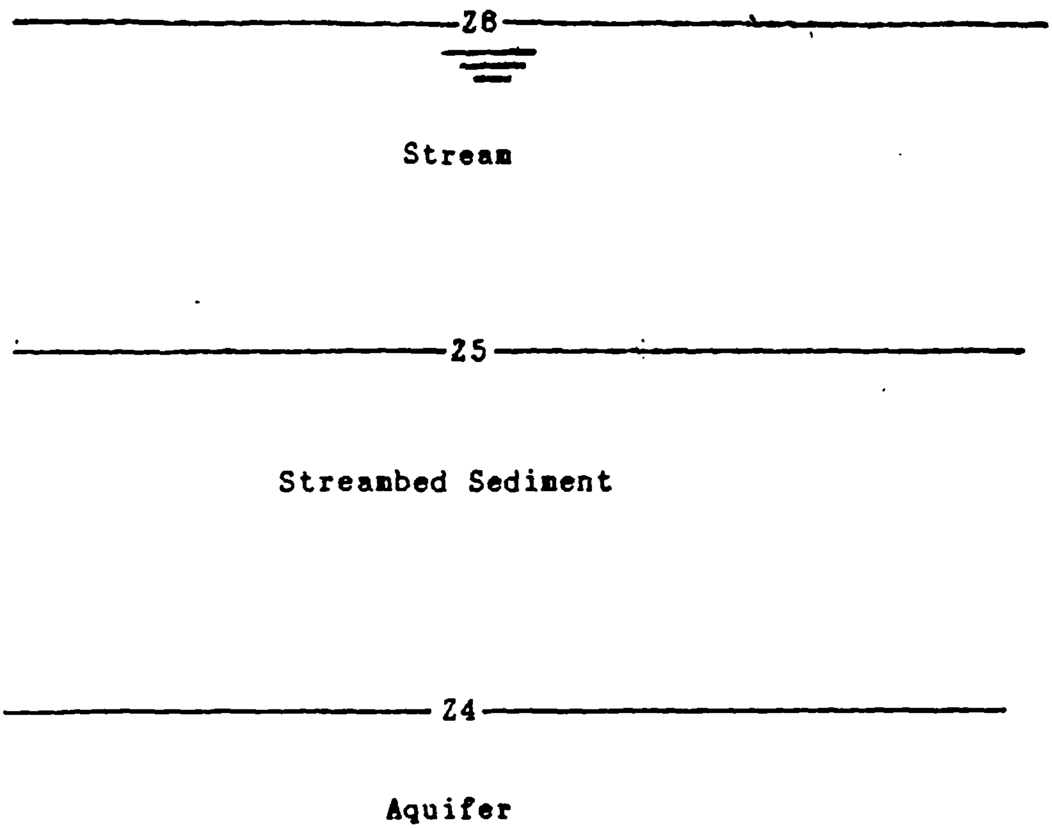
since Z1 is a no - flow boundary. The formulation of (6.28) includes the assumption that K is constant with depth in one - layer areas of the Chalk. The definition of b again introduces a non - linearity, as for equation (6.27) above. For the case of a single layer beneath the streambed sediment (case b), the appropriate expression is:

$$\frac{\partial}{\partial x}(Kb\partial h/\partial x) + \frac{\partial}{\partial y}(Kb\partial h/\partial y) + q_z\Big|_{Z4} = S\frac{\partial h}{\partial t}. \quad . \quad . \quad (6.29)$$

<u>The Streambed Sediment.</u> Derivation of the equation for flow in the streambed sediment differs from the derivations for the lower and upper aquifer layers. This is because the fine - grained nature of the sediment (Section 3.4.4) suggests that a solution in terms of depth - integrated potentials may be inadequate. Vertical flows are likely to dominate horizontal components in this sediment (Chapter Five).

In order to understand the relationship between surface water and groundwater gradients in this system, it is necessary to return to the basic definition of groundwater

Figure 6.3 -- The Streambed Sediment and its Relationship with Stream Stage.



Key: Z4 -- Base of Streambed Sediment (as in Figure 6.1); Z5 -- Surface of the Streambed Sediment; Z6 -- Surface of Water in River Channel.

potential (Φ), viz.:

$$\Phi = z + [p/\rho g] \quad . \; . \; . \; . \; . \; . \; . \quad (6.30)$$

where z = elevation of the point above a datum plane
p = water pressure at this point
and ρ and g are as defined for equation (6.11).

Now at Z5 (Figure 6.3), we can write:

$$\Phi \Big|_{Z5} = Z5 + [p/\rho g] \quad . \; . \; . \; . \; . \; . \; . \; . \quad (6.31)$$

But the second term on the right - hand side is equivalent to the depth of water in the overlying river = (Z6 - Z5).

Thus

$$\Phi \Big|_{Z5} = Z5 + (Z6 - Z5)$$

ie:

$$\Phi \Big|_{Z5} = Z6 \quad . \; . \; . \; . \; . \; . \; . \; . \; (6.32)$$

So from this equation, it can be deduced that the gradient of the groundwater potential ($\partial\Phi/\partial x, \partial\Phi/\partial y$) at the surface of the streambed sediment will be equivalent to $\partial Z6/\partial x$ and $\partial Z6/\partial y$, which are both negligible for flat lying silt. Whatever the values of $\partial\Phi/\partial x$ and $\partial\Phi/\partial y$ evaluated at Z4 turn out to be, the upper boundary effects, coupled with the refraction of groundwater flow lines through the low permeability streambed sediment, are sufficient to ensure that horizontal components of groundwater flow in the streambed sediment will be very small. They are here assumed to be negligible.

With these considerations in mind, let us return to a basic expansion of the mass continuity equation (6.1):

$$- \text{div} \; . \; q = \frac{\partial(K\partial\Phi/\partial x)}{\partial x} + \frac{\partial(K\partial\Phi/\partial y)}{\partial y} + \frac{\partial(K\partial\Phi/\partial z)}{\partial z} \quad . \; . \; . \; . \; (6.33)$$

From the assumption that / x and / y are constant and negligible in the streambed sediment, equation (6.33) reduces to:

$$- \text{div} \; . \; q = \frac{\partial(K\partial\Phi/\partial z)}{\partial z} \quad . \; . \; . \; . \; (6.34)$$

which for steady - state conditions becomes:

$$- \text{div} \; . \; q = \frac{\partial(K\partial\Phi/\partial z)}{\partial z} = 0. \; . \; . \; . \; . \; (6.35)$$

and for transient conditions:

$$- \text{div} \; . \; q = \frac{\partial(K\partial\Phi/\partial z)}{\partial z} = S \frac{\partial\Phi}{\partial t} \; . \; . \; . \; (6.36)$$

Solution of (6.35) or (6.36) will yield values for q_Z at any point in the domain bounded by Z4 and Z5, subject to the boundary conditions:

$$\Phi \Big|_{Z5} = Z6$$

and

$$\Phi \Big|_{Z4} = h(Z4)$$

where

$$h(Z4) = (1/b) \int_{Za}^{Z4} \Phi \, \partial z$$

and 'a' may be either 1 or 2. The value of h(Z4) is found by solution of either equation (6.26) or (6.29). Since solution of these equations is dependent on knowledge of q_Z evaluated at Z4, they may be solved simultaneously with the other equations in this term (ie (6.35) and (6.36)) by iteration.

Conclusions. Equations have now been developed for all settings in the stream - aquifer system. Figure 6.4 summarises these equations in a simplified manner. The need to solve non-linear terms in those equations describing phreatic conditions, and the attractions of using a coupled solution to the equations for superposed layers, suggest that an iterative solution to these equations is desirable.

6.2.2 -- Finite Difference Representations of the Specific Flow Equations.

6.2.2.1 -- Rationale for Selection of Finite Difference Method. Finite difference solutions to the equations derived in Section 6.2.1 have been chosen in preference to other numerical methods because of their simplicity and

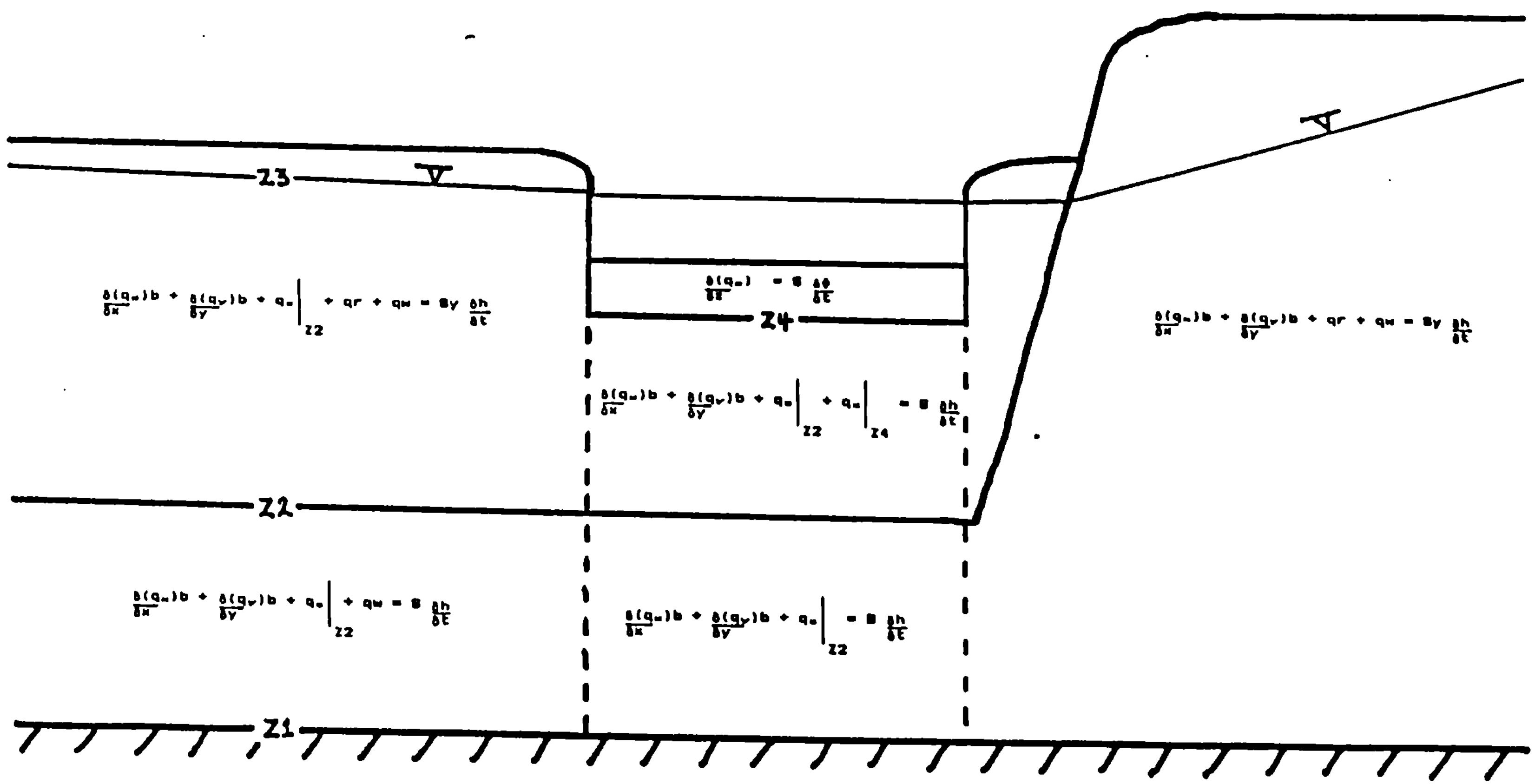


Figure 6.4 -- A Summary of the Groundwater Flow Model.

because of the ease with which they can be used to iteratively solve coupled systems of equations. In those finite difference methods which involve iteration, it is convenient to write computer programmes in such a way that solution of non-linear terms is accomplished by the same iterative cycle that solves the system of finite difference equations.

All finite difference methods involve 'discretising' the model domain into a number of regularly shaped cells or blocks, which join together to form a grid. Each cell in the grid is assigned certain values of the aquifer parameters according to field data or other estimates. These data are entered onto the model grid by laying a transparent copy of the grid over maps of field observations. Specific examples of this process are discussed in Chapter 7.

There are several iterative finite difference methods, most notably the various alternating direction implicit (ADI) methods, and the family of techniques which includes (in order of increasing refinement) Jacobi Iteration, Gauss-Seidel Iteration and Successive Over - Relaxation (Mercer and Faust, 1981, pp.29 - 30; Wang and Anderson, 1982, pp. 24 - 31; Bear and Verruijt, 1987, pp.229 - 233). For a comparative discussion of the merits of these various techniques, the reader is referred to Rushton and Redshaw (1979, pp. 162 - 185). Line Successive Over-Relaxation (LSOR) has been used in the US-FLOW module of UNCLESAM, since it is simple to understand and programme, and because it is unconditionally stable irrespective of the size of timestep used.

The implementation of LSOR requires that the equations of flow are re-written in finite difference form, and then arranged so that the head value at a node (I,J) for a particular timestep is placed on the LHS of the equation and all other terms on the RHS (thus giving a Gauss-

Seidel Equation for every node). When this has been accomplished, a nested DO Loop in a FORTRAN code can move through a rectangular grid node - by - node, calculating the value of head at each node in terms of its latest value at four surrounding nodes. The general equation on which the computer algorithm is based can be written (in FORTRAN algebraic notation):

HEAD2(I,J) = HEAD1(I,J) + RLXFCT * RESID . . . . (6.37)

where RESID = HEAD2(I,J) - HEAD1(I,J)

HEAD1(I,J) = head value at node (I,J) from the previous iteration

HEAD2(I,J) = head value at node (I,J) for the current iteration

RLXFCT = Relaxation Factor (with $1 < \text{RLXFCT} < 2$)

Now suppose the basic Gauss - Seidel equation for head at a node (I,J) is:

HEAD2(I,J) = (HEAD2(I,J-1) + HEAD2(I-1, J) + HEAD1(I, J+1) + HEAD1(I+1, J)) / 4 . . . . (6.38)

Then the LSOR equation will be solved by first calculating (6.38), then calculating RESID, then, finally, updating the latest value for HEAD2(I,J) using (6.37). One iteration is completed every time HEAD2(I,J) has been calculated for every point in the domain. Successive iterations are performed until such time as the value of RESID at every node is less than (or equal to) a prescribed tolerance (usually 0.0001). At this point, the solution is said to have converged for the timestep under consideration.

Narasimhan (1982) has outlined some of the pitfalls of the LSOR method, the most important of which is the dependence of convergence on the value of the relaxation factor. While an optimal value of this parameter can increase the speed at which convergence is attained, selection of a suitable value is extremely problem - dependent, and, if too high a value is assigned for a given problem, then the solution may fail to converge. Furthermore, if too large a value for the time step is chosen, then this convergence problem may be exacerbated. The safest course in case of doubt is to set the relaxation factor equal to 1, and thereby reduce the problem to a Gauss - Seidel formulation, which is far more robust than LSOR, though less rapid.

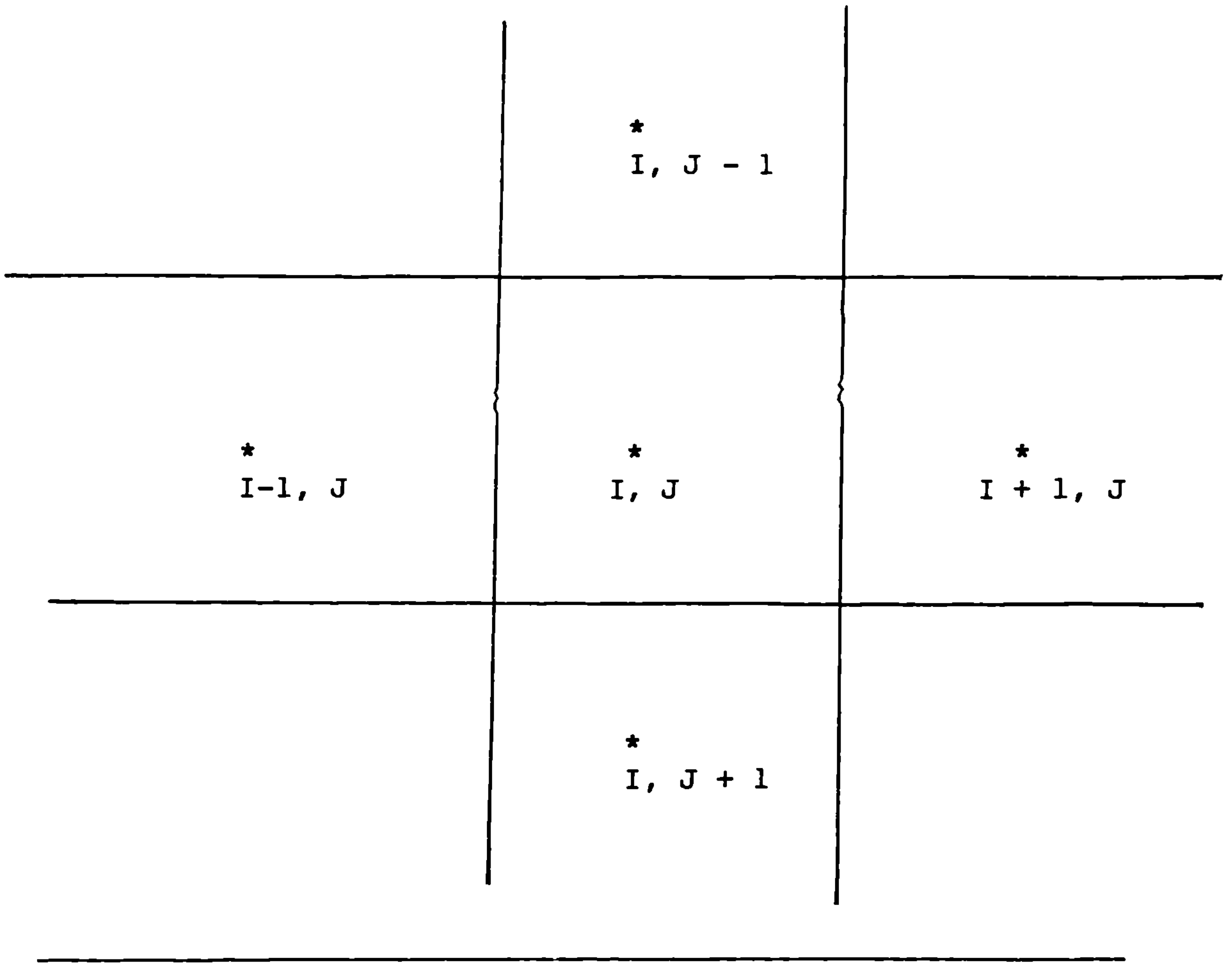
From this brief review of the numerical method used in US-FLOW it is clear that the various equations derived in Section 6.2.1 above must now be rendered into a form where they may yield values equivalent to HEAD2 in equation (6.37). A worked example of this process is given below.

6.2.2.2 -- Finite Difference Representations of the Groundwater Flow Equations.

To render the flow equations (6.25 - 6.29, 6.36) into their finite difference eqivalents, implicit finite difference approximations to the derivatives ($\partial h/\partial x$, $\partial h/\partial y$ etc) are substituted into them. Then the equations are re-arranged into the Gauss - Seidel form (cf equation 6.38). The derivation of the finite difference equivalent of equation (6.26) will be given in detail to illustrate this process. The same process was used to derive the finite difference equivalents of all the other flow equations.

The finite difference formulation adopted here assumes a block - centred grid, with the nodes placed in the centre of grid cells (Figure 6.5). An implicit representation (ie the discretisation of time uses a backward - differencing approach) is used in preference to an explicit formulation to avoid any stability restrictions (cf Rushton and Redshaw, 1979). For simplicity, equation (6.26) is re-written as:

Figure 6.5 -- Finite Difference Block - Centred Grid Lettering Convention.



$$\frac{\partial(T\partial h/\partial x)}{\partial x} + \frac{\partial(T\partial h/\partial y)}{\partial y} + q_{*}\bigg|_{Z2} + q_{*}\bigg|_{Z4} = S\,\frac{\partial h}{\partial t} \quad . . . (6.39)$$

with $T = Kb$ = Transmissivity.

b = saturated thickness

Now in the finite difference method, we are concerned with representing the derivatives in (6.39) by approximations defined according to the grid convention in Figure 6.5. The finite - difference version of (6.39) is given below (equation 6.40).

$$\frac{\dfrac{2T_{i-1/2}(Ht_{i-1,j}^{n+1} - Ht_{i,j}^{n+1})}{(dx_i + dx_{i-1})} - \dfrac{2T_{i+1/2}(Ht_{i,j}^{n+1} - Ht_{i+1,j}^{n+1})}{(dx_i + dx_{i+1})}}{dx_i} +$$

$$\frac{\dfrac{2T_{j-1/2}(Ht_{i,j-1}^{n+1} - Ht_{i,j}^{n+1})}{(dy_j + dy_{j-1})} - \dfrac{2T_{j+1/2}(Ht_{i,j}^{n+1} - Ht_{i,j+1}^{n+1}}{(dy_j + dy_{j+1})}}{dy_j} +$$

$$(Ht_{i,j}^{n+1} - Hb_{i,j}^{n+1}).B_{i,j} + q_{sa} = St_{i,j}(Ht_{i,j}^{n+1} - Ht_{i,j}^{n}) / dt$$

. . . . (6.40)

dx_i = Spatial step in x - direction

dy_j = Spatial step in y - direction

$St_{i,j}$ = Storage parameter for upper layer in a node

$Ht_{i,j}^{n+1}$ = Head in upper layer of a node (at current time level)

$Ht_{i,j}^{n}$ = Previous head in upper layer of a node (ie head value at last timestep)

$Hb_{i,j}$ = Head in lower layer of a node

$T_{i,j}$ = Transmissivity in the upper layer

$T_{i-1/2}$ = dx - weighted harmonic mean of $T_{i,j}$ and $T_{i-1,j}$

$T_{i+1/2}$ = dx - weighted harmonic mean of $T_{i,j}$ and $T_{i+1,j}$

$T_{j-1/2}$ = dy - weighted harmonic mean of $T_{i,j}$ and $T_{i,j-1}$

$T_{j+1/2}$ = dy - weighted harmonic mean of $T_{i,j}$ and $T_{i,j+1}$

$B_{i,j}$ = Harmonic mean of vertical hydraulic conductivities for upper and lower layers, weighted by the thicknesses of these layers

t = time

dt = timestep

qsa = stream - aquifer exchange flux

Now when (6.40) is re-arranged in $H_{t\,i,j}^{n}$ (*ie in* Gauss - Seidel form), the resulting equation is:

$$H_{t\,i,j}^{n+1} = (H_{t\,i-1,j}^{n+1} * (-A) + H_{t\,i+1,j}^{n+1} * (-C) + H_{t\,i,j-1}^{n+1} * (-D) + H_{t\,i,j+1}^{n+1} * (-E) - (qsa + Hb_{i,j} * (B_{i,j} / b_m)) * dx_i * dy_j + Ht_{i,j}^{n} * (-F)) / (-A - C - D - E - F - (B_{i,j} / b_m) * dx_i * dy_j) \quad \ldots\ldots\ldots (6.41)$$

Where:

$A = (T_{i-1/2} * dy_j) / ((dx_i + dx_{i-1}) / 2)$

$C = (T_{i+1/2} * dy_j) / ((dx_i + dx_{i+1}) / 2)$

$D = (T_{j-1/2} * dx_i) / ((dy_j + dy_{j-1}) / 2)$

$E = (T_{j+1/2} * dx_i) / ((dy_j + dy_{j+1}) / 2)$

$F = (St_{i,j} / dt) * dx_i * dy_j$

b_m = mean of thicknesses of upper and lower layers

This equation is used to obtain the first estimate of $H_{t\,i,j}$ prior to over - relaxation according to equation (6.37). The finite difference equivalents for all the remaining equations were derived using the technique shown above.

6.2.3 -- Development and Testing of the Flow Module.

6.2.3.1 -- Structure of the Computer Programme. After a considerable period of experimentation, testing and refinement, the structure of the FORTRAN 77 code for US-FLOW was finalised. Six subroutines survived the refinement period, out of an original complement of twelve (see the code listings in Appendix E). The links between the routines are shown in the hierarchical flow diagram (Figure 6.6), and brief descriptions of the routines are given in Table 6.1.

The execution of the US-FLOW code is controlled by an array which stores a node - type identifier for every node in the simulation domain. Table 6.2 summarises the assignments made, and with reference to these, the simple modular structure of the code can be readily interpreted.

The manner in which US-FLOW deals with the interfaces between two - layer cells and adjacent one - layer cells is worthy of remark. The method developed here was adapted from a technique developed by Rovey (1975) for interfacing adjacent 2-D and 3-D flow models. To maintain mass balance, it is necessary to ensure a partitioning of the total flow from a one - layer cell into the upper and lower layers of an adjacent two - layer cell. This is accomplished in the code by assigning 'apparent' values of transmissivity, thickness and head to imaginary upper and lower layers in the one - layer cell, based on the elevation of the upper / lower layer interface in the two-layer cell and the basic hydraulic properties of the one-layer cell (Figure 6.7). Thus in the equations in the TWOLYR and ONELYR subroutines, various coefficients and imaginary heads, transmissivities and thicknesses (ALFA, ALFB, ALFC, TTRAPP, BTRAPP etc) are included to make this interfacing possible. Although this makes the subroutines rather more complicated than they would be if they contained ordinary Gauss - Seidel equations, the increase

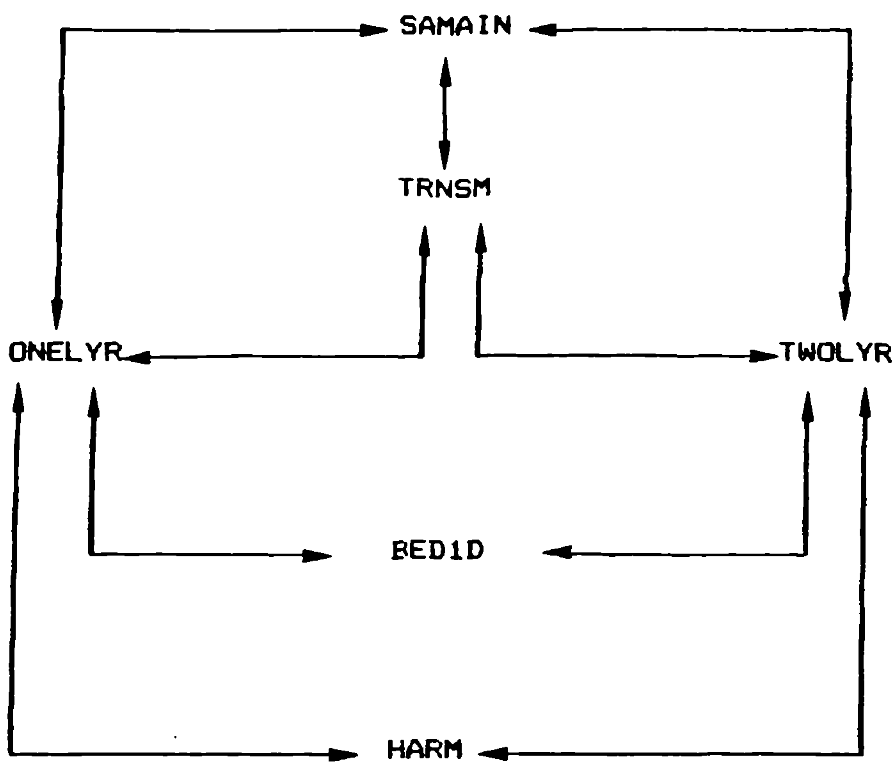
Table 6.1 Functions of Routines in the US-FLOW Code.

Routine.	Function.
SAMAIN	Main programme; reads and organises all data, and distributes it to various subroutines via common blocks. Calls TRNSM to calculate original transmissivity distribution, and the main flow subroutines (ONELYR and TWOLYR) to solve for head at each node. Prints results to files.
TRNSM	Calculates transmissivity values for upper and lower aquifer layers at all nodes. Called by the flow routines to update transmissivity at 'unconfined' nodes during iteration.
ONELYR	Simulates flow in nodes which represent only one aquifer layer, whether this be unconfined, or confined beneath the base of the streambed sediment. Calculates required FD coefficients, and allows for appropriate boundary conditions. The LSOR equations for single aquifer layers appear in this routine. Calls BED1D, HARM and TRNSM.
TWOLYR	Simulates flow where there are two aquifer layers. The upper layer may be unconfined or confined beneath the streambed sediment. Again, appropriate boundary conditions are considered when FD coefficients are evaluated. The LSOR equations for the two aquifer layers appear in this routine. Calls BED1D, HARM and TRNSM.
BED1D	Calculates steady - state or transient flow in the streambed sediment using the 1-D LSOR equations, Returns a value for the stream-aquifer exchange flux (QSA(I,J)) to the calling routine.
HARM	A Double Precision Function which calculates the weighted harmonic mean of two parameters with their respective weights. Mainly used in the calculation of internodal transmissivities in ONELYR and TWOLYR.

in modelling power afforded by this refinement is well worth the slight loss in clarity.

6.2.3.2 -- Testing of the Flow Code. All of the subroutines in US-FLOW were tested independently of each

Figure 6.6 -- Routine Hierarchy in US-FLOW



other, by creating separate programmes, which were run using test data sets for problems with analytical solutions. Finally, the full programme was also tested against a simple analytical solution. Output for the ONELYR, TWOLYR, BED1D and full US-FLOW test problems are given graphically in Figures 6.9 through 6.15. The analytical solutions used were:

(i) The Theis solution for drawdown around a well in a confined aquifer, which is described in numerous texts (eg Freeze and Cherry, 1979; Todd, 1980). This solution was used to test ONELYR and TWOLYR.

(ii) The Hantush (1967) solution for drawdown in two infinite leaky aquifers of equal diffusivity (T/S), where a well is pumping in the lower aquifer only. This solution was used to test the full US-FLOW code only.

Figure 6.7 -- Interfacing of One - Layer and Two - Layer Model Areas.

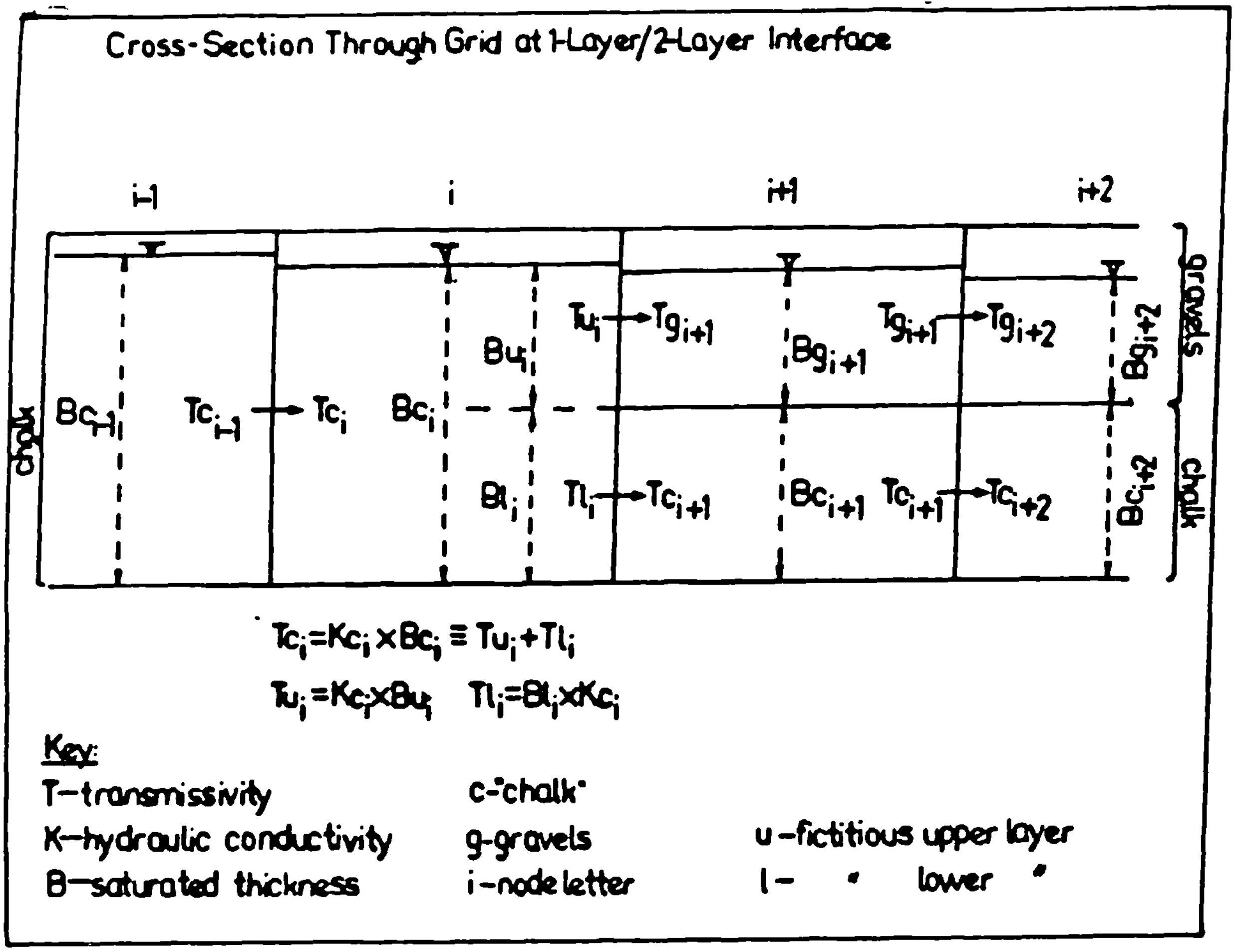


Table 6.2 -- Assignments of NODTYP Values Used to Control Execution in US-FLOW

NODTYP Value	Type of Node Simulated
1	One unconfined aquifer layer
2	Two aquifer layers, where the upper is unconfined
3	Two aquifer layers, where upper is confined beneath the streambed sed.
4	One aquifer layer confined beneath streambed sediment
5	Fixed - head boundary node
6	Known - flow boundary node; flow in x - direction only
7	Known - flow boundary node; flow in y - direction only
8	No - flow boundary node

(iii) A simple analytical solution to the one-dimensional steady state flow problem illustrated in Figure 6.8, which has been described by Rushton and Redshaw (1979, pp. 28 - 29). The geometry sketched in Figure 6.8 is such that a bounded aquifer abutting a fully penetrating stream (fixed - head boundary) is subject to an increment of recharge q. The equation describing this situation may be written:

$$T \frac{\partial^2 h}{\partial x^2} = -q \quad . \; . \; . \; . \; . \; (6.42)$$

where T = transmissivity (L^2/T)

h = groundwater head (L)

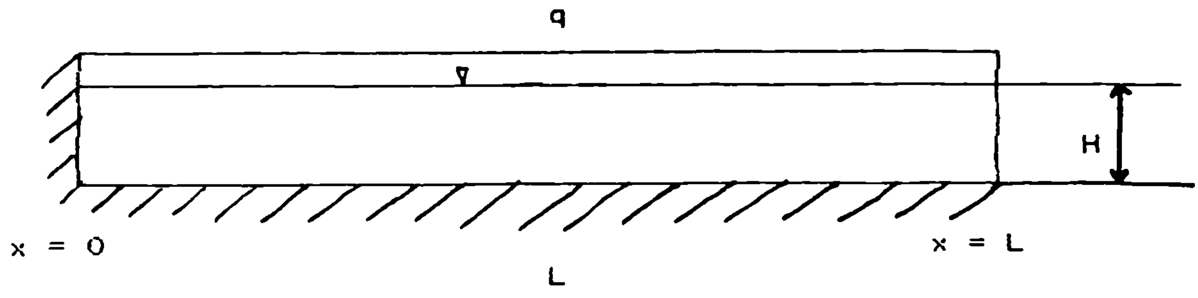
x = spatial co-ordinate (L)

q = recharge (L/T)

Integrating this equation twice yields:

$$h = (-0.5\, q\, x^2 / T) + Ax + B \quad . \; . \; . \; . \; (6.43)$$

Figure 6.8 -- Steady State Flow Problem.



where A and B are constants of integration. Employing the following boundary conditions:

at $x = 0$, $\partial h/\partial x = 0$, and

at $x = L$, $h = H$

A and B can be evaluated. Substituting these values into (6.43) results in this final expression for the solution of (6.42) in terms of the state variable h :

$$h = 0.5\, q\, (L^2 - x^2) / T + H \quad . \; . \; . \; . \quad (6.44)$$

This solution was used to test ONELYR and TWOLYR.

(iv) A simple solution for one - dimensional steady state flow in a homogeneous aquifer between two fixed heads, in which case the 'analytical solution' is simply a straight line (Todd, 1980). This solution was used to test BED1D only.

Slight problems arose in comparing numerical and analytical results for the two transient (Theis and Hantush) flow problems, since the mathematical formulations for the analytical solutions in both cases assume that the aquifer is infinite in lateral extent, whereas the numerical model requires boundary conditions for solution. Hence the time - drawdown curves for the transient ONELYR and TWOLYR tests, and for the full US-FLOW tests show a divergence of numerical and analytical results after a certain time due to the influence of boundary conditions. In all cases

Figure 6.9 -- Comparison of Analytical and Numerical Solutions to A Steady - State Test Problem, Routine ONELYR

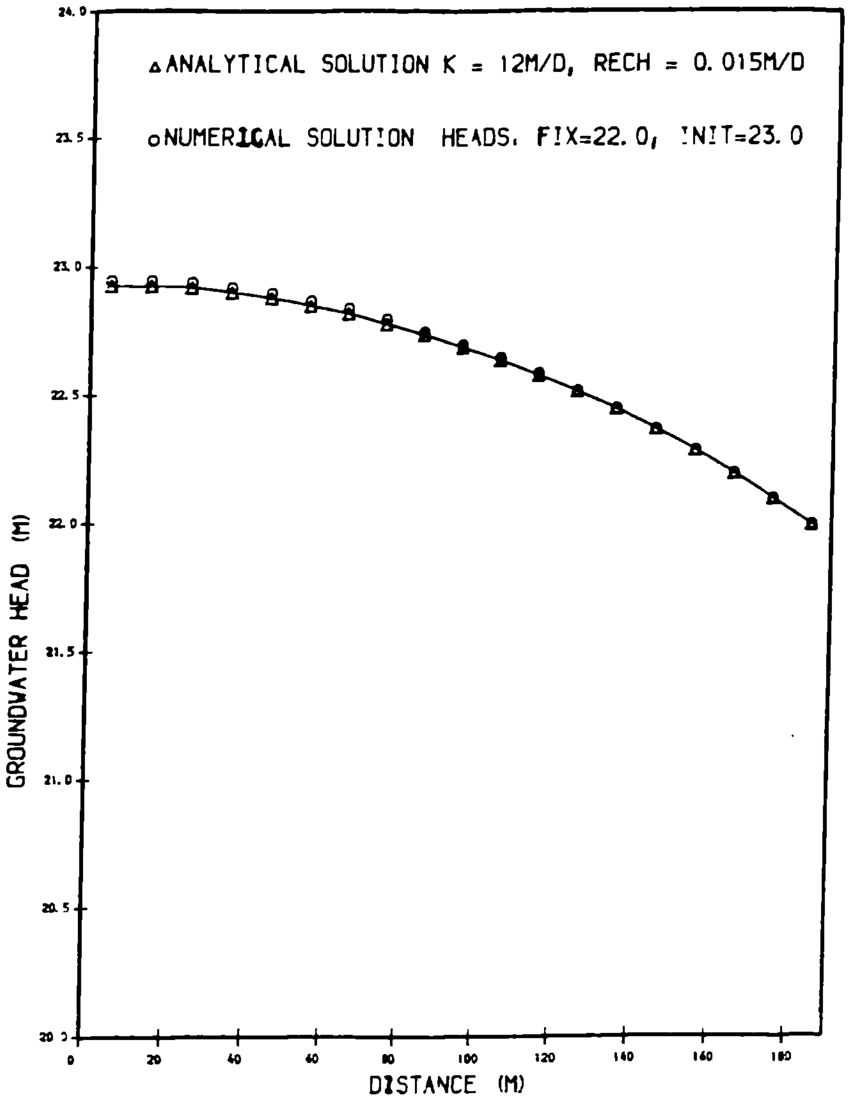


Figure 6.10 -- Comparison of Numerical Model Results with Image Well Analysis Results, Routine ONELYR

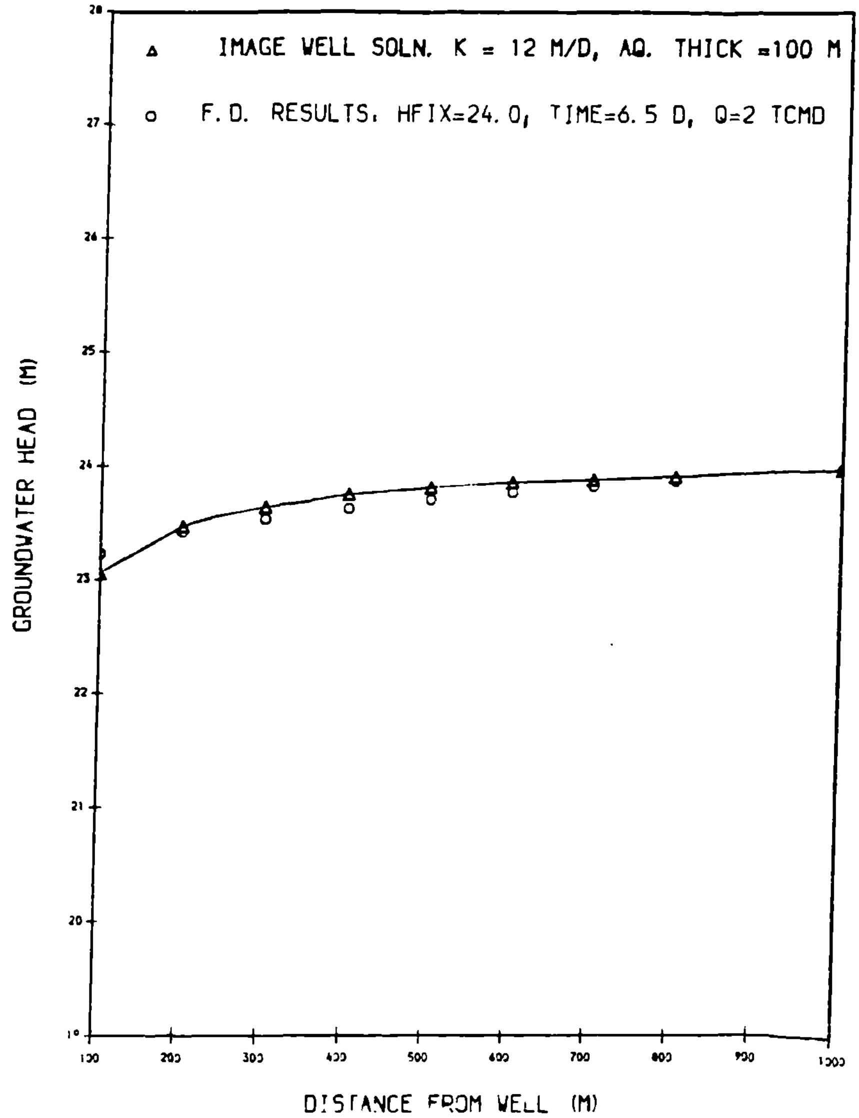


Figure 6.11 -- Numerical Model Approximation to a Theis problem for Routine ONELYR

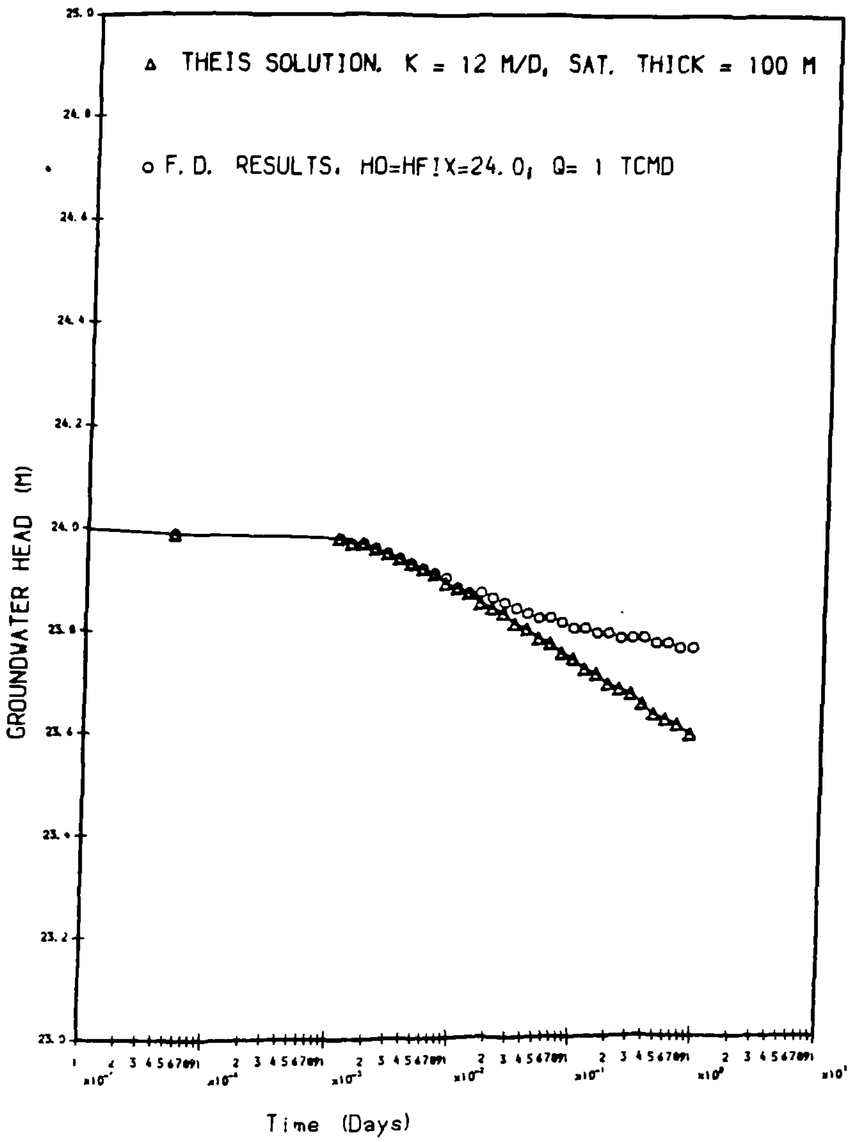


Figure 6.12 -- Comparison of Analytical and Numerical Solutions to A Steady - State Test Problem, Routine TWOLYR

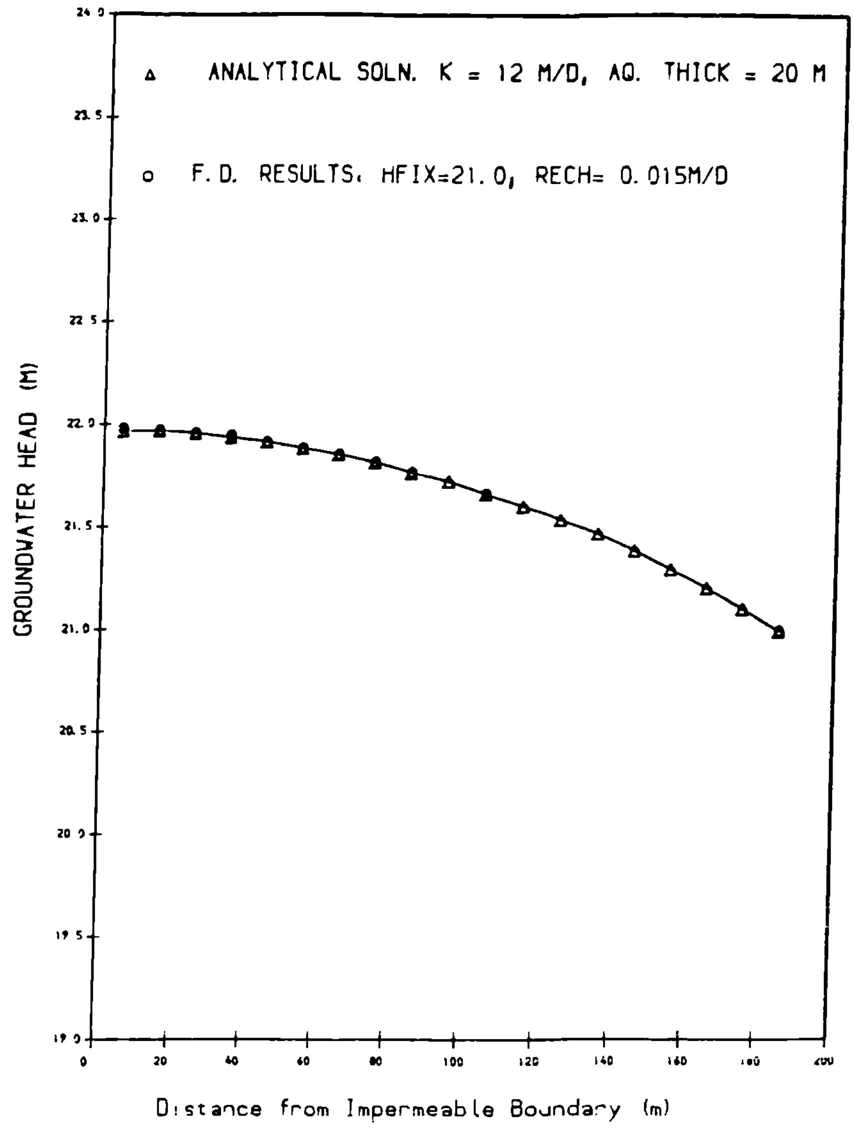


Figure 6.13 -- Numerical Model Approximation to a Theis problem for Routine TWOLYR

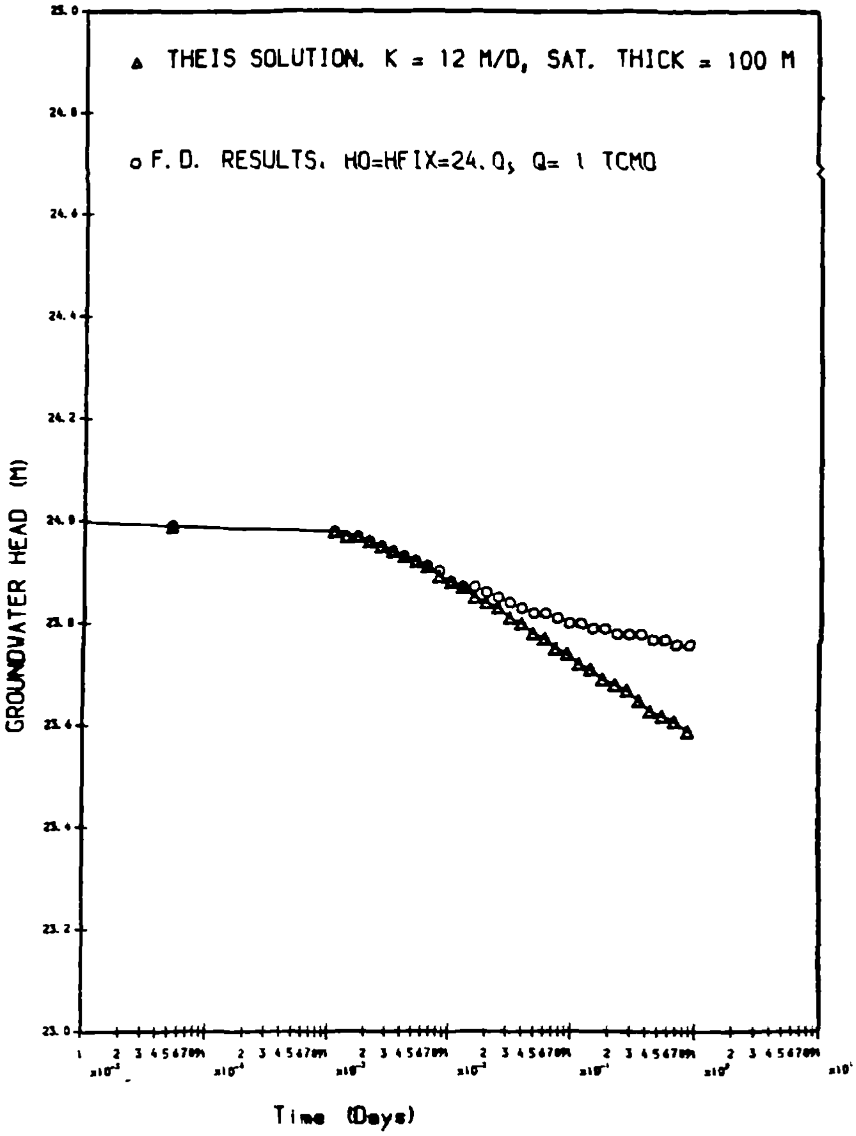
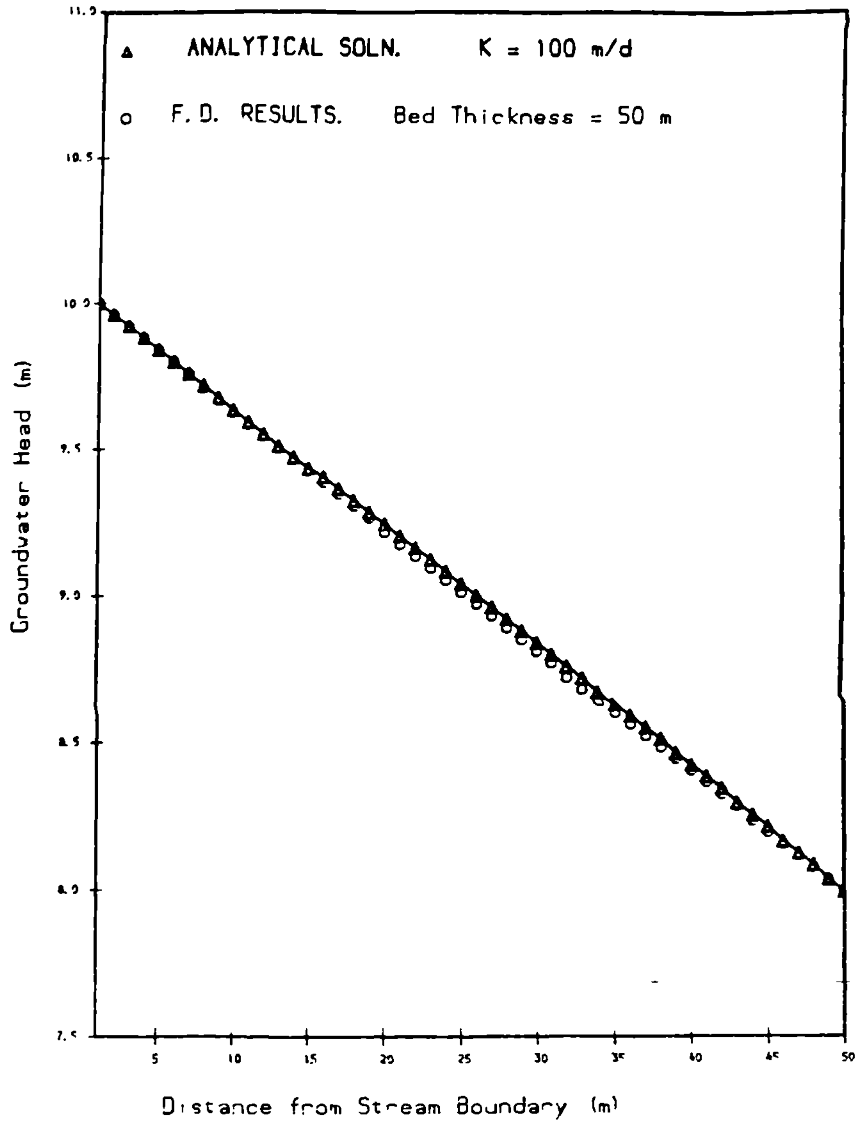


Figure 6.14 -- Comparison of Analytical and Numerical Solutions to a Simple Steady - State Test Problem, Routine BED1D.



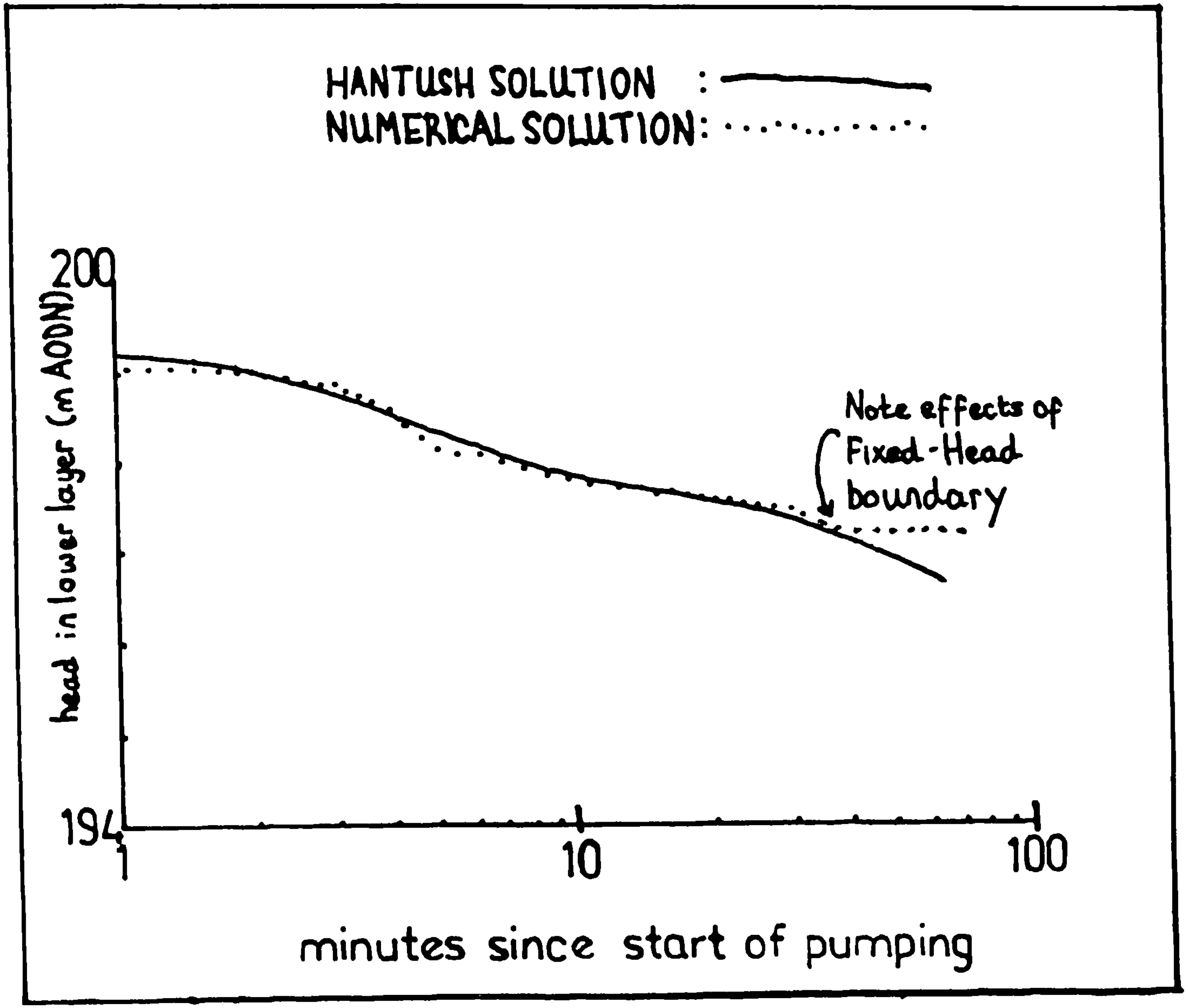


Figure 6.15 -- Two - Layered Aquifer Problem: Comparison of US-FLOW Output with Analytical Solution of Hantush (1967).

the finite difference results are higher than the analytical results after divergence because the fixed head boundaries 'buoy - up' the head distribution in the aquifer. To confirm this interpretation, image well analysis was used to construct distance - drawdown curves for each of the test problems, so that an analytical solution for the boundary effects at any one time was obtained. The results of one such analysis are given in Figure 6.10. The agreement between the numerical results and the image well analysis curves is excellent, confirming that the divergence effects are due to the boundary effects identified above.

After all of these tests had been successfully concluded, a few test data sets were constructed to make sure the integrated code would run in the simulation mode in which it was to be used. For the tests conducted, no analytical solutions are available, and thus interpretation of the results had to be based upon water balance calculations (for steady state solutions) and on mental comparison of the results with what would be intuitively expected. Final errors (due to inadequate formulation for one - layer / two - layer interfaces) were removed during this exercise, and the full US-FLOW code was finally ready to accept 'real world' data. The results of applying US-FLOW to Middle Thames field data are given in Chapter 7.

6.3 -- THE SOLUTE TRANSPORT COMPONENT OF UNCLESAM.

6.3.1 -- Introduction.

Various solute transport processes of importance in stream - aquifer systems were identified in Chapters 3, 4 and 5, where the geochemical properties of hydrogeological units in the Thames Basin were described and conceptualised. In this section, the mathematical representation of these processes is discussed. Further discussion of solute transport processes is therefore required here in order to facilitate mathematical description. However, the discussions in this section are of a generalised nature, and are thus complementary to the site - specific information already presented.

6.3.2 -- Mathematical Formulations for Solute Transport.

The equation most commonly used to describe solute transport in saturated porous media may be written, for a simple one - dimensional case, as:

$$\frac{\partial[(D_L/Rd)(\partial C/\partial x)]}{\partial x} - \frac{V}{Rd}\frac{\partial C}{\partial x} \pm CsQ = \frac{\partial C}{\partial t}$$

(Dispersion) - (Advection) ± (Production or Decay) = (Temporal Change in Concentration)

. . . . (6.45)

where

V = average linear groundwater velocity

D_L = coefficient of longitudinal hydrodynamic dispersion

x = space dimension

t = time

Rd = retardation factor

C = concentration of solute

CsQ = source or sink function having a concentration Cs and a flux rate Q.

As will be seen below, a direct solution of equation (6.45) is not sought in the present model. For this reason a formal derivation is not included in the present discussion (derivations may be found in many standard texts, eg Freeze and Cherry, 1979). Equation (6.45) is quoted here simply because it provides a suitable conversation piece for the discussion of the mathematical treatment of solute transport processes which follows.

As shown in equation (6.45), two major processes govern the migration of solutes in groundwater, namely advection and dispersion. Advection is defined as the transport of solutes by the bulk motion of flowing groundwater, so that transport occurs "at the same speed as the average linear velocity (V) of groundwater" (Anderson, 1984), where

$$V = K\ (\partial h\ /\partial x)\ /\ n\ .\ .\ .\ .\ (6.46)$$

and

K = hydraulic conductivity
n = mean effective porosity
$(\partial h\ /\partial x)$ = head gradient

This interstitial velocity is, in fact, the specific discharge (qx) divided by the mean porosity of the porous medium. This division is necessary because the true velocity of groundwater in the pore space will be somewhat higher than the specific discharge (which assumes flow across the entire cross sectional area of a unit volume of the medium).

Dispersion, or 'hydrodynamic dispersion', can be defined as the spreading of a stream or discrete volume of solutes in excess of the displacement attributable to advection alone. Two processes are generally held to account for dispersion; mechanical mixing and molecular diffusion. At high groundwater velocities, mechanical mixing is the dominant component of dispersion, while molecular diffusion is most important at low velocities. Dispersion is also sometimes differentiated into micro- and macro-scopic dispersion (Anderson, 1984). Microscopic dispersion processes include molecular diffusion, and interstitial mixing. Interstitial mixing is caused by deviations of actual pore velocities from the average linear velocity (V) and the small scale diversion of flow paths around the grains which comprise the porous medium. Macroscopic dispersion, on the other hand, is caused by large scale heterogeneities in the subsurface. These may, for example, take the form of lenses of high permeability material embedded in a matrix of sediments of lower permeability. In such a case, small zones of rapid advection associated with the high permeability lenses can lead to considerable dispersion from the flow path anticipated from the average linear velocity distribution. In this sense, macrodispersion may be viewed as a description of how advection (and microdispersion) deviates from the mean on the scale of measurement or the scale of modelling. The longitudinal dispersion coefficient in (6.45) is a term which includes both mechanical mixing and molecular diffusion thus:

$$D_L = \alpha_l V + D_D \quad . \; . \; . \; . \; . \; . \; . \; (6.47)$$

where α_l = longitudinal dispersivity, which is taken to be a 'characteristic length' of the porous medium.

$D_D = D_o \tau / n$ = coefficient of molecular diffusion in the porous medium.

D_o = diffusion coefficient in free solution

τ = tortuosity of the porous medium (generally ≈ 0.7), which is an approximate expression of pore geometry

n = porosity

V = average linear velocity

Discussions of the various components of the dispersion coefficient may be found in many groundwater texts (eg Freeze and Cherry, 1979; Bear, 1979). Gillham and Cherry (1982) and Domenico (1977) give detailed discussions of molecular diffusion in porous media. Therefore no detailed discussion of these components is given here. However, it is worth noting that, because (6.45) is one - dimensional, only longitudinal dispersion (ie dispersion in the direction of flow) has been mentioned so far, whereas dispersion in directions normal to the direction of flow also occurs in nature. In two - dimensional modelling, this is referred to as 'transverse dispersion' and it is described mathematically as:

$$D_T = \alpha_t V + D_D \quad . \; . \; . \; . \; . \; . \; . \; . \; (6.48)$$

where α_t = transverse dispersivity, which is taken to be a 'characteristic length' of the porous medium.

Further reference to the mathematical treatment of dispersion is made in Section 6.3.4.4 below.

The "Production or Decay" term in equation (6.45) is a catch-all expression which covers the panoply of processes which add solutes to, or remove them from, the main body of fluid. These processes include dissolution / precipitation, oxidation / reduction, decay of one species leading to formation of another (by both radioactive or biological pathways), complexation, hydrolysis and acid / base reactions.

The "Retardation Factor" (Rd) in (6.45) is a simplified representative of a family of expressions of varying complexity which can represent adsorption / desorption processes which occur in the saturated zone. Where these processes may be regarded as instantaneous, linear and entirely reversible, the representation reduces to the division of the average linear velocity and the dispersion coefficient by a simple coefficient (Rd), as shown in equation (6.45). Rd is defined as:

$$Rd = 1 + (\rho_b / n).K_d \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; (6.49)$$

where ρ_b = bulk dry mass density of the porous medium which is equal to $\rho_s(1 - n)$, where ρ_s is the particle mass density (approximately 2.65 gm/cm^3 for most mineral soils)

K_d = distribution coefficient for a given solute on the solid grains of the porous medium under investigation.

For zero sorption, Rd equals 1, otherwise it is greater than 1.

If sorption is not instantaneous, linear, or entirely reversible, the retardation factor approach ceases to be valid, and a more detailed mathematical representation is called for (Hounslow, 1983). In lieu of any evidence to the contrary, however, it is assumed that a simple retardation factor is an adequate description of all sorption processes modelled in this project.

6.3.3 -- Solution Techniques for Solute Transport.

Direct solution of (6.45) by a finite difference or finite element scheme is hindered by a phenomenon known as "numerical dispersion". This arises from the fact that the error in the FD or FE approximation of the advection term is of the same order of magnitude as the absolute value of the dispersion term, leading to a swamping of actual dispersion by false numerical "dispersion" (Marsily, 1986, p. 388).

Two alternative approaches to the advection - dispersion problem which reduce or eliminate numerical dispersion have been proposed and widely used. The first to be devised was the Method of Characteristics (MOC; Konikow and Bredehoeft, 1978). In the MOC, the advection term in equation (6.45) is solved by moving particles (which represent solute concentrations) according to the local velocity vectors of the groundwater flow field, expressed in terms of co-ordinates of the finite difference grid used to solve the flow equation. From the particle distributions thus obtained, concentrations are calculated at all positions in the flow domain. Then a second finite difference grid, associated with the solute concentration distribution, is used to solve the dispersion term in (6.45). However, despite mathematical simplicity, the MOC is extremely awkward to programme and requires great amounts of computer time and storage. Because of these shortcomings, a method known variously as the Discrete Parcel Random - Walk Method (DPRW; Marsily, 1986, p. 393) or as the Particle - Tracking Method (PTM; Bear and Verruijt, 1987) has been developed. The main sources of reference for this technique are the detailed treatises of Ahlstrom et al (1977) and Prickett et al (1981). A recent application of this method to a field problem has been described by Sauty et al (1989). The advantages and disadvantages of the PTM are discussed by Prickett et al (1981) and by Marsily (1986). Table 6.3 summarises these.

The essentials of the PTM are as follows. With a head distribution obtained from solution of the groundwater flow equations, the average interstitial velocity of the groundwater is obtained from Darcy's Law and the effective porosity of the aquifer using equation (6.46). Once values for V have been obtained for the boundaries of all the quadrilateral finite difference cells in the solution grid, an interpolation scheme can be used to obtain an accurate estimate of velocity at any point in the solution domain whenever this is required.

Particles representing a specific mass of solute (not a concentration as in the MOC) are routed through the velocity field along the flowlines, thereby solving for the advective component of transport. At the end of the calculation of advective displacement for a given timestep, the position of each particle is modified to allow for the effects of dispersion. It is at this stage that the PTM differs from the MOC. In the PTM the effect of dispersion is represented by moving each particle according to a vector obtained by randomly sampling a normal (Gaussian) distribution with a mean of zero and a variance equal to S_D^2, where:

$$S_D^2 = 2D_L\Delta t \quad . \; . \; . \; . \; . \; . \; . \; . \; . \quad (6.50)$$

with D_L = longitudinal dispersion coefficient
Δt = timestep

This random sampling procedure, known as a "Random Walk", is based on the common assumption that dispersion is a

Table 6.3 - Advantages and Disadvantages of the PTM[1]

ADVANTAGES	DISADVANTAGES
Avoids Numerical Dispersion	As with MOC, concentrations greater than initial ones are possible if coarse discretising is used.
Only one finite - difference grid is required for the solution.	An unusually large number of particles may be needed for the acceptable solution of some problems.
Particles are needed only where water quality is of interest (unlike MOC).	The solution can become unstable when large numbers of particles are used.
Concentration distributions are calculated only when needed (again unlike MOC, in which the calculation of concentrations after each time - step is a source of some numerical dispersion).	Book-keeping of a large number of particles can be expensive.
Relatively easy to programme by comparison with MOC and FEM.	Considerable experience is needed before success will be met with in field applications.
Satisfies the principle of mass conservation (MOC can violate this).	

[1]Summarised from Prickett et al (1981) and Marsily (1986).

random process tending to a normal distribution (cf. Scheidegger, 1961; Prickett et al, 1981, p. 8). While this assumption is clearly compatible with molecular diffusion (which results from Brownian Motions), the statistical nature of mechanical mixing is not as clearly defined. For example, certain parameters which govern mechanical mixing (including grain size and permeability) commonly have log-normal rather than normal distributions (Marsily, 1986, p. 307; Davis, 1986, pp. 87 - 92). Thus it is not surprising that mechanical mixing often results in spatial and temporal concentration distributions which are non - Gaussian (Anderson, 1984). Nonetheless, at the time of writing, the assumption of random motions tending to a normal distribution is the most widely used approach in modelling dispersion by mechanical mixing. It should be noted that in the original formulation of Prickett et al (1981), molecular diffusion is assumed to be negligible, so that D_L is reduced to the product of dispersivity and velocity (with or without retardation as appropriate).

The PTM was selected for use in this project because the advantages it offers were felt to outweigh the disadvantages. However, the technique required further development before it could be used to represent the conceptual model for the stream - aquifer flow and transport systems developed in Chapter 5. In particular, the velocity interpolation schemes had to be modified to allow representation of vertical flow components, and further modifications were introduced to represent the effects of rock matrix diffusion in the Chalk and processes of molecular diffusion in the streambed sediment. These developments of the PTM are described in the next section.

6.3.4 -- Particle Tracking Formulation in UNCLESAM.

6.3.4.1 -- Introduction. In all major respects, the particle tracking formulation adopted here closely resembles that described by Prickett et al (1981), which was summarised above. Practical details of the main components of the method will now be given, with emphasis given to new developments and modifications which have been introduced by the present author. The description falls into three parts. First the general structure of the particle tracking code is described; secondly, velocity interpolation methods are discussed; and finally, details of particle movements by advection, dispersion and matrix diffusion are presented.

The two FORTRAN-77 codes which comprise the solute transport module of UNCLESAM are frequently mentioned in the following sections. The first is US-VEL, which takes the output from US-FLOW and calculates x and y velocity components across the boundaries of each block - centred finite difference cell. The second code, US-TRACK, performs particle tracking using the velocities delivered by US-VEL. Full listings for US-VEL and US-TRACK can be found in Appendix E.

6.3.4.2 -- The Structure of US-TRACK.

(i) Representation of stream pollution. As mentioned in Sections 5.2.1 and 6.2.1.1, US-FLOW is an externally coupled stream - aquifer model, in which stream flow is represented simply by mass balance techniques. In practical terms, this approach means that field data on stream stage are directly input to US-FLOW without satisfying any sort of boundary condition, and the agreement between observed and modelled baseflow discharges is used as a criterion for accepting calibrations of the flow model (see Section 7.1.3 below). As an extension of this approach, the input of pollutants to the aquifer is based upon a mass balance of dissolved solutes in the river pollutant plume (Section 5.3.1). In all simulations, it is assumed that the pollutant under investigation is at saturation in the river, and is mixed throughout the the body of polluted water. Knowledge of the solubility of the particular pollutant enables the total mass of solute which passes a given area of streambed to be calculated. Information on the percentage of river flow which is lost to the aquifer is readily obtained from the flow model solution, and this information can be directly used to estimate the total mass of solute entering the aquifer. The number of particles used in a given run is based on this value, so that as fine a discretisation as possible can be obtained for the solute load in the aquifer. For any point on the streambed, there is a possible range of time during which polluted stream water is passing overhead, depending on the velocity of the stream, the distance of the point from the pollutant source, and the duration of the pollutant input. This information is used to determine the time at which a given particle begins its journey through the streambed sediment.

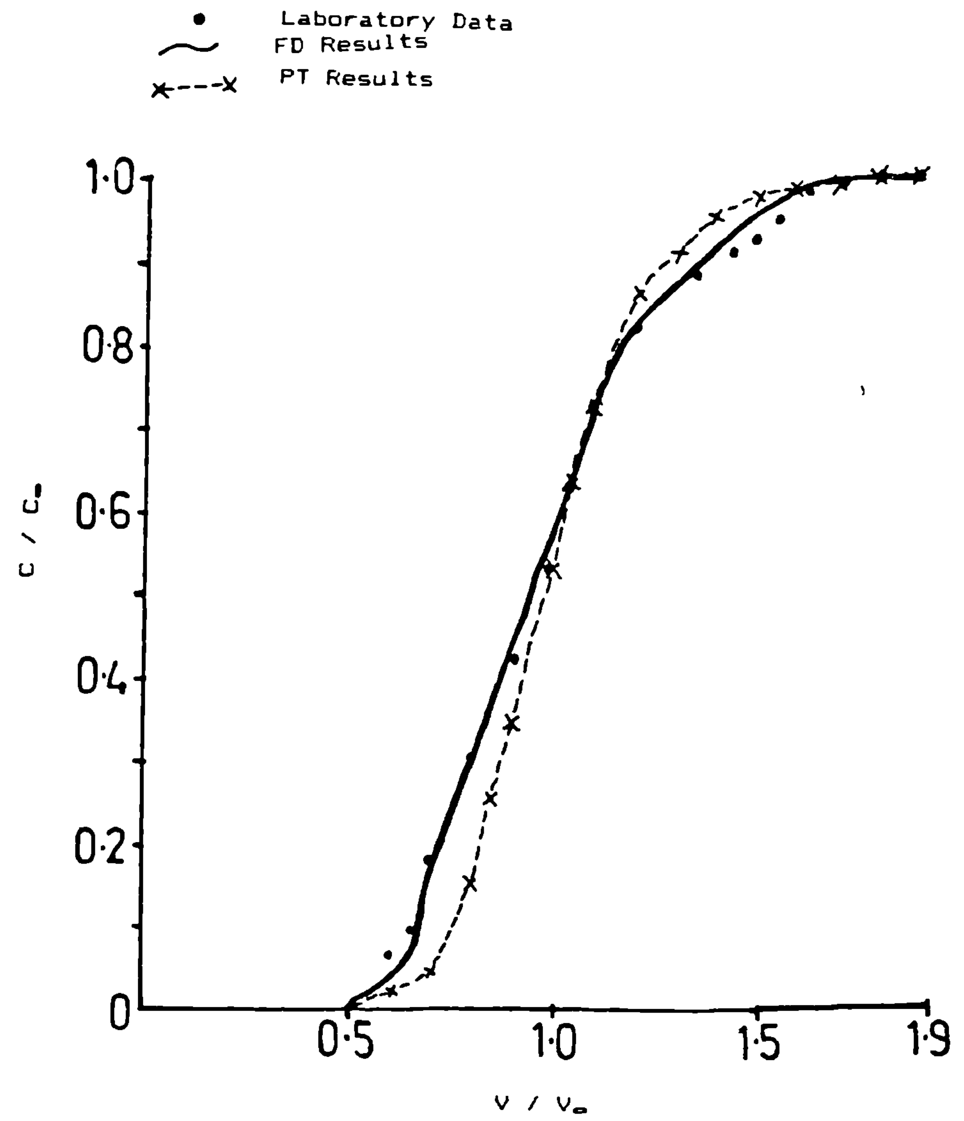
(ii) Particle Movement. The starting position for each particle is obtained as follows. The code checks to see which stream cells are losing water to the aquifer, and then randomly selects one of these for an individual particle. Within the selected cell, random selection of x and y co-ordinates is undertaken, and a random starting time within the possible range for that cell is also established (this takes place in subroutine START). From this point in space and time, each particle is tracked through the solution domain by successively calculating displacements by advection and dispersion until the particle position (in terms of x, y and z co-ordinates) lies within a designated 'sink' area of the grid. There are four possible fates for a particle in the model; it may exit to a well, it may be caught up in a flowline leading back to the stream, it may exit the domain boundaries, or it may cease to exit within a specified time. Checks for all four contingencies are made after every time step (in routine EXITS).

Advection and dispersion calculations in US-TRACK are controlled by the same system of node - type descriptors as is used in US-FLOW, with individual subroutines representing the streambed sediment (SEDMOV), the gravels (GRAMOV), and the Chalk (CHKMOV). Selection of a particular routine is made on the basis of the latest x-y-z position of the particle. When each routine is called, it calculates a new value for the timestep according to the magnitudes of the velocity components at the latest particle position. In this way, particles can be speeded through homogeneous low - permeability zones (eg the streambed), and slowed through heterogeneous high-permeability zones (eg the Chalk), so that maximum use is made of all available information on velocities without making the solution unnecessarily expensive in execution time.

Before discussing particulars of the PTM formulation in US-TRACK, one final point about the flow of the code must be made, and this concerns co-ordinate systems. Particle movements are calculated on the basis of 'real world' co-ordinates, defined as metres from a reference point (which is invariably the top left hand corner of cell (1,1), designated the 'real world' position (X = 0.0, Y = 0.0)). The positions of nodes, which must be known for the purposes of deciding exactly which subroutine is to be called, are defined according to model co-ordinates (I,J integers, as in US-FLOW). It is therefore necessary to convert co-ordinates from one system to the other throughout the execution of the code, and this is accomplished by the subroutine COORDS. Incidentally, the reason for using two separate co-ordinate systems is that all model parameters are defined in 'real world' units (m/d etc), and a great amount of scaling of input data would be required to transform everything to values consistent with the (I,J) system.

(iii) Testing of the Code. Before applying US-TRACK to field data, comparisons of output with solutions to simple problems were made to ensure that reasonable results were being produced. The results of one such comparison are given in Figure 6.16. The data and finite difference solutions presented in the Figure are from an experiment reported by Rao et al (1980), in which breakthrough curves for chloride from columns of porous glass beads were obtained. Simulation of this experiment allowed testing of the modified dispersion coefficient approach to matrix diffusion modelling (see Section 6.3.4.4 below).

Figure 6.16 -- Comparison of the US-TRACK Particle Tracking Results (Including the Effective Dispersion Approach) with Laboratory Data and Finite Difference Results of Rao et al (1980).



Notes: C_o is concentration of injected fluid; C is concentration of fluid at breakthrough. V is total volume of fluid passed through column, V_o is the total pore volume of the column.

6.3.4.3 -- Velocity Interpolations. In order to perform particle tracking it is important to be able to estimate the components of velocity at any point in the domain of interest. In US-VEL, velocity components at cell boundaries are readily obtained by the application of equation (6.46) to the output from US-FLOW. During particle tracking, it is necessary to interpolate between these known values of velocity to find the components of velocity at a given point. In US-TRACK, this is accomplished by calling an interpolation subroutine (INTERP) each time a particle reaches a new position. In the next movement of the particle, the new velocity vector is used to perform the advection.

The interpolation algorithm used in subroutine INTERP is well established for two dimensional (x,y plane) modelling (Prickett et al, 1981). In essence the interpolation method for a block - centred finite difference grid (as used in US-FLOW) is as follows (with reference to Figures 6.17 to 6.19):

(i) From the latest particle position (XP,YP), the four nearest known values for velocity (priovided by US-VEL) are identified. Obviously two of these values will be x-direction velocity components (VX(I,J)) and the other two y-direction velocity components (VY(I,J)) (Figure 6.17). Then the values of the VX1P and VY1P at the particle position are linearly interpolated from these pairs of VX and VY values on the basis of relative distance from the relevant boundaries to the particle. The expressions resulting from this linear interpolation are:

$$VX1P = VX(I,J)(1 - y) + VX(I,J+1)y \quad . . . . . (6.51)$$

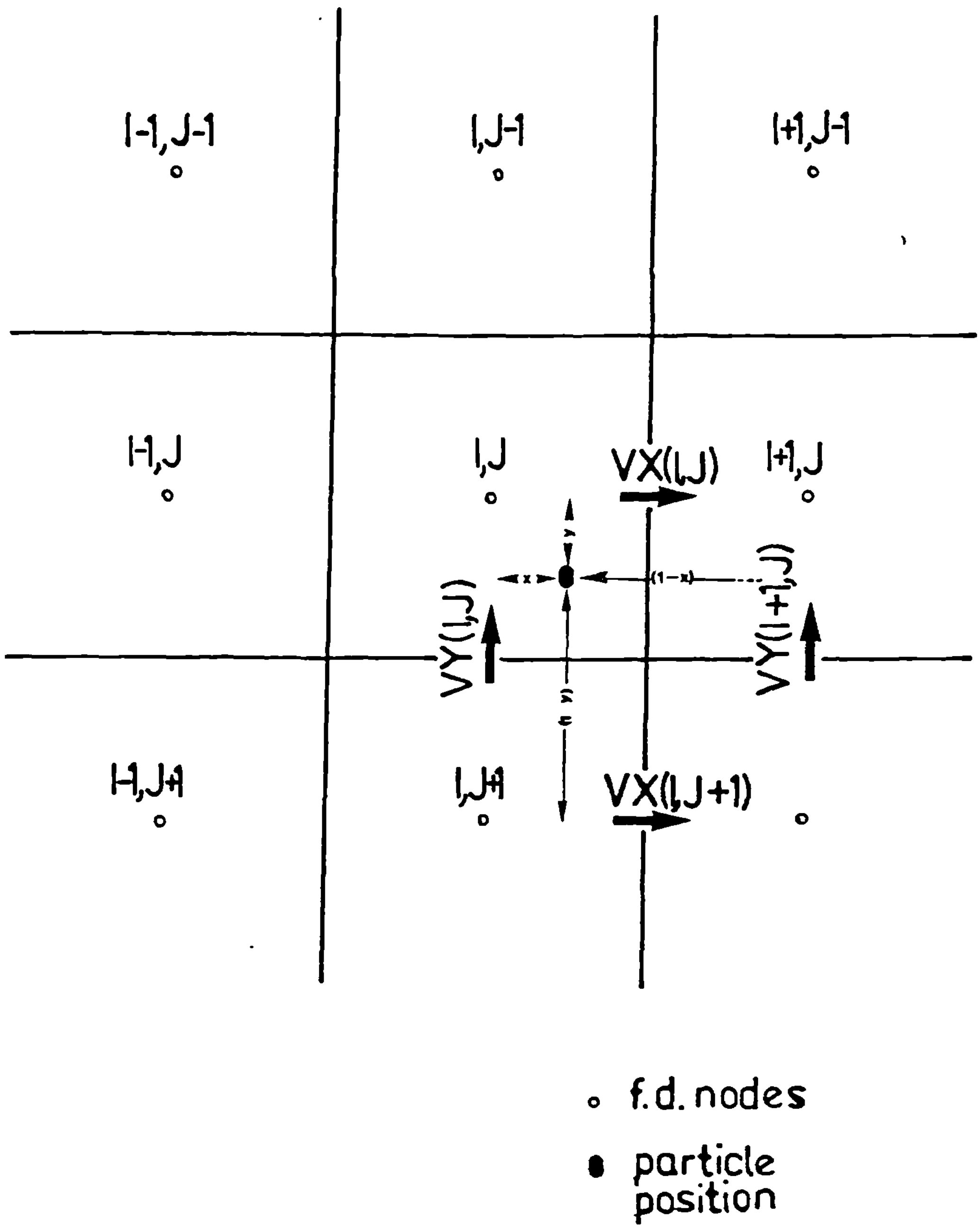
and

$$VY1P = VY(I,J)(1 - x) + VY(I+1,J)x \quad . . . . . (6.52)$$

where all definitions are as shown in Figure 6.17.

(ii) Since the values of VY and VX at the next nearest boundaries may be different from those just used, a

Figure 6.17 -- First Step in Velocity Interpolations.



further interpolation is required to extract information concerning the velocity trends from these boundaries also. This is illustrated in Figure 6.18. As before, a simple linear interpolation scheme is used, so that the new values of velocity at the particle (VX2P and VY2P) are given by:

$$VX2P = VX(I-1,J)(1 - y) + VX(I-1,J+1)y \quad \ldots\ldots \quad (6.53)$$

and

$$VY2P = VY(I,J-1)(1 - x) + VY(I+1,J-1)x \quad \ldots\ldots \quad (6.54)$$

where again all definitions are given in Figure 6.18.

(iii) Having used all the available information, the values obtained from equations (6.51) through (6.54) are combined and a final linear interpolation is made on the basis of the distance of the boundaries from the particle (Figure 6.19). The resultant expressions yield the values of VXP and VYP at the particle position thus:

$$VXP = VX1P(1 - XTOT) + VX2P(XTOT) \quad \ldots\ldots\ldots \quad (6.55)$$

and

$$VYP = VY1P(1 - YTOT) + VY2P(YTOT) \quad \ldots\ldots\ldots \quad (6.56)$$

where YTOT and XTOT are defined as shown in Figure 6.19.

The algorithm just described was originally formulated for the case where the horizontal components of hydraulic conductivity (Kx and Ky) are assumed to be constant with depth, and where all solutes are evenly mixed throughout the saturated thickness of the aquifer (Prickett et al, 1981). In that approach, vertical velocity components are effectively ignored.

When modelling systems which have considerable vertical velocities (eg near partially penetrating streams, or in aquifers, such as the Chalk, where permeability varies markedly with depth), vertical velocity components cannot be ignored with impunity (see Section 2.4.1 and Rushton,

Figure 6.18 -- Second Step in Velocity Interpolations.

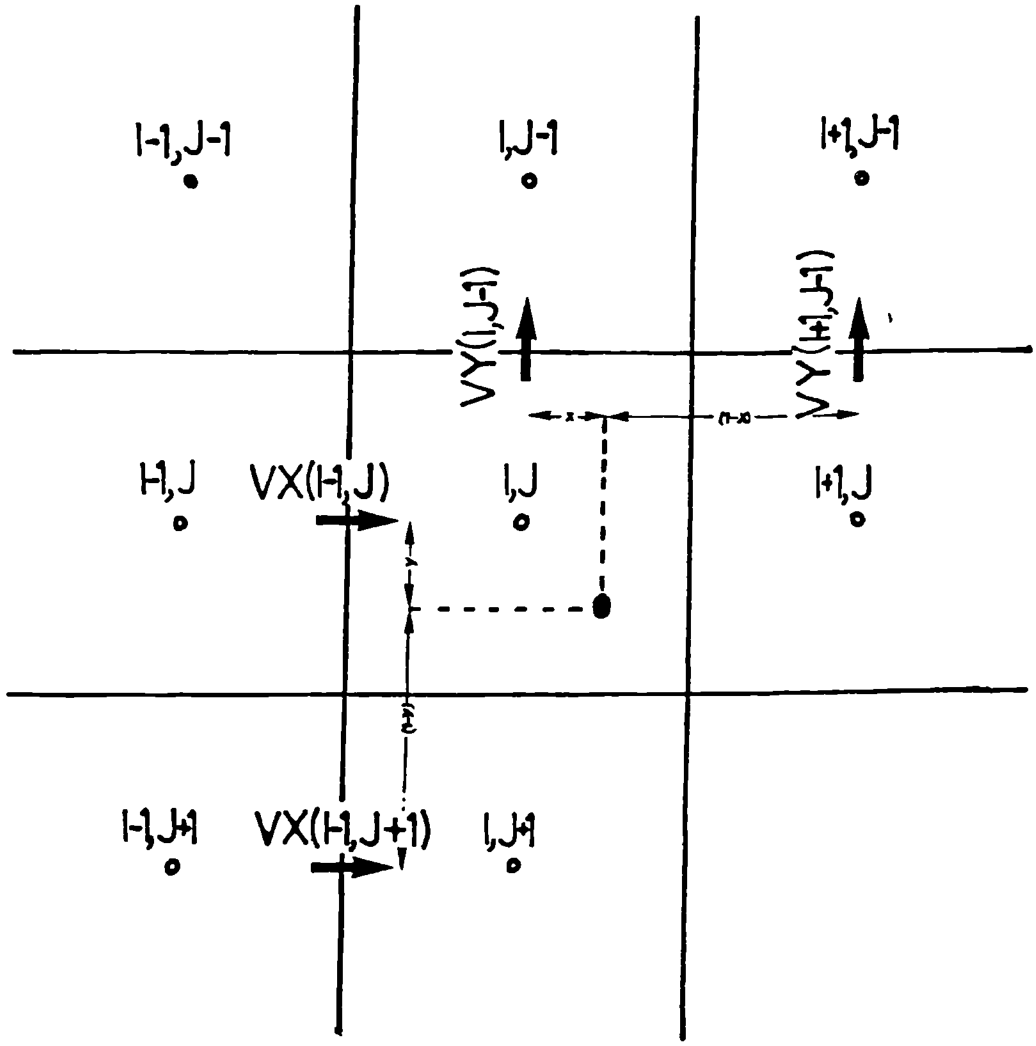
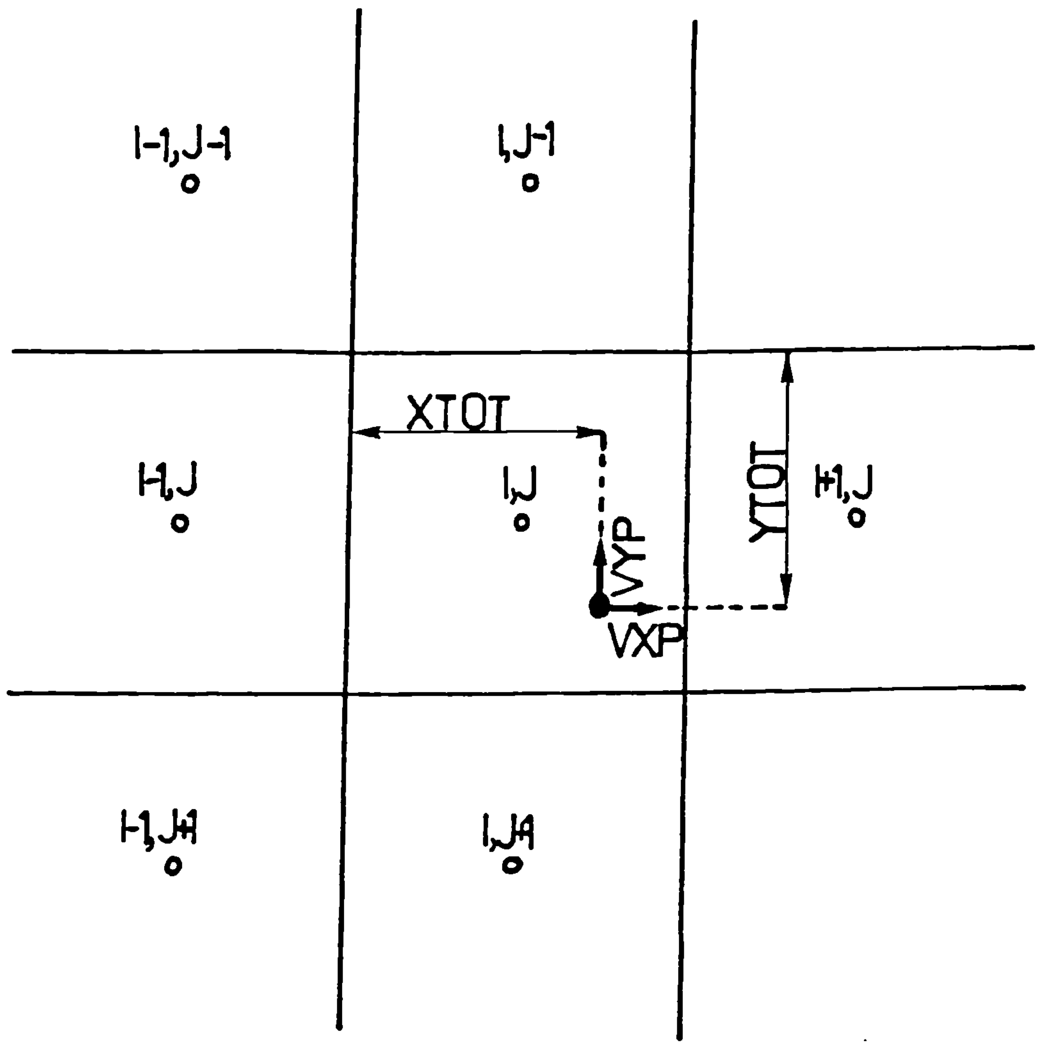


Figure 6.19 -- Third Step in Velocity Interpolations.



1989). Thus in the present study, the PTM has been developed further to allow the inclusion of vertical velocity components and vertical variations in horizontal hydraulic conductivity.

The two main effects of a variation in hydraulic conductivity with depth on the velocity field in an aquifer are:

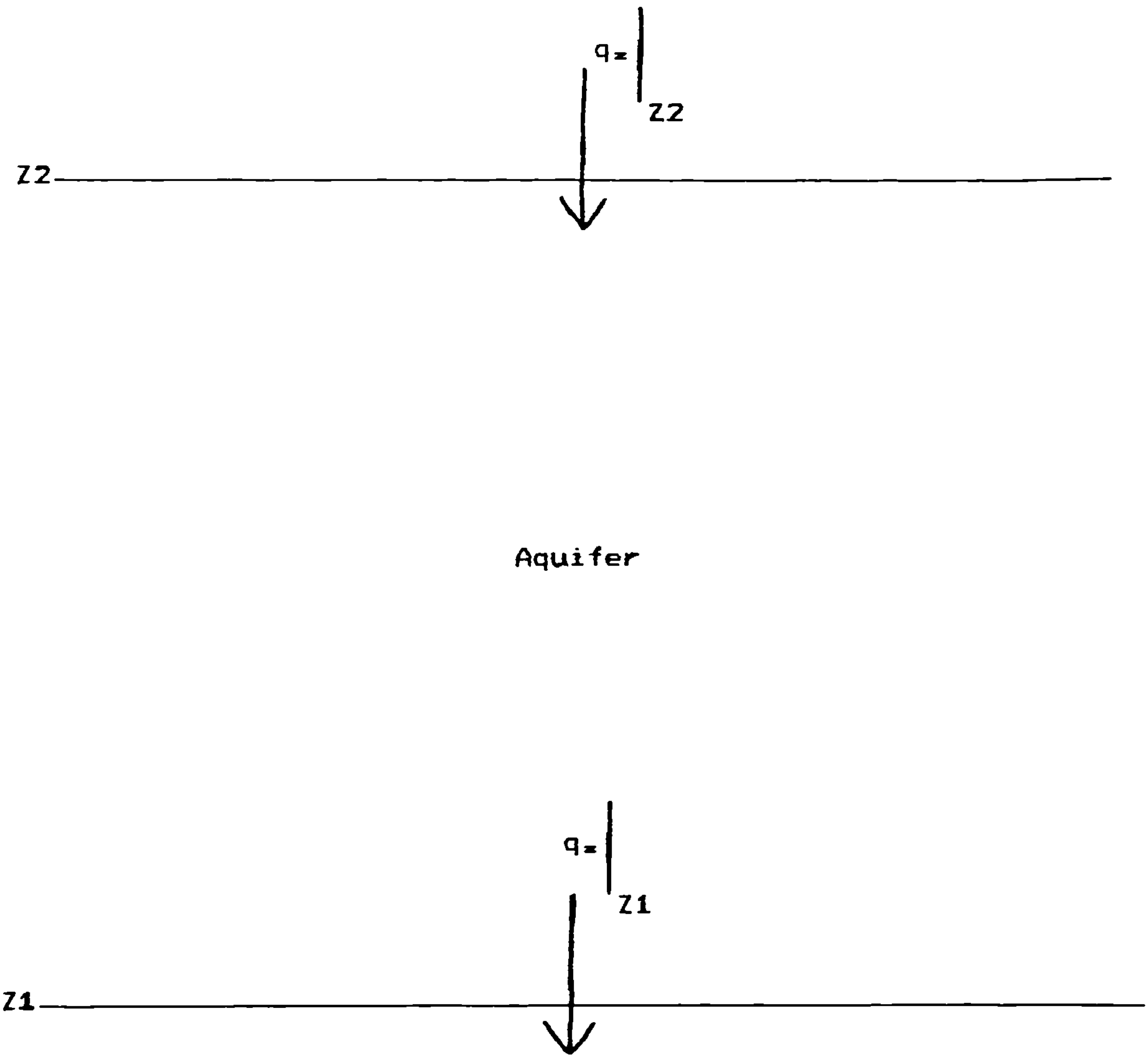
(a) the velocity components in the x and y directions will obviously vary with depth, so that the x - y plane interpolations described above will use different values of VX and VY according to the vertical position (ZP) of the particle being tracked.

(b) the magnitude of the vertical velocity component will vary non - linearly with depth, and thus the vertical component of the particle displacement can only be determined if some method for describing this variation can be found.

In the development which follows it is assumed that the values of Kx and Ky are explicitly known over specified depth intervals, and that horizontal hydraulic conductivity is isotropic. These assumptions are concordant with the method of estimating changes in hydraulic conductivity with depth used in this study (ie estimation from borehole flowmeter logs; Appendix B), and are also consistent with the formulation for transmissivity used in US-FLOW (Section 6.2.1.2).

Obtaining horizontal velocity components for different depth intervals within a given aquifer layer is straightforward. From US-FLOW, head is known in each aquifer layer only as some average over depth. Therefore the difference in head between any two adjacent nodes is constant with depth, and variations in the magnitude of horizontal velocity components between different intervals

Figure 6.20 -- Definition Sketch for the Development of qz Interpolator.



Key: Z1 -- Base of Aquifer; Z2 -- Upper Boundary of Aquifer
For explanation see text.

within each layer depends only on variations in the hydraulic conductivity. Values of VX and VY at cell boundaries for all depth intervals can be easily obtained from the depth -averaged head distribution according to equation (6.46), using the value of K appropriate for that interval. US-VEL includes this feature (Appendix E). Subsequently, during particle tracking in programme US-TRACK, the basic x-y plane interpolation scheme described above can be used to obtain the values of VXP and VYP according to the current vertical position (ZP) of the particle.

While representation of variations in vertical velocity components over depth is not quite so straightforward, a simple and effective method has been devised. Consider the aquifer shown in Figure 6.20. A flow of known magnitude enters the aquifer through the upper boundary (Z2) and another flow of known magnitude leaves the aquifer at the lower boundary (Z1). Using the same terminology as in Section 5.1, these two flows are designated as:

$q_z\Big|_{Z2}$ for the vertical flow evaluated at the upper

boundary, and $q_z\Big|_{Z1}$ for the vertical flow evaluated at the

lower boundary. In terms of the formulation of US-FLOW, the former may be recharge, a stream - aquifer exchange flux (qsa), or an upper / lower layer exchange flux. The latter may be an upper / lower layer exchange flux, or else it will simply equal zero at the impermeable base of the aquifer. Whatever the particular configuration, the total change in qz over the aquifer thickness (Δqz) may be written as:

$$q_z\Big|_{Z2} - q_z\Big|_{Z1} = \Delta qz \quad . . . . (6.57)$$

For simple aquifers, where Kx and Ky are constant with depth, it is commonly assumed that qz changes linearly with depth. In other words the rate of change of qz with depth is constant, so that we can write:

$$\frac{\partial(qz)}{\partial z} = \frac{\Delta qz}{(Z2 - Z1)} \quad . \; . \; . \; . \; . \; . \; . \; . \quad (6.58)$$

Now where Kx and Ky vary with depth, the total decrease in qz with depth (Δqz) will be the same, but the local value of $\partial(qz)/\partial z$ will be variable, and therefore equation (6.58) will not be valid. Because of this, several methods for relating $\partial(qz)/\partial z$ to a known variation of K with depth were considered. Initially, data describing the value of K for given depth intervals were subjected to polynomial regression to obtain second and third order expressions for the variation of K (and therefore qx and qy) with depth. However, no satisfactory method could be derived to relate these equations directly to the distribution of qz with depth. Returning to the original data, the aquifer was next conceived as being composed of superposed horizontal layers, each having its own thickness (b) and hydraulic conductivity (K). Assuming that the drop in qz across each layer is linear, the following expression was derived to relate the drop in qz across the *ith layer in a system* of (n) such layers in relation to the hydraulic conductivity (K_i) and thickness (b_i) of this layer:

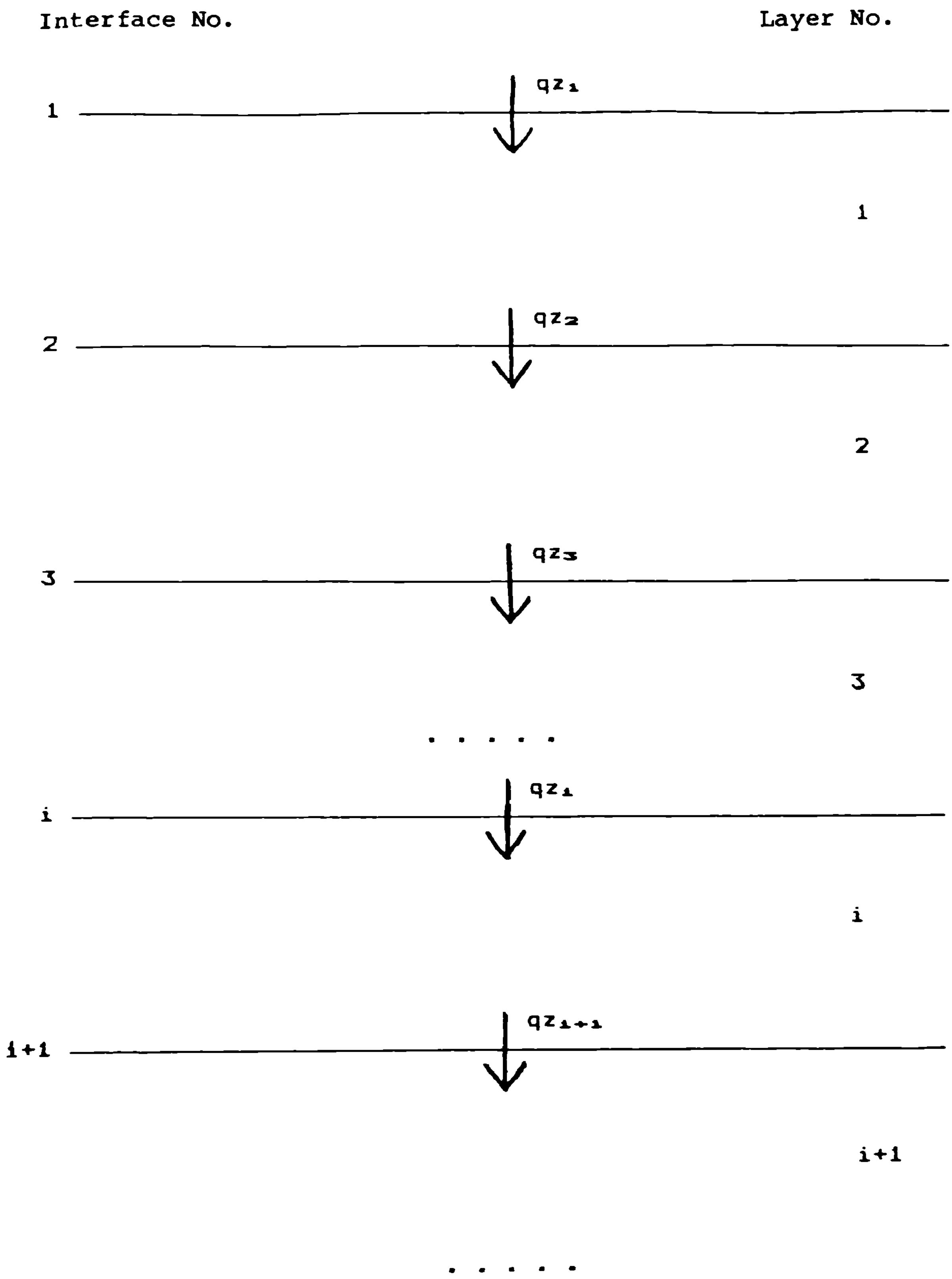
$$\Delta qz_i = \Delta qz \;\; [\,(K_i b_i) \,/\, s_t] \quad . \; . \; . \; . \; . \; . \; . \quad (6.59)$$

where Δqz_i = the drop in qz across the ith layer
qz = the total drop in qz from Z2 to Z1, as defined in equation (6.57) above.

$$s_t = \sum_{i=1}^{n} K_i b_i$$

Once the value of Δqz_i has been obtained for each layer, the value of qz at the bottom of each layer can be easily obtained by subtracting Δqz_i from the value of qz at the top interface of each layer. Using the convention shown in Figure 6.21, the following expression is obtained:

Figure 6.21 -- Conventional Notation for the qz Interpolator.



$$qz_{i+1} = qz_i - \Delta qz_i \quad \ldots\ldots\ldots\ldots \quad (6.60)$$

So, given values for qz evaluated at Z2 and Z1 (Figure 6.20), and values for the thickness and hydraulic conductivity of the constituent layers of the aquifer (Figure 6.21), then the values at the interfaces between all of these layers are readily obtained by application of equations (6.59) and (6.60). US-VEL performs these calculations (Appendix E). Within each layer, the variation in qz with depth is calculated by linear interpolation from the upper and lower interface values wherever a vertical velocity component is required during particle tracking (in US-TRACK).

To test this algorithm, a number of test problems were constructed. For each test problem, a given layered system was modelled using a two dimensional steady - state vertical profile model (using an implicit finite difference formulation, based on the US-FLOW code), and also analysed using the algorithm developed above. In all cases, the basic flow domain was as shown in Figure 6.22, with a uniform recharge of 0.567 m/d at the upper boundary and fixed head boundaries of 45.00 and 43.00 metres at the left and right boundaries respectively. The median values of qz for each interface were compared with the values obtained using the interpolation algorithm. Data for three of the test data sets are given in Table 6.4, and graphs showing the results of the simulations are given in Figures 6.23 through 6.25. The results obtained show excellent agreement between the 'full' solution and the estimated values. While it is not known how well this interpolator would perform under transient flow conditions, or with more extreme head and conductivity distributions, it was felt that these preliminary results were sufficiently encouraging to justify application of the algorithm to the field problems analysed in Chapters 7 and 8.

Figure 6.22 -- Flow Domain for Vertical Interpolator Test Problems.

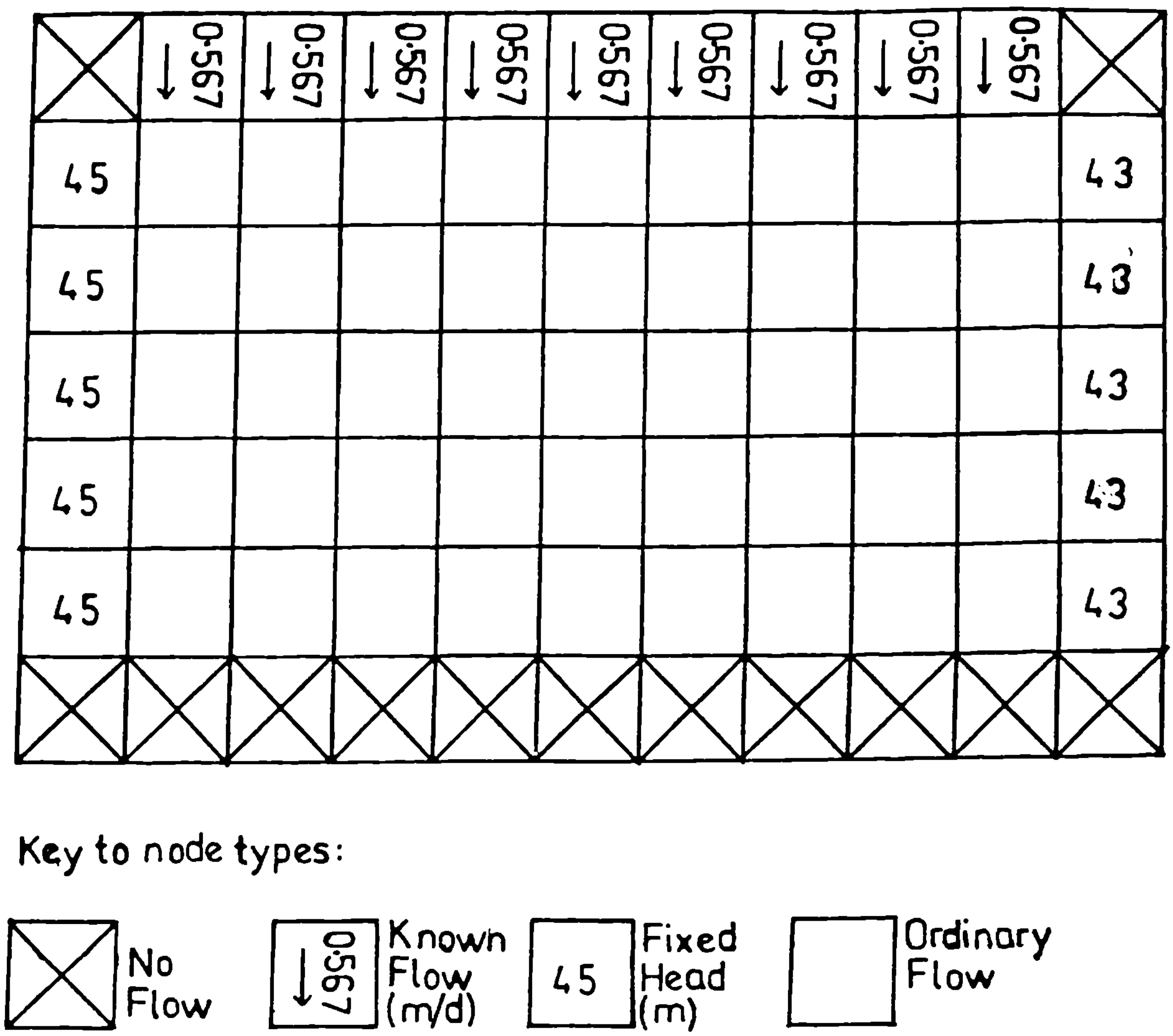


Table 6.4 -- Data for Test Problems used to Check the Interpolation Algorithm.

Data Set:	1			2			3		
Layer	K_i	b_i	K_ib_i	K_i	b_i	K_ib_i	K_i	b_i	K_ib_i
2	1000	25	25000	1000	25	25000	1000	25	25000
3	890	25	22250	890	25	22250	890	15	13350
4	723	25	18075	723	25	18075	723	32	23136
5	149	25	3725	890	25	22250	149	17	2533
6	23	25	575	920	25	23000	23	36	828

Notes: K_i values in m/d; b_i values in m; K_ib_i values in m^2/d.

Further Descriptions:

Test Number	*Comments*
1	K_i monotonically decreasing with depth, but b_i constant. Therefore K_ib_i monotonically decreasing with depth also.
2	K_i not monotonically decreasing with depth, but b_i constant. Therefore K_ib_i not monotonically decreasing with depth.
3	K_i monotonically decreasing with depth, but b_i variable. Therefore K_ib_i not monotonically decreasing with depth.

6.3.4.4 -- Advection, Dispersion and Matrix Diffusion in US-TRACK.

Advection. Advection calculations in US-TRACK are simple; with velocity components defined according to the latest particle position, the three dimensional displacement (d_x, d_y, d_z) due to advection in any time interval Δt is given by:

$$
\left.\begin{aligned}
d_x &= (VXP / Rd).\Delta t \\
d_y &= (VYP / Rd).\Delta t \\
d_z &= (VZP / Rd).\Delta t
\end{aligned}\right) \quad . \; . \; . \; . \; . \; (6.61)
$$

where Rd is the retardation factor, discussed in Section 6.3.2. If no sorption is occurring, then Rd equals 1. According to the conceptual model of Section 5.3, adsorption is assumed to occur in the streambed sediments and the gravels, but to be negligible in the Chalk.

Dispersion. Dispersion calculations in US-TRACK are generally identical to those given in Prickett et al (1981), save that three extensions of the method are made:
(i) A transverse dispersion component in the vertical direction is added.
(ii) A representation of molecular diffusion is added to the dispersion calculations in the streambed sediment subroutine (SEDMOV).
(iii) The effects of matrix diffusion on dispersion after long travel times is accounted for in the Chalk subroutine (CHKMOV). This effect is discussed in more detail below, in the general discussion of matrix diffusion.

For normal dispersion, the calculation takes place in two steps. Firstly, the variance of the dispersion distribution (S_D^2) is calculated. For longitudinal dispersion, this is given by:

$$S_D^2 = 2 \, \alpha_l \, \sqrt{(dx^2 + dy^2)} \quad . \; . \; . \; . \; . \; . \; . \; . \; (6.62)$$

Which is simply the dispersivity times twice the total advective displacement. This is mathematically equivalent to equation (6.50) (since $D_L = \alpha_l \, (V / Rd)$).

In the second step, the standard deviation (S_D) is used to sample the normal distribution for dispersion. This involves multiplication by a number (between -6 and +6)

Figure 6.23 -- Results of Interpolator Test 1.

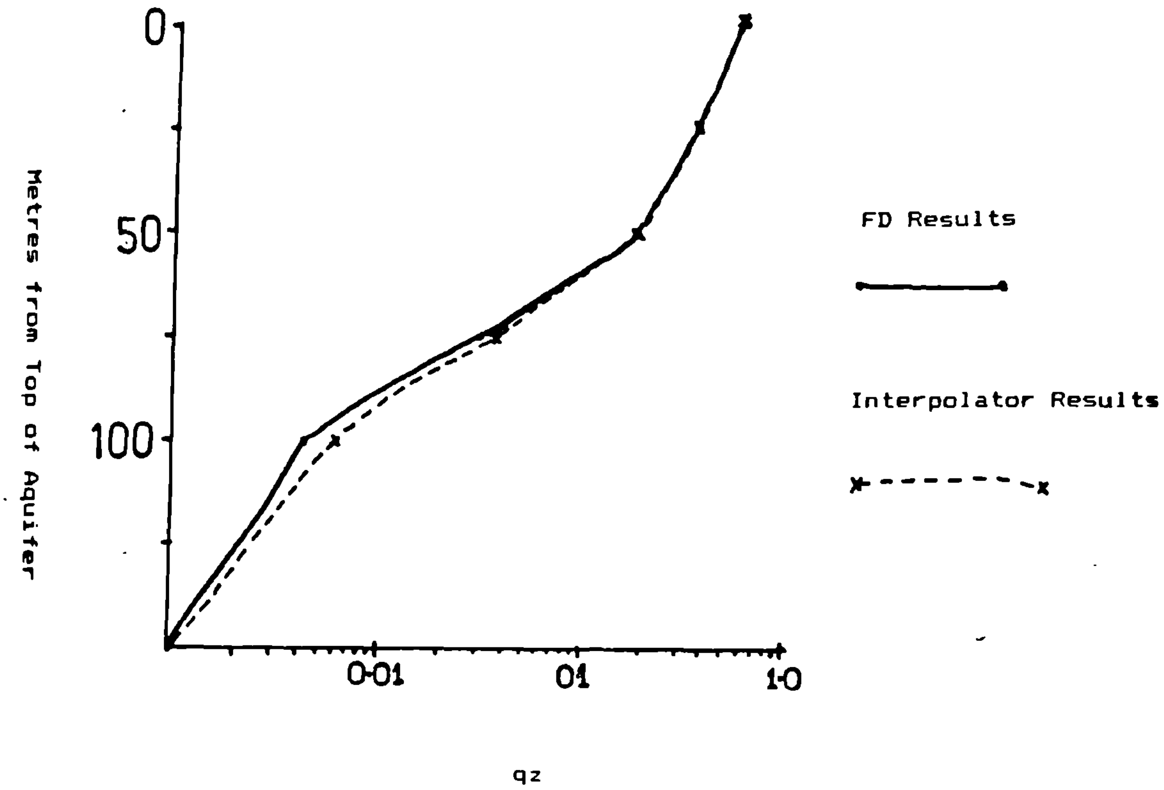


Figure 6.24 -- Results of Interpolator Test 2.

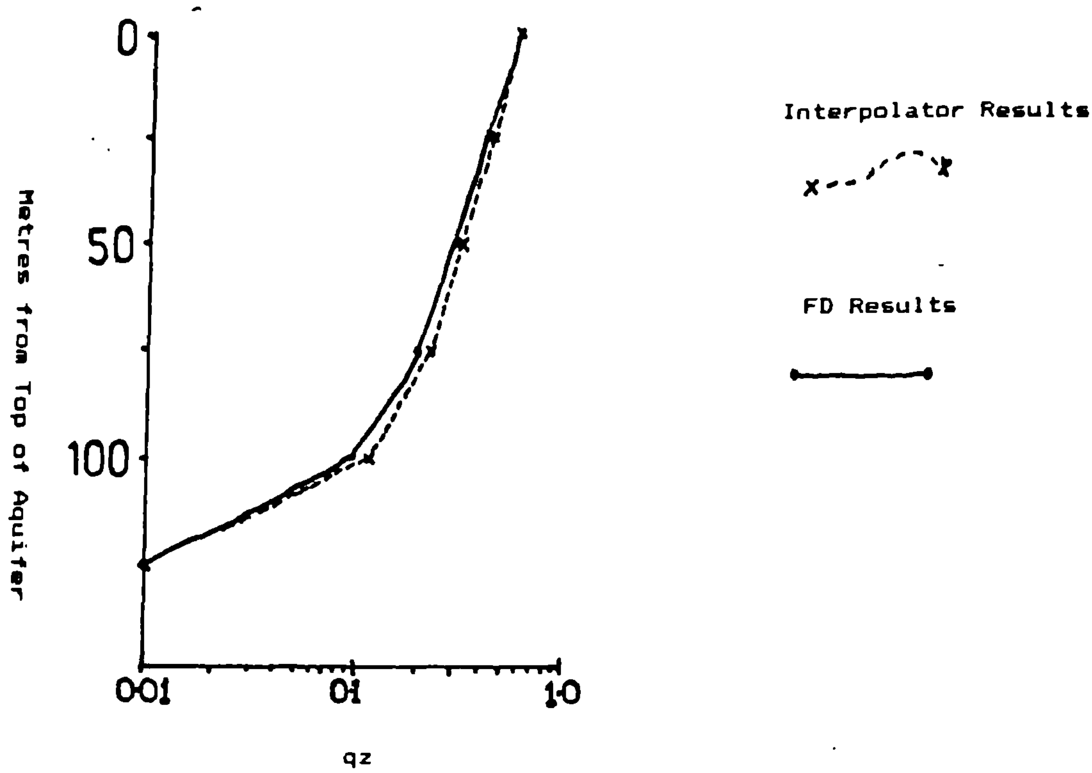
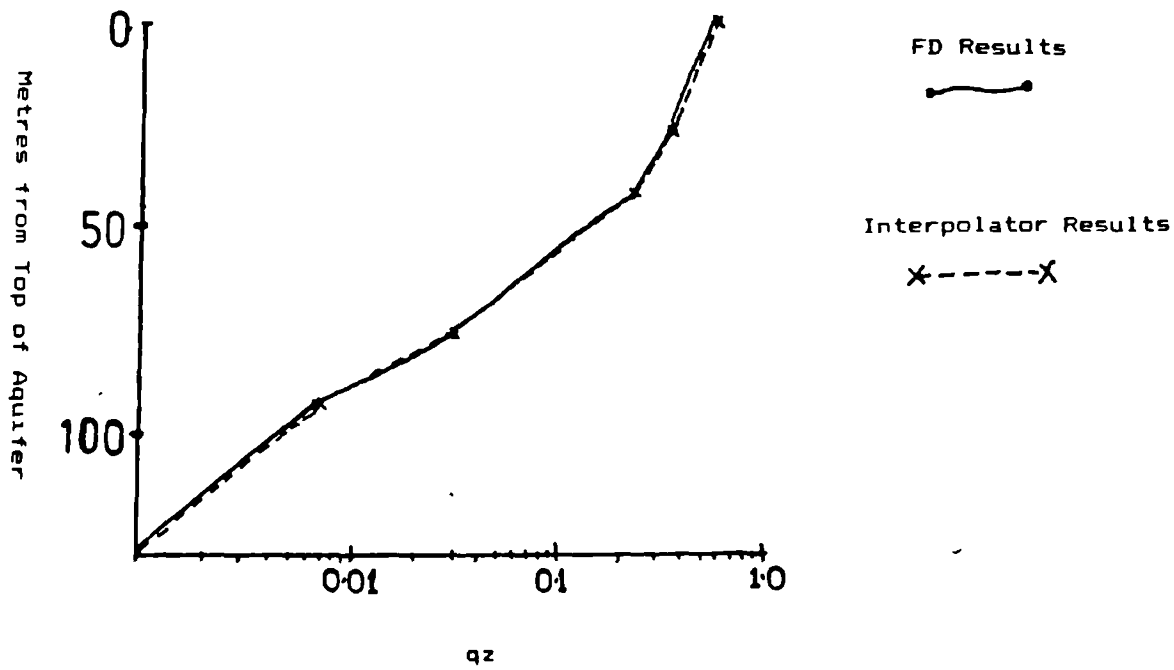


Figure 6.25 -- Results of Interpolator Test 3.



selected randomly from the distribution. This step gives the magnitude of the dispersive flux. Resolution of longitudinal and transverse displacements into x - y - z components is accomplished by simple geometry. Transverse dispersion is accounted for in a similar manner, using a transverse dispersivity (defined in 6.48). Extension to the vertical dimension is accomplished by defining an analogous vertical dispersivity, acting normal to the horizontal advection resultant.

For molecular diffusion, equation (6.50) is used directly to obtain S_D, with the coefficient for molecular diffusion in the porous medium (D_D) substituted for D_L. The calculation then proceeds as for mechanical mixing.

It should be noted that these extensions of the random walk procedure have previously been applied with success in a geostatistical model of radionuclide migration described by Mackay et al (1988, pp. 43 - 44).

Matrix Diffusion. Even though retardation by sorption is negligible in the Chalk, the process of matrix diffusion is known to cause retardation and additional dispersion of solutes moving through the fissure system of the Chalk (Section 5.2.2), and some consideration must be given to this phenomenon in any study of solute transport in the Chalk. Mathematical models of matrix diffusion have been extensively studied by Lever et al (1983). Where matrix diffusion takes place, the simple one - dimensional advection - dispersion equation (6.45) is re - written:

$$\frac{\partial[D_L(\partial C/\partial x)]}{\partial x} - \frac{V}{}\frac{\partial C}{\partial x} + \frac{2n_m D_L}{a}\left.\frac{\partial c'}{\partial w}\right|_{w=0} = \frac{\partial C}{\partial t}$$

(Dispersion) - (Advection) + (matrix diffusion) = (Temporal Change in Concentration)

. . . . (6.63)

where

V = average linear groundwater velocity

D_L = coefficient of hydrodynamic dispersion (in fissures)

x = space dimension in domain

w = space dimension into matrix block at any x

t = time

C = concentration of solute in fissure system

c' = concentration of solute in matrix blocks

n_m = porosity of the matrix blocks

a = fissure aperture

Since the PTM deals in masses of solute rather than in concentrations, concentration - dependent calculations cannot easily be incorporated into a PTM formulation. Thus, while the other terms in (6.63) have obvious particle tracking equivalents as described above, the matrix diffusion term does not. Direct solution of (6.63) in a particle tracking code would demand that concentrations be calculated for portions of the model grid after *every time* step, so that a solution of the matrix diffusion term could be obtained. It is not certain whether this could be accomplished, but even if it were, the expense in computer time and storage thus incurred would be vast. Moreover, such an approach would rob the PTM of its main advantages over the MOC, namely simplicity and the avoidance of numerical dispersion. It is therefore clear that an alternative approach is needed. One possibility would be to represent the effects of diffusion into and out of storage by assigning a stochastic retardation to each particle trajectory. However, the basis on which such stochastic assignments could be made is far from clear. Another possibility is suggested by the discussions of solutions to (6.63) presented by Lever et al (1983).

Studies of various solutions to (6.63) have revealed that there are three different 'regions' in the solution (Lever et al, 1983, p. 100). These are summarised below:

Region 1 -- This is the proximal region, where very little of the matrix block has been invaded by solutes. When a solute has just begun to migrate through a dual porosity medium, matrix diffusion effects are negligible compared to the effects of advection and hydrodynamic dispersion in the fissure system. Within this zone, the third term on the LHS of equation (6.63) tends to zero, and so that the solution is identical to the that for the ordinary advection - dispersion equation.

Region 2 -- This is the intermediate region, where active exchange of solutes between the fissure system and the matrix blocks exerts a profound influence on solute transport in the fissure system. In this region, the third term is of great importance, and a full solution of (6.63) provides the only full description of solute transport. The interface between Region 1 and Region 2 is customarily expressed as a distance from the start of solute ingress (designated the symbol L_i). When there is no sorption in the fissure system or the matrix blocks, L_i is approximately given by:

$$L_i = 3 \left[\frac{\alpha_1 \ V \ (a/2)^4}{(D_D \ n_m)^2 C_F^2} \right]^{1/3} \quad . \ . \ . \ . \ . \ . \ . \ . \ . \ (6.64)$$

where $C_F = n_m + \rho_S$ Rd = rock matrix capacity factor

ρ_S = density of mineral grains (= 2.715 for calcite)

and all other symbols have their previous meanings.

Region 3 -- This is the distal region, in which solute exchange between the fissure system and the matrix blocks has developed to a state where the amount of solute leaving the fissures is approximately equal to the amount re-entering them from the matrix blocks. In other words, a quasi - equilibrium exchange has been established. For this region, equation (6.63) can be re-written as:

$$\frac{\partial}{\partial x}\left[(De/R')(\partial C/\partial x)\right] - \frac{V}{R'}\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; (6.65)$$

(Dispersion) - (Advection) = (Temporal Change in Concentration)

where

V = average linear groundwater velocity

De = enhanced coefficient of hydrodynamic dispersion, which includes effects of matrix diffusion

x = space dimension

t = time

R' = apparent retardation factor, due to matrix diffusion

C = concentration of solute

Equation (6.65) is simply the advection - dispersion equation with an 'apparent retardation factor' (R') and an enhanced dispersion coefficient (De) which describes the increased spreading of solute caused by the matrix diffusion. The retardation factor expresses equilibrium partitioning of the solute between the fissure system and the matrix blocks as a function of the differing porosities of the two zones. Following Lever et al (1983), this is written:

$$R' = \frac{1 + n_m (1 - n_F)}{n_F} \quad . \; . \; . \; . \; . \; (6.66)$$

where n_m = porosity of the matrix blocks

n_F = porosity of the fissure system

The enhanced dispersion coefficient is defined by the following expression:

$$De = D_L + \frac{\pi^2 V^2 n_m (1 - n_F)}{12 F_T n_F R'^2} \quad \ldots\ldots (6.67)$$

where all symbols have their previous meanings, and F_T is the transfer function, given by:

$$F_T = \pi^2 D_D / b^2 \quad \ldots\ldots\ldots\ldots (6.68)$$

with b = fissure spacing

D_D = coefficient of diffusion *in the matrix* block

The distance beyond which the intermediate region solutions may be replaced by the distal region solution (using equation (6.65)) is given by the length L_d, which is defined as:

$$L_d = \frac{3 V a b}{2 D_D n_m} \quad \ldots\ldots\ldots (6.69)$$

where all symbols have their previous meanings.

By analogy with the discussions in Sections 6.3.2 to 6.3.4, it is obvious that equivalent particle tracking statements can be written for all terms on the LHS of (6.65). Thus for both Regions 1 and 3, simple particle tracking representations are possible which do not involve any concentration - dependent calculations. Thus, even though the effects in Region 2 cannot be adequately represented, a method for accounting for the possible range of matrix diffusion effects suggests itself: For each simulation involving Chalk, two calculations can be performed. In the first calculation, Region 1 can be represented by a straightforward advection - dispersion model. In the second calculation, the 'extreme' case of quasi-equilibrium exchange, as in Region 3, can be represented by using the particle tracking equivalents of equations (6.65), (6.66) and (6.67). This approach will be termed 'the matrix diffusion range approach (MDRA)' in subsequent discussions.

6.4 -- CONCLUSION.

In this Chapter, mathematical models for both flow and solute transport have been derived. These models are consistent with the conceptual model (Chapter 5), and overcome many of the shortcomings of earlier models which were identified in the literature review (Chapter 2). FORTRAN-77 codes to numerically solve these models have been developed and tested. While the formulations adopted here were based primarily on the hydrogeology of stream-aquifer systems in the Thames Basin, an attempt has been made to retain generality so that the models can be applied to other sites in future. Results obtained from applying these codes to the field sites at Gatehampton and Dorney are presented in Chapters 7 and 8.

CHAPTER SEVEN
FLOW MODELLING OF FIELD SITES

7.1 -- RATIONALE OF THE FLOW SIMULATIONS.

7.1.1 -- Introduction.

In this Chapter, the two flow models which were developed for the field sites of Gatehampton and Dorney are described. As a preliminary to these descriptions, it is necessary to briefly discuss the rationale which was followed in developing these models.

Three shortcomings hinder the development of mathematical models for field sites: Lack of data, lack of knowledge about physical and chemical processes and lack of mathematical methodologies for describing these processes in a meaningful way. Notwithstanding these problems, however, mathematical models can provide a "disciplined format for assessing the consistency within and between:
(1) concepts of the governing processes and
(2) data describing the relevant coefficients" (Konikow, 1981).

It is with this understanding of the general purpose of modelling in mind that the following models have been developed.

The primary aim of the flow modelling described below was to assimilate all of the information on the physical hydrogeology of the field sites into models which would provide estimates of head and hydraulic conductivity throughout the problem domains. These hydraulic parameters could then be used to calculate groundwater velocities, for use in predicting the movement of pollutants from the Thames to the well fields. This ultimate purpose of the flow modelling coloured the approach taken throughout the modelling exercises.

7.1.2 -- Deterministic versus Stochastic Approaches.

It is important to stress that the approach used in this project is 'deterministic', that is, it is assumed that all of the parameters used in the model can be represented by a single, unique, value at any one point in space and time. With one set of parameters, one solution to the problem is obtained from the simulation. By contrast, if any of the parameters in a model are regarded as random variables (ie samples from some probability distribution), then the model is said to be 'stochastic' (Freeze, 1982). In this case, a range of randomly selected values for the input parameters are used, so that a number of possible solutions (or 'realisations') are obtained in place of a single deterministic solution. For the purposes of prediction, it is in many ways preferable that a stochastic approach be used, since it is clearly the case that there is great uncertainty in the specification of input parameters (cf Chapter 3). However, as observed by Narasimhan (1982);

> '. . . . Probabilistic solution of realistic problems is mostly uneconomical at present, even with the availability of big computers. The increased effort stems from two considerations. The first is of course the fact that every mathematical operation has to be performed on two strings of numbers rather than just two numbers. The other more interesting one is that the algebra of distributions may not be governed by exactly the same axioms governing the algebra of real numbers. . .'

For these reasons, it was felt that the benefits to be obtained from a stochastic approach to the present, somewhat preliminary, appraisal of pollution potential did not justify the vast increase in computing time and effort required by such an approach.

7.1.3 -- Calibration and Verification.

The calibration and verification method used in this study was as follows:

(1) Steady - state solutions to the flow model were obtained and the results compared with field head data from a period in which the field heads were at quasi-equilibrium. In both cases, the field head data were from periods of steady baseflow during periods when the recharge rate had been approximately uniform for several months. Model output heads could then be readily compared with observed heads, and the input hydraulic conductivity distribution altered to obtain a 'best fit'. To remove some of the subjectivity from the selection of the best fit solution, the observed data were entered into an array in the US-FLOW code, allowing the error between observed and computed heads at each node to be calculated after each run. The root mean square error (RMSE) in water table elevation is here defined as:

$$\mathrm{RMSE} = \left[\frac{1}{N} \sum (h_{im} - h_{io})^2 \right]^{1/2} \quad \ldots\ldots (7.1)$$

where h_{im} = modelled head at a given node (i)

h_{io} = observed head at the same node (i)

N = total number of nodes

This parameter became the 'objective function' in the simulations, allowing overall model performance in the entire domain to be assessed by examination of this single output variable. Later, when sensitivity analyses were performed (Section 7.4), the RMSE was also very useful as an indicator of model sensitivity. With RMSE minimised, 'steady - state calibration' was said to have been achieved. The benefit of starting the calibration procedure with a steady - state problem is that all storage parameters are set to zero and the problem therefore reduces to the estimation of hydraulic conductivities and aquifer geometry. Furthermore, steady state calibration is a simple and effective way of establishing a set of initial conditions for use in subsequent transient models.

(2) After a 'steady - state calibration' had been obtained, values of storage coefficients (estimated on the basis of existing field data) were inserted into the models, and transient runs were performed. In these runs, variable well pumping rates were included and the hydrographs of nodes representing abstraction and observation boreholes were compared with field hydrographs. If the agreement between 'observed' and 'predicted' heads was close, then the calibrated hydraulic conductivity distribution was taken to be correct.

Having decided to use the above deterministic approach, however, the problem of 'non-uniqueness of solution' inherent in deterministic modelling (which has been discussed by many authors, eg Wang and Anderson, 1979; Lerner, 1985; Freyberg, 1988) remains unresolved. In an attempt to minimize the damage caused by this problem, it was decided to constrain the calibrations of the flow models so that they would satisfy several conditions. Apart from the minimisation of RMSE, therefore, two stream - aquifer criteria were used as constraints:

(a) The modelled baseflow discharges should agree with the estimated baseflows for the modelled reaches. Baseflow for all modelled reaches was estimated from records of flow accretion between weirs upstream and downstream of each study site (provided by the Thames Water Authority).

(b) While calibration of the model to agree with heads in the unconfined part of the aquifer (the only parts for which information is available) may be relatively straightforward, it is possible that the head gradients across the streambed sediment predicted by the model could be so high that they would imply establishment of quick conditions leading to loss of strength, increase in permeability and erosional removal of the sediment (cf

Section 3.4.4.2 and Figure 3.9). It is clear that erosion of sediment by baseflow is not occurring at present in the Thames. Therefore, to ensure that unreasonable gradients were not implied by a given calibration, the critical hydraulic gradient (i_c) above which quick conditions would be established in the streambed sediment was calculated in the code according to the following expression (Capper and Cassie, 1976, p. 63):

$$i_c = \frac{G_s - 1}{1 + n_s} \qquad \ldots\ldots\ldots (7.2)$$

Where G_s = the specific gravity of the streambed sediment, and

n_s = the porosity of the streambed sediment.

The above expression is obtained quite simply by equating the forces acting downwards and upwards, the latter being due to friction of groundwater on the sediment grains. Use of (7.2) is based on two conservative assumptions. Firstly, it is assumed that uplift of the sediment is due solely to seepage forces, so that shear stresses due to the flow of water in the stream neither impede nor enhance erosional removal; secondly, it is assumed that the yield stress in the sediment (due to compaction, cementation etc) is insufficient to impede uplift. Calibrations were only accepted if equation (7.2) was satisfied at all stream nodes.

Due to limitations of time and data, the above process of calibration and limited verification was taken to be adequate for present purposes.

Having achieved acceptable transient runs, final steady-state flow fields were calculated for the central portions of each domain by setting all storage parameters to zero, defining a long-term mean recharge rate, and retaining all the wells in the model, pumping at their licensed abstraction rates. These final steady - state models were used as input to the velocity calculation module (US-VEL), to obtain the velocity fields used in the particle tracking solutions (Chapter 8).

7.1.4 -- Grid Design and the Nested Grid Approach.

In designing model grids, an attempt was made to satisfy the sometimes conflicting demands of simplicity (allowing easy data input), accuracy (keeping cell dimensions as small as possible, and keeping changes in cell dimensions between adjacent cells fairly small), and consistency with real hydrogeological boundaries. Because no information on aquifer anisotropy was available for either site, grid axes were aligned with the National Grid lines on the Ordnance Survey base maps, thus making future use of model results straightforward.

In the case of the Dorney model, the original finite difference grid was used for all modelling runs, with the head information abstracted for a central finely-discretised portion at the end of the simulation. The nature of the site allowed grid design to include a 30 x 30 central portion with a uniform grid - spacing of 25m.

By contrast, for the Gatehampton model the size of the main simulation domain had to be so large to incorporate the full details of lateral variations in Chalk permeability that the finest divisions on the main grid were still on the order of 50m. Therefore a 'nested grid' was inserted into the centre of the main grid, and parameter values were interpolated onto the nested grid from the successfully calibrated main grid. Fixed head boundaries were adopted on the nested grid according to values calculated by the main grid. In this way, a 50 x 50 grid with 10m spacing could be used for the Gatehampton wellfield. The main advantage of the nested grid approach is that, while the final grid is restricted to the main area of interest and is finely discretised to represent flow as accurately as possible, the parameter values which are used on this fine grid were derived from a calibration which used information from a much wider area. Therefore much more hydrogeological information is implicitly included in a nested grid than would be the case were the fine grid used straight away. After running the nested model, head values at well nodes were compared with those predicted by the large - scale model, and the close agreement obtained was taken as proof of the validity of the nested model. A successful previous application of this approach to a field problem has been described by Ward et al (1987). In their study, the nested grid approach (which they termed the 'Telescopic Mesh Refinement Technique') was used with a three dimensional finite difference flow code and a particle tracking solute transport code to model a hazardous waste site in Ohio. Three grids were used; a regional grid (covering a 16 km stretch of the aquifer), a local grid (covering 3.2 km) and a site model (covering a square domain 500m across). All grids included the Great Miami River, and the study revealed the suitability of the nested grid approach for the modelling of stream - aquifer interactions.

7.2 -- THE GATEHAMPTON FLOW MODEL.

7.2.1 -- Data Selection and Preparation.

The main sources of data for the Gatehampton flow model were:

(a) Site - specific information, especially the site investigation reports of Robinson (1984) and Robinson et al (1987), which were reviewed at some length in Section 3.5.2.1 above. The data from Gatehampton presented in Appendices B and C were also used, as were lithological logs from the BGS archive at Wallingford.

(b) General published information on the permeability and storage properties of the Chalk and gravels, which was reviewed in Sections 3.2.3 and 3.4.2.2.

(c) Recharge Data and River Data, which were obtained from various sections of the Thames Water Authority. In *particular*, recharge data (see Section 1.2.1) were provided by Brian Greenfield and Cathy Glenny, who calculated the figures using a model which is based on modifications to the classic Penman equation (Glenny and Greenfield, 1982). Information on river stage, gradient, discharge and velocity were gleaned from copious records held at the River Control Room, Nugent House, Reading, by Mel Slingo and Denis Boreham. Channel profiles provided by Dick Greenaway were used to calculate streambed elevations where needed.

Before composing data files based on these sources of information, a certain amount of processing and preparation was necessary. In particular, maps showing the spatial distribution of values of various parameters had to be prepared.

Point data for gravel base elevation from various borehole records were compiled onto a 1:10,000 base map of the site, and contoured. At first, the mainframe contouring package SURFACE II was used to do this (Figure 7.1). However, the resulting plot was not logically consistent with the knowledge that the erosion surface being contoured was formed by down-cutting river channels. Therefore a second version of the contour map was prepared by hand, and in this case, because geological knowledge was added to point estimates of elevation, a more meaningful pattern emerged (Figure 7.2). This second map was used to provide estimates of gravel base elevation (variable TBASE(I,J)) for all cells in the domain.

A map of 'steady - state' water table elevation was adapted from a map of the water table position in September 1986 (prior to pumping and after summer depletion) presented by Robinson et al (1987). While it is clear that a true steady - state will never be realised in nature, this

Figure 7.1 -- Gravel Base Elevation (m AODN) Contoured by *SURFACE II.*

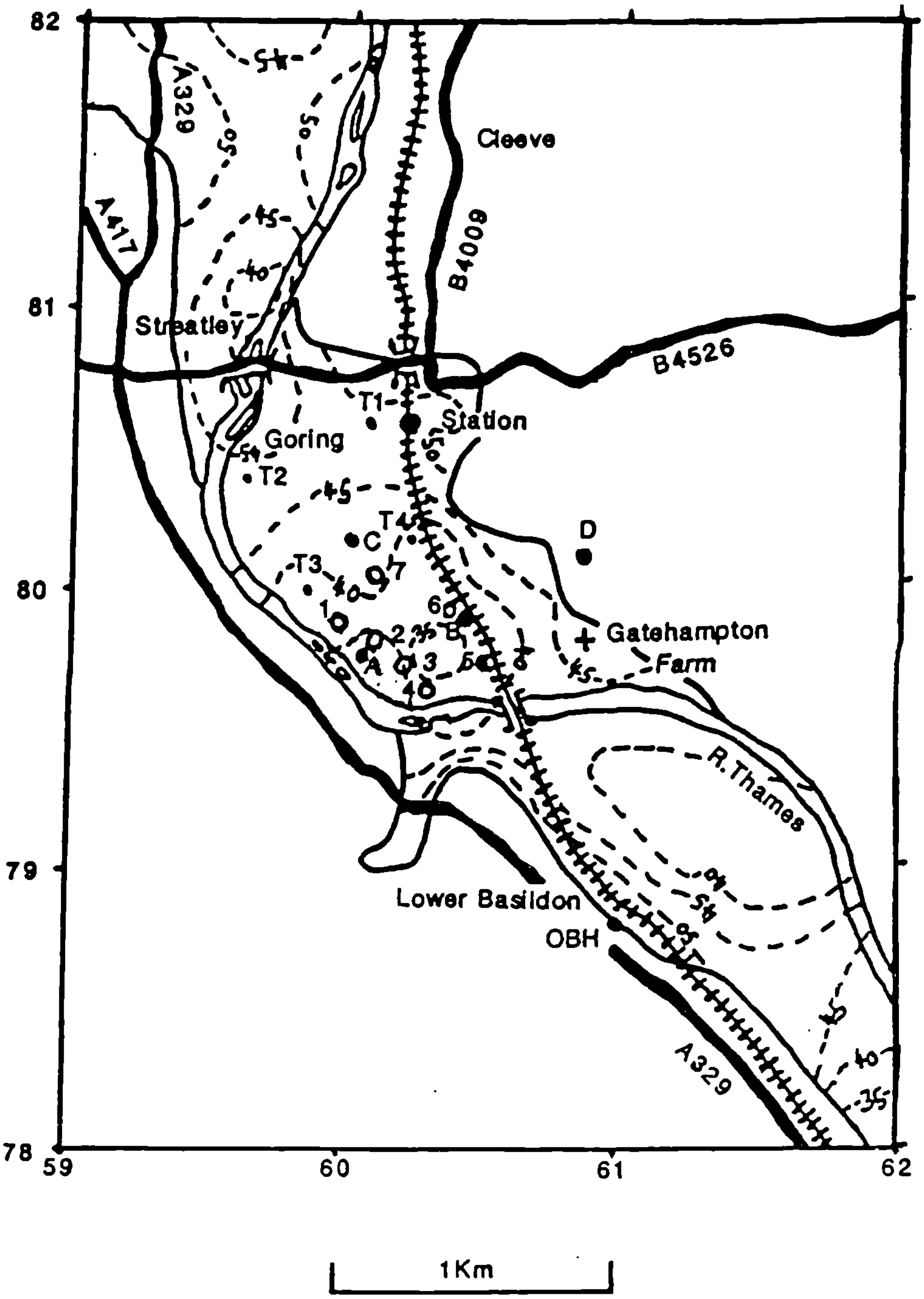
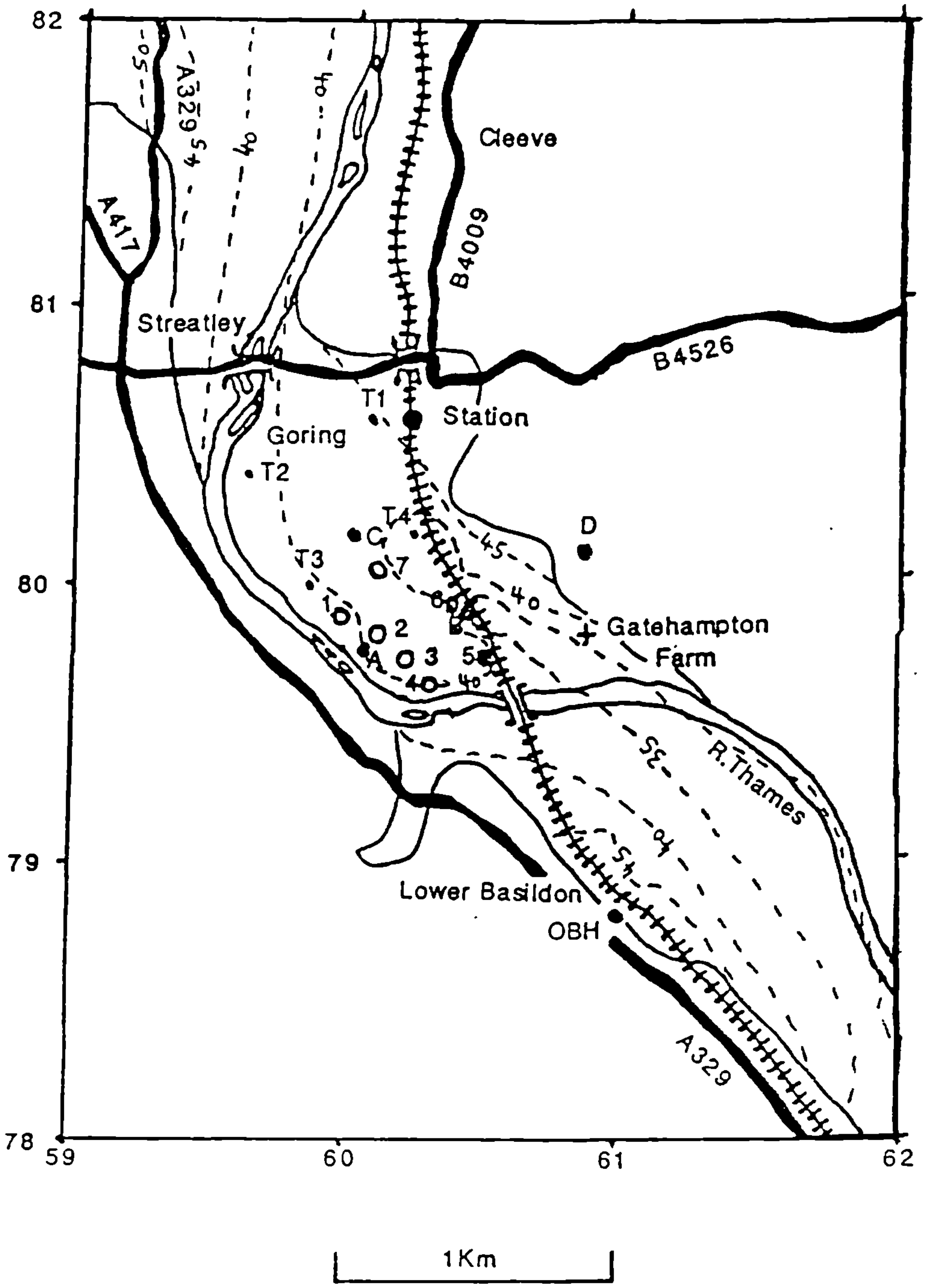


Figure 7.2 -- Gravel Base Elevation at Gatehampton Contoured by Hand.



map was felt to be the closest approximation available. Nonetheless, the divergence between assumptions and reality implicit in the selection of this map will be the source of some modelling error.

The lateral and vertical variability of Chalk permeability has been described in great detail in Chapters 3 and 4, and the information presented there was used as the basis *for* defining the spatial structure of Chalk permeability for input into US-FLOW. During the development of US-FLOW, it had been decided to use a system of 'relative hydraulic conductivities' (RHCs) for representing input data. In this approach, a key value for the hydraulic conductivity of the aquifer (usually the maximum feasible value) is entered in the main data file, and for each node an RHC value is assigned. This RHC value will be a positive real number less than or equal to 1 in most cases (although there is no reason why RHCs greater than 1 cannot be used in principle). Then at each node, the hydraulic conductivity is calculated from an expression such as:

COND(I,J) = CONMAX * RHC(I,J) . . . . . . (7.3)

where COND(I,J) = the hydraulic conductivity at node i,j
CONMAX = the 'key' value of hydraulic conductivity (usually the local maximum)
RHC(I,J) = relative hydraulic conductivity at node i,j

The advantage of the RHC approach is that the general structure of spatial variations in permeability may be held constant during calibrations while absolute values are adjusted up and down. Obviously RHCs at individual nodes can be, and were, altered during the later stages of calibration, but the correct order of magnitude for hydraulic conductivity was obtained first.

Maps of the variation in Chalk transmissivity around river valleys are available in numerous publications (eg

Woodland, 1946; Ineson, 1962; Connorton and Reed, 1978; Owen et al, 1977). However, because transmissivity is an integral of hydraulic conductivity over the aquifer thickness, transmissivity maps confound two separate pieces of information; namely information on the hydraulic conductivity distribution and information on variations in aquifer thicknesses. Because saturated thickness is not constant spatially or temporally in the unconfined Chalk it seems more logical to map hydraulic conductivities than transmissivities. Prior to the start of calibration, therefore, a map of RHCs for the Goring Gap was prepared. To facilitate preparation of this map, the relationship between elevation of ground surface and RHC had to be estimated. A logarithmic relationship was adopted on the basis of linear regression of published data, and on the basis of information presented by Morel (1979) and Robinson (1976). For the Goring Gap, this was of the form:

$$\left.\begin{array}{ll} (E_S < 45) : & RHC = 1.0 \\ (45 < E_S < 160) : & \log_{10}RHC = 1.169 - 0.026\ E_S \\ (E_S > 160) : & RHC = 0.001 \end{array}\right\} \quad (7.4)$$

Where E_S = Elevation of land surface

In other words, all Chalk beneath the Gravels (surface elevation 45m or less on the geological maps) has the maximum RHC (cf Chapter 4), while all land at or above the crest height of the Chilterns (160 m) is underlain by Chalk with minimal RHC (0.001). Between these two extremes, the approximate relationship between surface elevation and the RHC of the underlying Chalk is given by the logarithmic equation. While this mathematical description was derived more from geological inference than from strict quantitative analysis, it did allow a map of RHC distribution in the Goring Gap to be prepared by simply calculating the RHC value represented by topographic contours on the Ordnance Survey 1:10,000 base map. The usefulness of this simple model may be gauged by the success of its application in the numerical modelling.

The RHC method is also applicable to vertical variations (see Appendix B and Connorton and Reed, 1978), and it was applied to the Gatehampton site for all nodes where the Chalk underlies the Shepperton Gravels, in accordance with the geological model of Chapter Four. The spatial structure with depth was assumed constant across the site, and was determined according to flowmeter data from ABH 3, the analysis of which is presented in Appendix B (Table B.6).

The elevation of the effective base of the Chalk aquifer is a difficult parameter to quantify, for, unlike many other aquifers, the stratigraphic base of the Chalk usually lies well below the depth at which it ceases to contribute to the main flow regime. Previous workers in the Middle Thames area have suggested that the Chalk beneath the river valleys is permeable to depths of 50 to 60 metres, but that below this depth, enlarged fissures are generally absent and the Chalk is effectively impermeable (Robinson et al, 1987; Owen et al, 1977). As a starting point for calibration, therefore, it was simplistically assumed that the effective base of the Chalk aquifer could be calculated as 'ground level minus 60 metres' throughout the domain. During calibration, this was found to be unsatisfactory in the lower areas of the interfluves, and adjustments were made accordingly.

7.2.2 -- Steady - State Calibration.

The grid used in the steady - state calibration for the Gatehampton site is shown in Figure 7.3. As shown in the Figure, variable grid spacings were used, so that greater detail could be represented in the 'key' areas of the domain, ie the wellfield and all stream nodes. Two types of boundary condition were used; fixed - head boundaries (in the interfluve areas) and no - flow boundaries (along flowlines which intersected the stream away from the

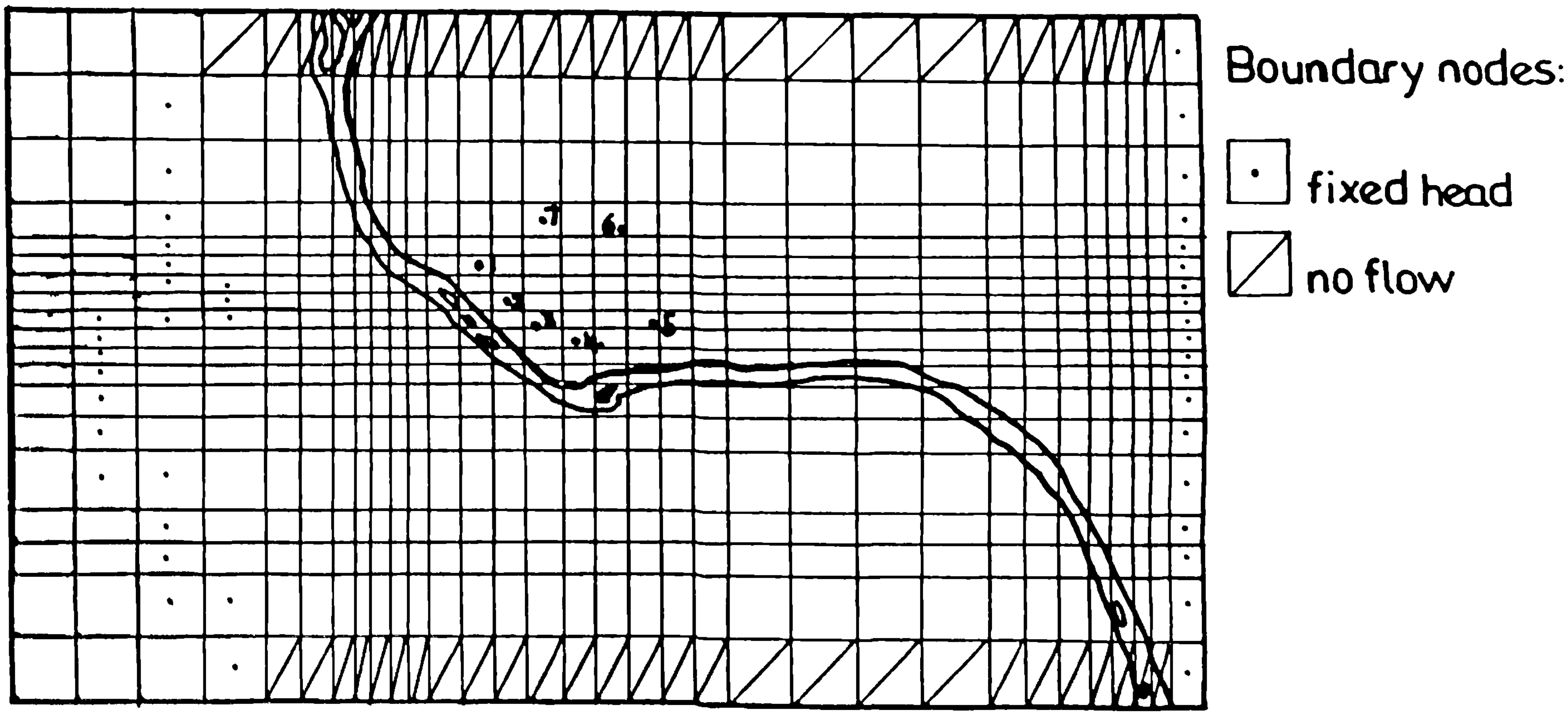


Figure 7.3 -- Main Gatehampton Finite Difference Grid.

wellfield). The long - term mean recharge rate for the Chiltern area (350mm per annum) was assumed for this exercise.

Initial Values. Permeabilities were set uniformly high in the gravels (RHC = 1.0 at all nodes), but were spatially varied in the Chalk according to the constraints (7.4) given above. Initial values for maximum hydraulic conductivity were 100 m/d for the Chalk, and 1500 m/d for the gravels. The thickness of the streambed sediment was initially set at 0.1m, but was soon raised to 0.5m to avoid problems with the critical hydraulic gradient. Streambed hydraulic conductivity was initially set at the laboratory value of 0.002 m/d at all stream nodes, but it was found to be impossible to reduce the root mean square error (RMSE; equation 7.1) between computed and observed water table elevations below 3m without increasing the value of this parameter considerably.

Final Values. After a long period of trial and error, a set of values emerged which gave the lowest RMSE values (0.338m), produced no problems with the critical hydraulic gradient and gave good agreement between observed and modelled baseflow discharges (7776 $m^3/d/km$ and 6280 $m^3/d/km$ respectively) in the modelled reach. This set of values is listed in Table 7.1 below. It must be stressed that a certain amount of variation in gravel hydraulic conductivities was represented, although for the most part values other than that quoted in Table 7.1 were restricted to positions close to the gravel feather edge (where the preservation of F1 facies in the main body of the Shepperton Gravels is more likely) and near model boundaries (where effects of slight inaccuracies in the positioning of the no - flow boundaries had to be countered). Very little adjustment of the estimated Chalk RHC distribution was necessary to achieve the final calibration, suggesting that equation (7.4) and its related conditions are a reasonably accurate description of lateral

Table 7.1 -- Parameter Values in the Steady - State Calibrated Model for Gatehampton.

Parameter	Value
Hydraulic Conductivity:	
(a) Chalk (maximum, below gravels)	170 m/d
(b) Chalk (minimum, interfluves)	0.17 m/d
(c) Gravels (majority of nodes)	1500 m/d
(d) Streambed Sediment	0.2 m/d
Thickness of Streambed Sediment	0.5 m

variations in permeability for the Chalk of the Goring Gap.

The streambed sediment parameters were held constant at all stream nodes, save at sharp bends in the river, where a slight thinning of the sediment (to 0.40 or 0.45 m) was represented. This thinning is consistent with sedimentological considerations (scouring at bends), and it led to improvements in the calibrated head distribution and the RMSE.

Superimposed contour maps for observed and modelled steady - state heads are given in Figure 7.4. Agreement is best in the centre of the domain, where it is most crucial, but less accurate high in the interfluves (where effects of the model boundaries are most acute).

The modelled water budget for the Gatehampton area is quite simple, since there are only two inflow routes (recharge and flow through model boundaries) and one outflow route (baseflow to the Thames). The figures produced by the model are given below in the form of an annotated equation, in which the total inflow (on the LHS) can be seen to equal the total outflow (on the RHS). All figures are in m^3/d.

7814	+	11026	=	18840
Recharge	+	Inflow from Regional Chalk Aquifer	=	Baseflow

These figures indicate that recharge to the aquifer in the direct vicinity of the river valley (ie the domain modelled here) accounts for only 42% of the total amount of water which flows into the river as baseflow. Thus, despite their lower transmissivities, those portions of the Chalk which lie below the interfluves behave as a vast reservoir of slowly moving water, contributing 58% of the baseflow in the Gatehampton area. From this result it might be anticipated that wells constructed in the river valleys have the potential to exploit a much larger total resource than may have at first seemed likely.

7.2.3 -- Transient Simulation Exercise.

As there is a vast body of data from aquifer testing at Gatehampton, it was decided to concentrate on the most important phase of group test pumping (September to October 1986) when devising a transient simulation exercise to test the calibrated hydraulic conductivity distribution. Since the 'observed' head distribution used in the steady - state calibration was that exhibited by the aquifer prior to the start of the main group test, it was possible to use the output head distribution from this calibration as the initial conditions for the transient simulation.

Wells are represented in the model by the nearest node. Modelled heads for observation wells can be compared directly, but corrections have to be made to modelled heads for pumping well nodes to allow for two effects;

(a) the difference between finite difference cell dimensions and actual well diameters (Rushton and Redshaw, 1979), and

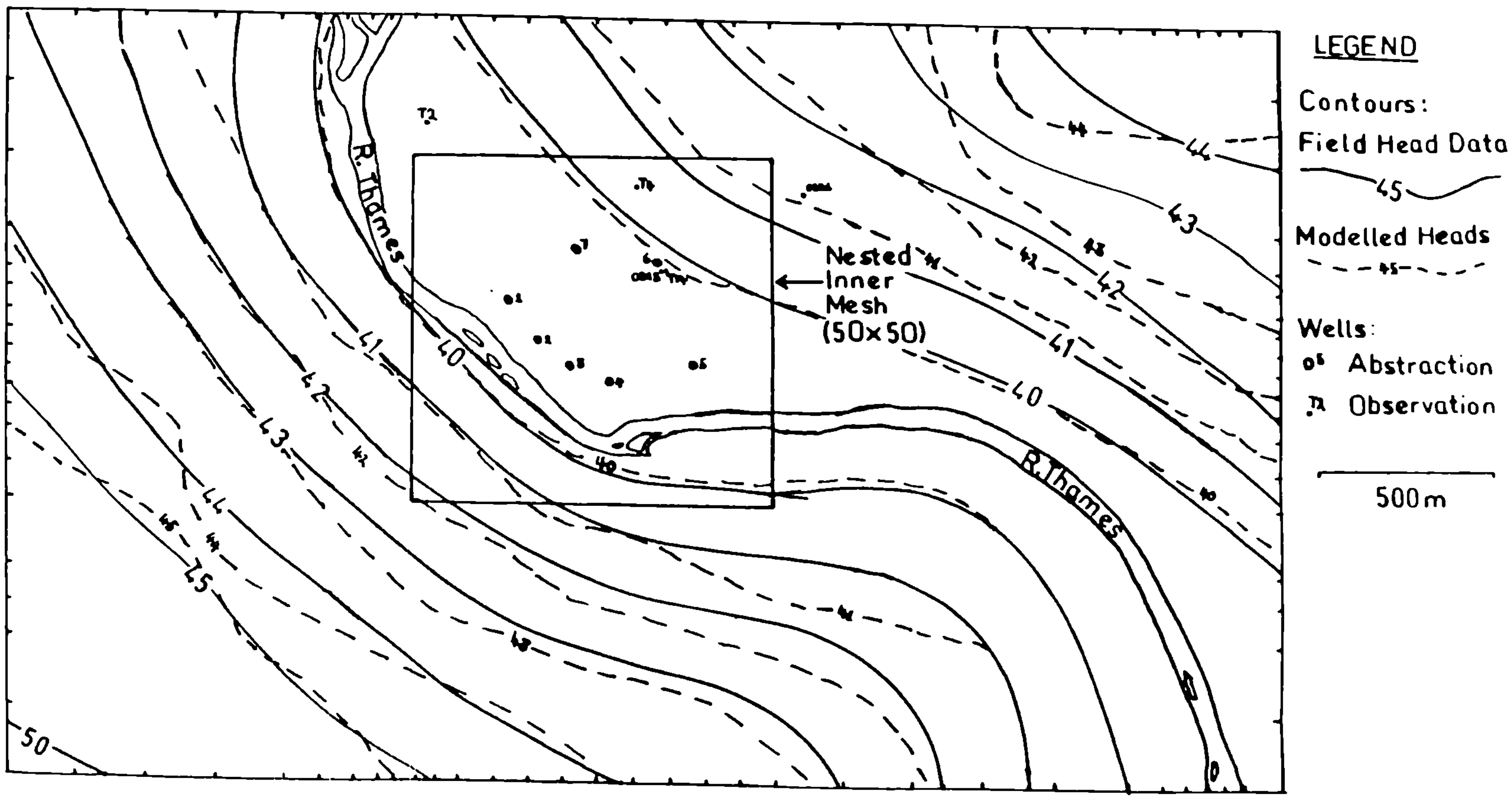


Figure 7.4 -- A Comparison of Observed and Modelled 'Steady - State' Groundwater Heads for Gatehampton.

(b) well loss, due to turbulent flow in the well screen, gravel pack and/or within the casing (Todd, 1980).

Since corrections for these effects have been reviewed recently by Lerner (1989), detailed discussion is omitted here. The cell dimension correction technique, which invokes the Thiem equation for radial flow, was taken directly from Rushton and Redshaw (1979). To determine the well loss coefficient (C_{wl}) for a given well, the step-drawdown data presented by Robinson et al (1987) were used. For each well, values of the ratio (drawdown / pumping rate) were calculated for the various pumping rates in the step - test, and the public domain programme CURVEFIT was used to fit optimal straight lines to the data sets so formed. The C_{wl} is simply the gradient of such a line (Todd, 1980, pp. 152 - 156). Once a value for C_{wl} has been obtained, the turbulent well loss (W_l) for the well at a given pumping rate (Q) is given by:

$$W_l = C_{wl}Q^2 \quad . \; . \; . \; . \; . \; . \quad (7.5)$$

Table 7.2 gives the values of C_{wl} obtained for each of the Gatehampton ABHs. Using these values, the modelled drawdown at each well was calculated from the finite difference head at the end of each timestep using (7.5).

Storage parameters for the model were estimated from the sources cited in Chapter 3 and Section 5.2.3, and, in lieu of any information to the contrary, were assumed to be constant throughout each hydrostratigraphic unit. The values for specific yield (Sy) and storativity (S) used were as follows:

Unconfined Chalk (Sy): 0.01
'Confined Chalk' below gravels (S): 0.0008
Unconfined Gravels (Sy): 0.25
Streambed Sediment (S): 0.00005

Drawdown data for the Gatehampton test are available for tubewells (which are restricted to the gravels),

Table 7.2 -- Values of the Well Loss Coefficient (C_{wl}) for the Gatehampton Wells.

ABH Number	C_{wl} (d^2/m^5)
1	1.6×10^{-8}
2	1.4×10^{-8}
3	1.5×10^{-8}
4	7.2×10^{-9}
5	4.1×10^{-8}
6	1.4×10^{-8}
7	1.4×10^{-8}

observation wells and abstraction wells (both types cased through the gravels and screened in the Chalk). Coverage of the site was extremely thorough (Robinson et al, 1987) and therefore detailed comparisons of observed and modelled heads could be made for many points in the simulation domain. Selected examples of these comparisons are given in Figures 7.5 and 7.6. In Figure 7.5, the best (ABH 3) and worst (ABH 5) examples of abstraction borehole comparisons are given. The agreement of observed and modelled heads is remarkably good, especially in view of the difficulties which are commonly experienced by modellers in predicting drawdowns at pumping wells (Lerner, 1989). When it is considered that the caliper log for ABH 5 shows fissuring to be less well developed here than elsewhere in the site (indicating a departure from the assumption that the distribution of Chalk permeability with depth is constant across the site), and that ABH 5 has the worst yield - drawdown characteristics of all the Gatehampton ABHs (Robinson et al, 1987, pp. 9 - 10), even the errors in the match for this borehole seem pleasingly small.

Figure 7.5 -- Observed and Modelled Drawdown Behaviour for Abstraction Boreholes in the Main Gatehampton Pumping Test.

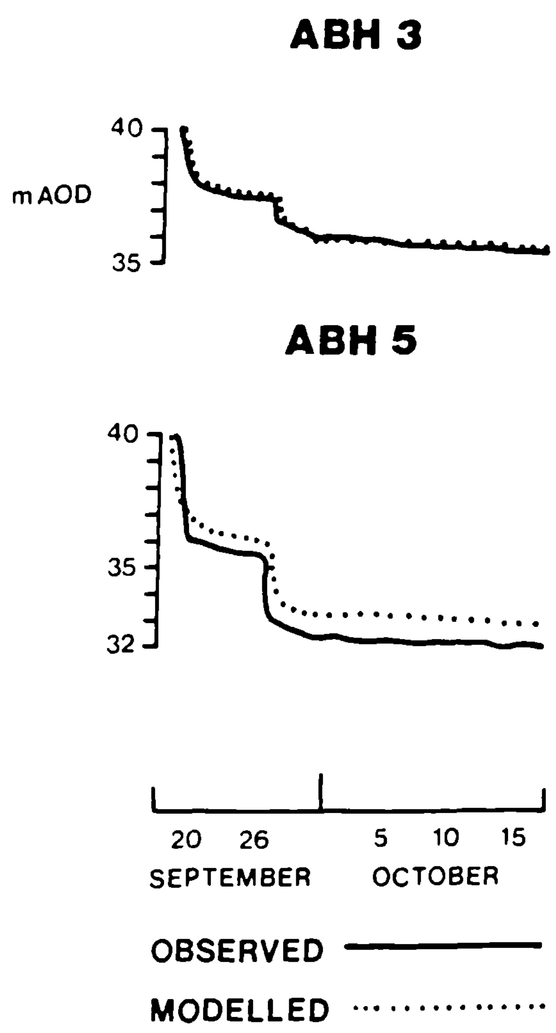
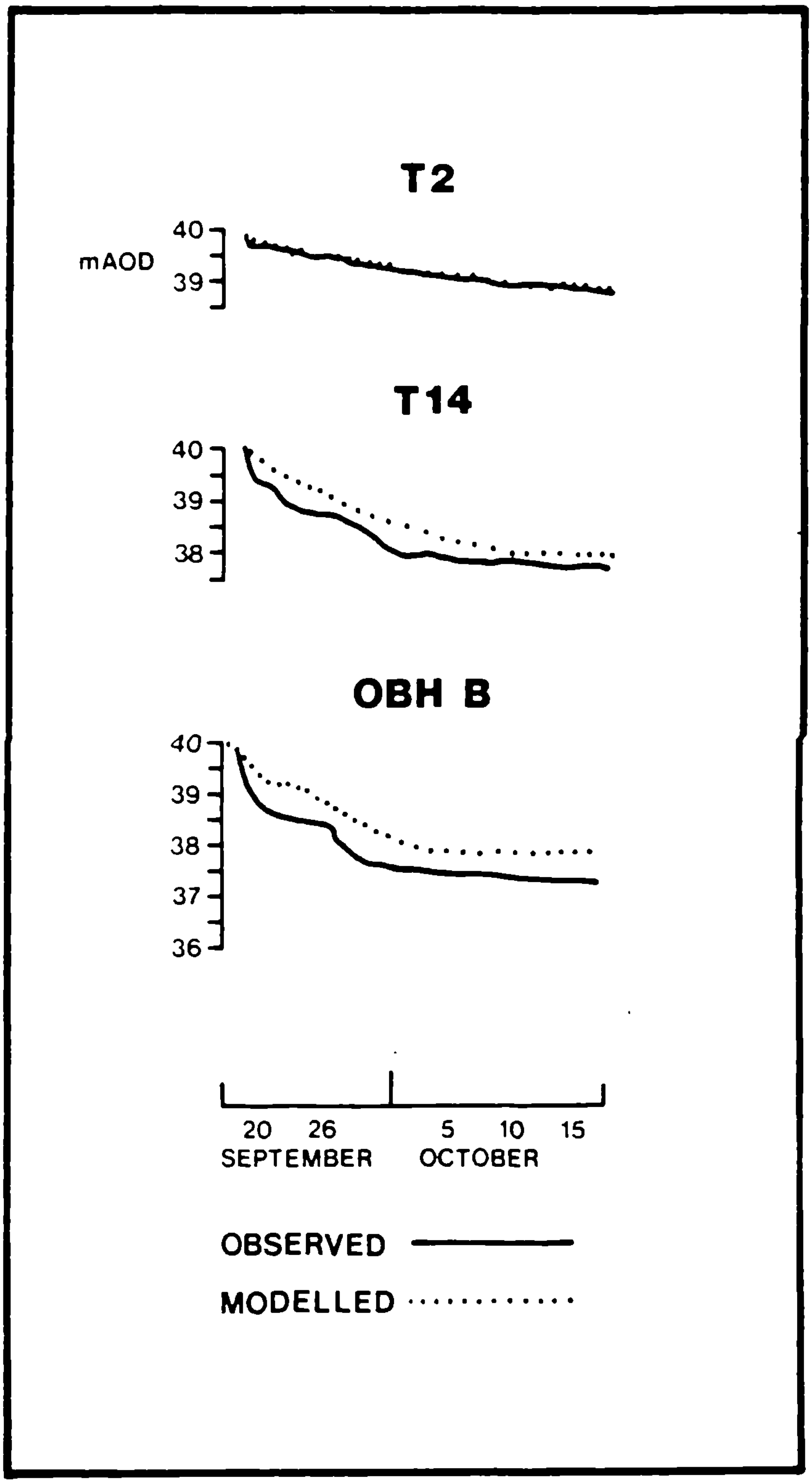


Figure 7.6 -- Observed and Modelled Drawdowns for Tubewells and Observation Wells in the Main Gatehampton Pumping Test.



While the ABH data suggest that the drawdowns have been modelled correctly, it is satisfying to note that head behaviour elsewhere in the aquifer has also been adequately represented. In particular the excellent agreement between observed and modelled heads for gravel tubewell T2, which is remote from the pumping wells (Figure 7.6), is very encouraging. The other two plots in Figure 7.6 allow some appreciation of the performance of the two-layered formulation of US-FLOW, since tubewell T14 monitored gravel heads immediately adjacent to the Chalk observation well OBH B. Both wells lie close to ABH 6, and might be expected to show considerable errors due to non-Darcian turbulent flow in the vicinity of the ABH. Since T14 is a piezometer, measuring head at a specific depth within the gravels, rather than the averaged head predicted by US-FLOW, it is felt that the hydrographs show reasonable agreements between observations and model results. This suggests that the two - layer coupling method used in US-FLOW performs adequately for field problems.

7.2.4 -- Steady - State Site Model.

Having obtained a satisfactory transient simulation for the Gatehampton site, heads from the final timestep of the transient run (when the model was pumping at licensed capacity) were used to define fixed heads around the entire boundary of the 50 x 50 nested grid shown in Figure 7.4. A steady - state head distribution was then obtained, using the parameter values interpolated from the main grid along with licensed well yields and the estimated average annual recharge. Comparison of the heads at pumping wells with the final heads from the pumping test simulation showed little difference, suggesting that the transient regime had reached a dynamic equilibrium by the end of the main pumping test.

On the basis of this site model, the amount of river-derived water in the total site yield at steady - state was calculated. A figure of 5.316 TCMD was obtained, which corresponds to about 8% of the site yield. Because flows from stream nodes outwith the site domain were not included in this figure, it is likely that the true figure is slightly higher, but it is not expected to exceed 10%. This figure is low compared to the value of 70% quoted by Edmunds, Owen and Tate (1976) for riverside chalk boreholes at Taplow. However, at the latter site, streambed sediment is known to have been absent during test pumping due to scouring in the tail pool of the weir adjacent to the wells (Edmunds, Owen and Tate, 1976). Furthermore, the transmissivities at Gatehampton far exceed those at the Taplow suggesting that far more 'native' groundwater water is available at Gatehampton than at Taplow. In the light of the comments made in Section 7.2.2 above (where the water budget for the main model domain was discussed) it seems reasonable to conclude that the modelled river contribution is compatible with the inflow of large quantities of groundwater from the regional Chalk aquifer.

This model was based on a typical 'summer flow' regime in the river. The amount of water entering the aquifer under these conditions is minute compared with the total discharge of the river in this reach (864 TCMD), amounting to only 0.6%. In passing, it should be noted that the total depletion of river flow caused by the Gatehampton site will be greater than this, since interception of groundwater that would otherwise have discharged to the river as baseflow must also be taken into account. The 'mean' baseflow for the reach during typical summer flow is estimated at 3.888 TCMD. If it is assumed that this 'mean' baseflow equals the intercepted flow at the site, then the total river discharge depletion for the site will be about 9 TCMD (ie about 1%).

Since particle tracking results for Gatehampton presented in Chapter 8 were obtained from simulations based on the steady - state site model, further discussion of the modelled flow regime may be found in that Chapter.

It is worth noting that, during the course of this project, a separate flow model of the Gatehampton site was independently developed at the Water Research Centre, Medmenham (WRC, 1988) in order to test a newly developed multi - layered finite element flow code. Comparison of the input and output of the two models revealed close agreement. Calibrated transmissivities and storage parameters in the two models were very similar. On the whole, the correspondence between observed and modelled drawdowns was better in the present model than in the WRC (1988) model, probably because a wider domain was modelled in this case, which reduced the effects of fixed head boundaries (cf WRC, 1988, p. 13). Nonetheless, the good agreement between the two independent flow models is very encouraging.

7.3 -- THE DORNEY FLOW MODEL.

7.3.1 -- Data Selection and Preparation.

The main sources of data for the Dorney flow model, which were similar to those used for the Gatehampton model (Section 7.2.1), were as follows:

(a) Site - specific information used was mainly obtained from the site investigation report of Ridings et al (1977), supplemented by information from reports by Edmunds, Giddings and El Agib (1977) and Flavin (1986), which were reviewed in Section 3.5.2.2.

(b) General published information on the permeability and storage properties of the gravels, which was reviewed in Section 3.4.2.2.

(c) Recharge Data and River Data were obtained from the same sources as for the Gatehampton model (Section 7.2.1). On account of the low relief in the Dorney area, the mean annual recharge rate is thought to be somewhat lower than for the hilly area around Gatehampton (Greenfield, 1988, personal communication), and accordingly, the steady-state calibration was based on an annual rate of 200mm.

Because the geology of the Dorney site (Section 3.5.2.2) is much more simple than at Gatehampton, very little processing and preparation of data was needed before commencing calibration runs. It was felt, for example, that assuming constant elevations for the major hydrostratigraphic interfaces (gravel base, streambed sediment base, ground level) involved no major departures from reality, while affording considerable advantages in data input to the model. Streambed sediment properties and gravel hydraulic properties were also assumed constant throughout the domain as a first approximation.

A map of 'steady - state' water table elevation was adapted from a map of the water table position in April 1976 (prior to pumping) which was drawn up by Ridings et al (1977). The same cautions apply to use of this map for steady-state calibration as to the Gatehampton map (ie uncertainties about the accuracy of the map, and the fact that a true 'steady - state' is a fiction in nature).

<u>7.3.2 -- Steady State Calibration.</u>

Design of the model grid for the Dorney site was undertaken in such a manner that the wider aquifer and the wellfield area could both be represented in sufficient detail on the same grid, thus avoiding any need to use a nested modelling approach. The final design is shown in Figure 7.7, where it may be observed that a square central portion (30 x 30) with a constant 25m spacing covered the wellfield, while spacings up to 350m were used for outlying cells near the model boundaries. Altogether a 3.5km by 2km area was represented by the model grid.

<u>Initial values</u> for the hydraulic properties of the gravels and the streambed sediment in the Dorney calibration were set equal to the final values obtained for the same properties in the Gatehampton simulation. The RMSE value obtained from the very first run (0.342m) was encouragingly

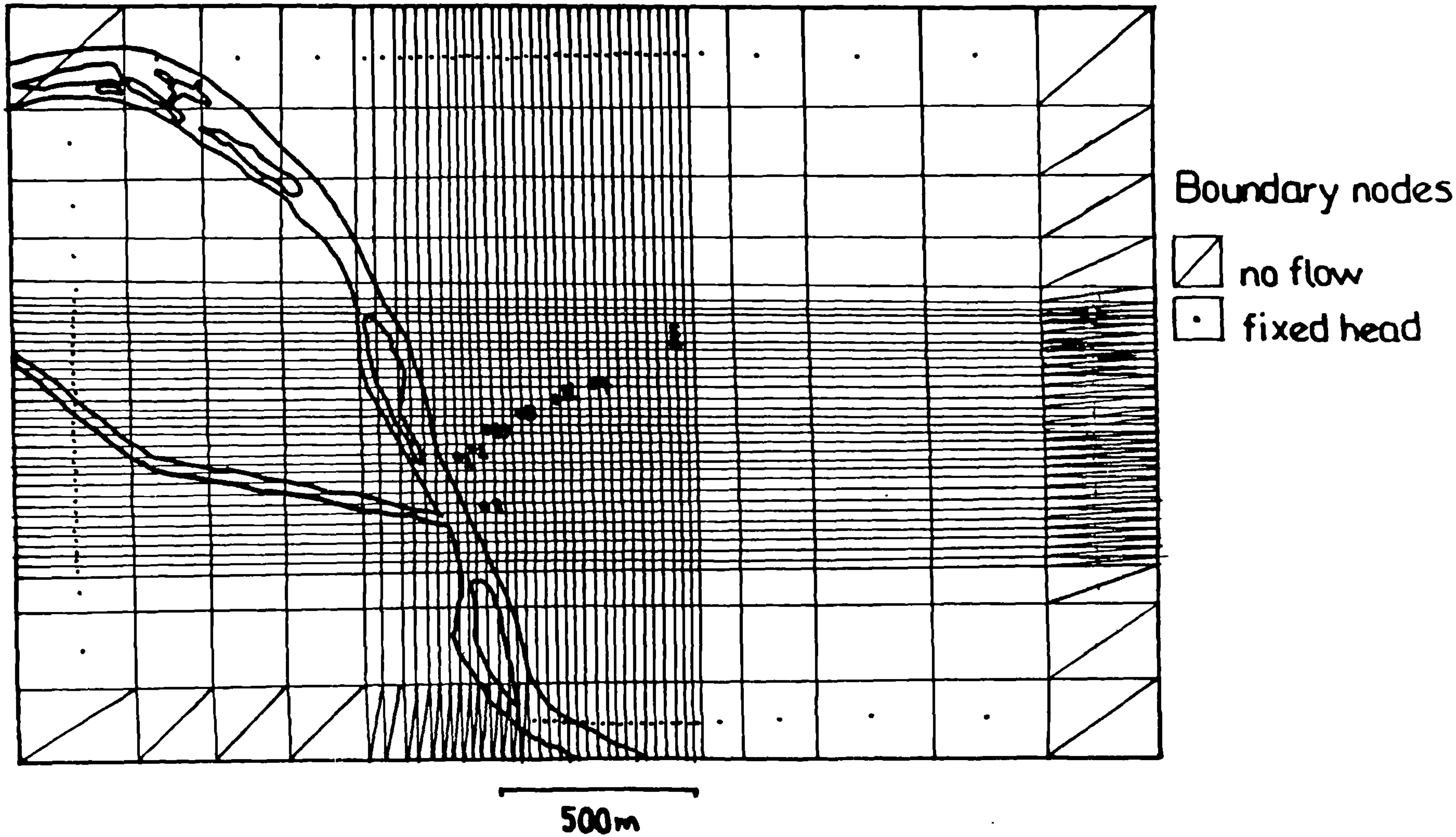


Figure 7.7 -- The Dorney Finite Difference Grid.

low, but because the contour spacing on the field data map was very fine (0.1m, compared with 1.0m at Gatehampton), the difference between maps of observed and predicted heads was still quite marked.

Final Values. Trial and error eventually resulted in the selection of a set of parameters which minimised RMSE at 0.148m, gave good agreement between observed and modelled baseflow discharges (818 m^3/d/km and 820 m^3/d/km respectively), and gave no problems with the critical hydraulic gradient. Since the final calibrated model proved rather insensitive to rather wide variations in gravel hydraulic conductivity (Section 7.4), however, a range of possible values is quoted for this parameter. The final values were as follows:

Gravel hydraulic conductivity (m/d): 700 to 1200
Streambed sediment hydraulic conductivity (m/d): 0.015
Thickness of the streambed sediment (m): 0.4

The most remarkable feature of these results is that the streambed hydraulic conductivity is an order of magnitude lower than the value used in the Gatehampton model (0.2 m/d). However, the model was quite sensitive to changes in this value (Section 7.4), and attempts to use higher values caused considerable increases in RMSE. Although the value used is still an order of magnitude higher than the lab permeameter value for Dorney sediment (0.0017 m/d; Appendix C), further explanation of this low value is desirable. The occurrence of lower hydraulic conductivities at Dorney than at Gatehampton is consistent with sedimentological observations (Section 3.4.4.2) that the Dorney sediments have a higher proportion of fines than the Gatehampton sediments (see Figure 3.8), and that lamination and compaction have been described from sediment samples taken near Dorney while no such features have been described from Gatehampton.

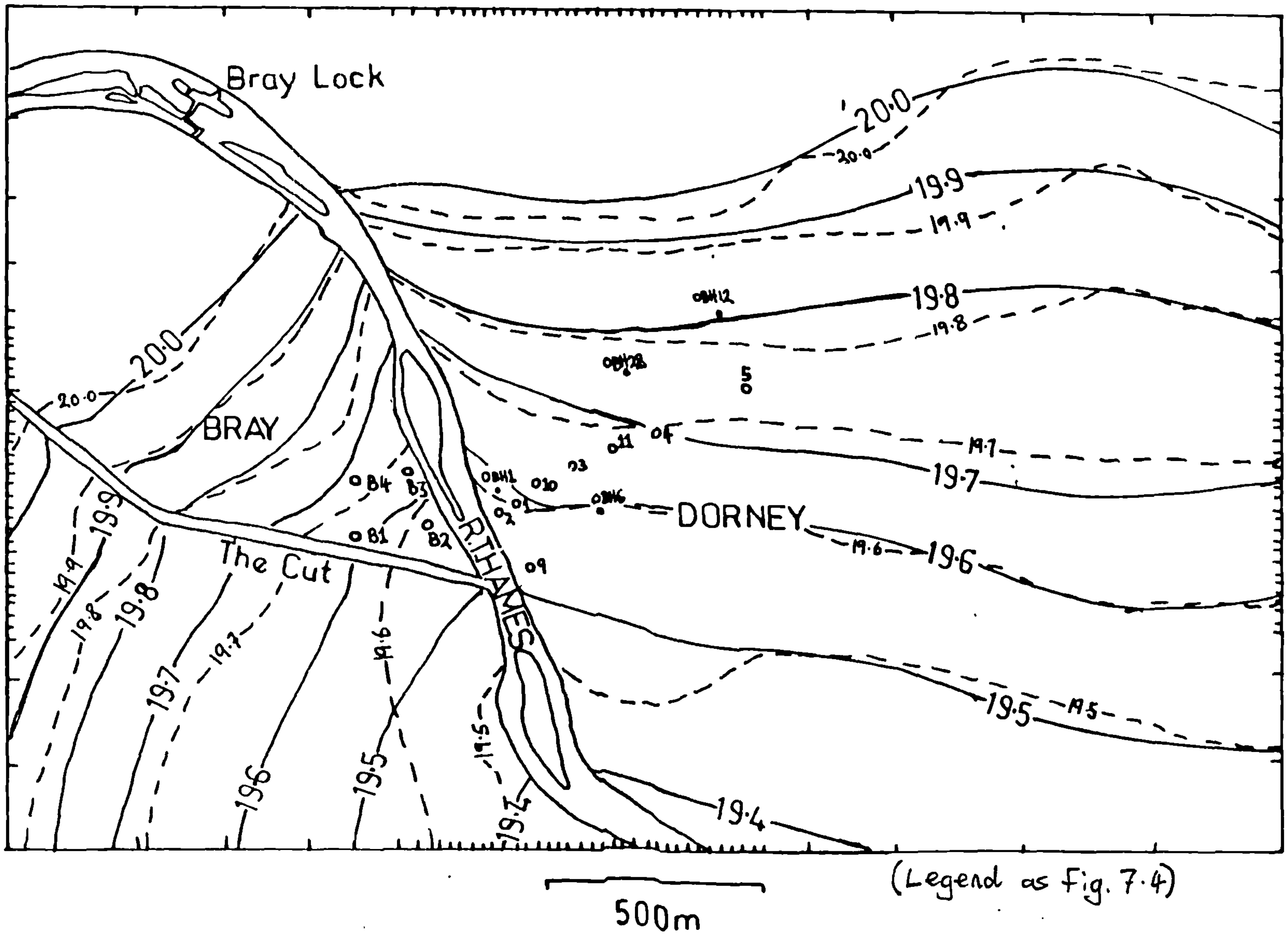


Figure 7.8 -- Observed and Modelled 'Steady - State' Groundwater Heads at Dorney.

The gravel hydraulic conductivities are very high, though still somewhat lower than the 1500 m/d obtained in the Gatehampton calibration. Banks (1989) has recently reported values for gravel hydraulic conductivity at Bray which are somewhat lower than usual. Reflecting upon the geological model presented in Chapter 4, it is likely that the exceptional width of the depositional valley of the Shepperton Gravels at Dorney (4 km) led to the development of a great number of anabranch channels, thus increasing the frequency of abandoned channels, thereby favouring the preservation of silty channel fills in the sequence. A somewhat lower mean hydraulic conductivity than at Gatehampton therefore seems geologically reasonable.

Observed and modelled heads from the steady - state calibration (contoured on Figure 7.8) show good agreement in the vicinity of the wellfield, but are less accurate towards the no - flow boundaries at the southern edge of the domain. It must be stressed, however, that the contours of field head are at their most conjectural in that area in any case (Robinson, personal communication, 1989).

The water budget calculated for the calibrated steady-state model indicates that, even though recharge is lower than at Gatehampton, it is more than sufficient to supply all of the baseflow in the modelled reach. In the form of an annotated equation (with all values in m^3/d), the full budget can be written:

3190	+	4322	=	2460	+	5052
Recharge	+	Inflow through northern model boundary	=	Baseflow	+	Outflow through southern model boundary

The substantial inflows and outflows through the model boundaries are the inevitable consequence of the head distribution which was used in the calibration (Figure 7.8), and the true significance of these flows needs a little explanation. The general east - west disposition of groundwater contours east of the Thames in the modelled domain are a local expression of two hydrogeological features which lie immediately outside the modelled domain. To the north, the gravels form a feather edge along the edge of the chalk scarp which runs eastwards from Taplow towards Slough; along this line, the gravels receive a substantial inflow of chalk groundwater. To the south, the Thames swings into an easterly direction at Ruddles Pool (SU 937772), and maintains this orientation as far as Eton, some 4km downstream. These two features explain the presence of a north - south through - flow, in which water contributed to the gravels by the regional chalk aquifer flows south to sustain baseflow in the Ruddles Pool - Eton reach of the Thames. The water flowing through the modelled area clearly represents a large resource available to production wells in this area.

7.3.3 -- Transient Simulation Exercise.

Available data from pumping tests at Dorney (Ridings et al, 1977) are far less detailed than those from Gatehampton. For instance, there is no step - drawdown test information, and therefore the facility in US-FLOW for incorporating well losses into the calculation of total drawdown at pumping wells could not be used. In any case, data on the pumping rates and drawdowns of individual wells during the main group test are not available for comparison. Only aggregated pumping rates are recorded. Nonetheless, the available data are adequate for the formulation of a transient simulation, although a greater tolerance of error is called for than was needed in the Gatehampton simulation.

The simulation period adopted was the main phase of group test pumping from 26th April to June 30th 1976. As before, the steady - state calibrated head distribution had been obtained with reference to a map showing the water table elevation prior to the start of pumping, which meant that the output heads from the calibrated model could be used as initial conditions for the transient run.

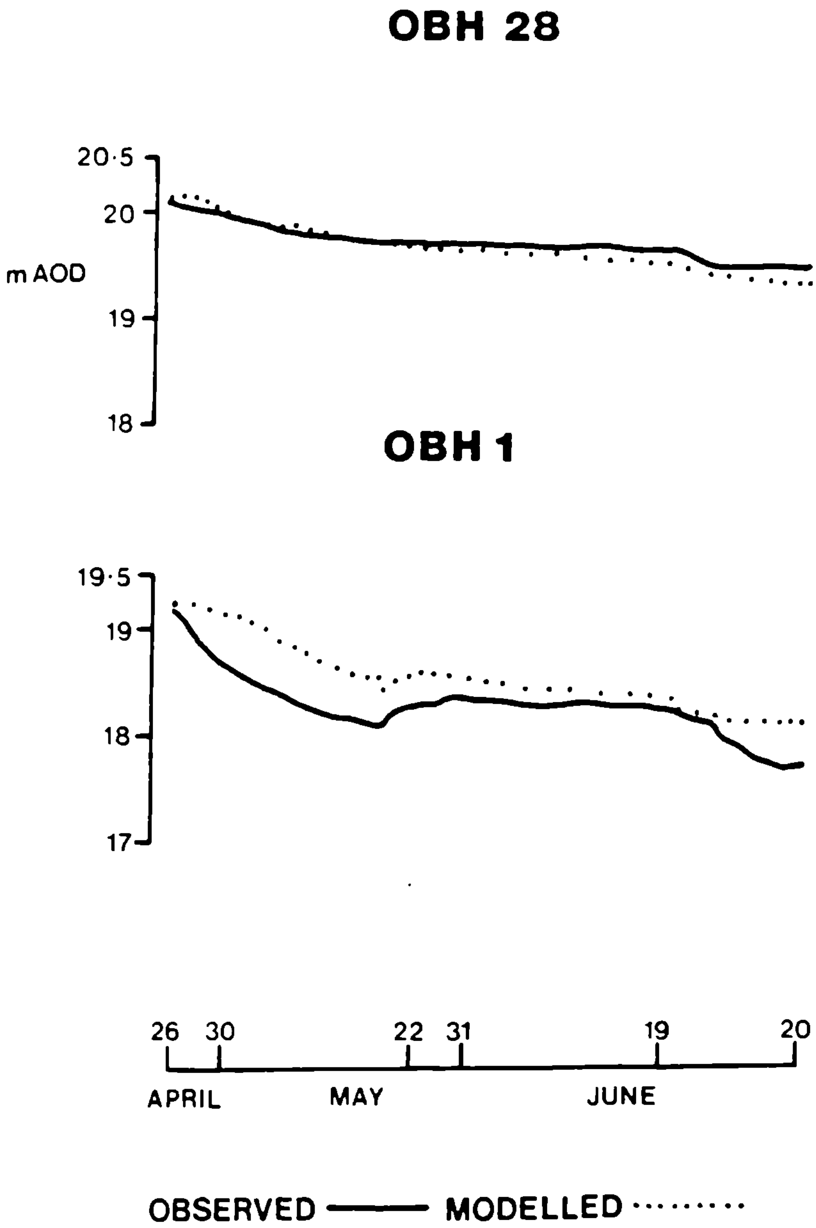
Unfortunately, pump failures bedeviled the early stages of the pumping test at Dorney, resulting in extremely complex pumping schedules and drawdown patterns prior to the start of continuous pumping (at a combined rate of 21 TCMD from eight ABHs) on April 26th. These complexities defied analysis, introducing considerable uncertainties into the simulation of the crucial early phases of the pumping test. The rest of the main group test was simulated as faithfully as possible, including a reduction in the combined rate at Dorney to 16 TCMD on May 22nd, the switching - on of the four Bray boreholes on June 19th (which reached a combined abstraction rate of 16 TCMD by June 30th), and further reductions (to 12 TCMD) at Dorney.

Given the complexities and uncertainties surrounding the Dorney test, the agreement between observed and modelled drawdowns (Figure 7.9) is reasonably satisfying. To obtain these results, a specific yield of 0.25 was used for the unconfined gravels (cf the discussion in Section 5.2.3), and a storativity of 0.001 was assigned to the gravels where they are confined beneath the streambed. As at Gatehampton, a very low storativity (0.00005) was used for the streambed sediments (cf Section 3.4.4.3).

7.3.4 -- Steady - State Site Model.

After obtaining satisfactory transient run results, all storage parameters were set to zero, all pumping rates to their licenced values, an average annual recharge rate was added to the input data, and a steady - state head distribution was obtained for use in particle tracking (Chapter 8). Since the future of the Bray site was in doubt at the time this model was developed, only the Dorney wells were included in the site model.

Figure 7.9 -- Observed and Modelled Drawdowns for the Main Dorney Pumping Test.



After the steady - state head distribution had been obtained, values for the 30 x 30 central portion of the grid were copied to separate files, so that the well field could become the sole focus of the solute transport simulations without wasting computing resources on irrelevant areas of the aquifer.

Calculation of the river contribution to the Dorney wells at steady - state yielded surprising results. A figure of 430 m^3/d was obtained, which represents only 2% of the site yield (which is 22.5 TCMD). This is considerably lower than the minimal estimate of 26% given for the site by Edmunds, Giddings and El Agib (1977).

When the modelled figure was discussed with the Thames Water Authority staff responsible for the Dorney site, however, the consensus was that the figure does not seem unreasonable in light of recent experiences at the site, where the sustainable yield now appears to be rather lower than the figure proposed by Edmunds, Giddings and El Agib (1977) after the initial test pumping (Robinson, personal communication, 1989).

It may well be that the river - derived proportion of the site yield was anomalously high in 1976 (during site development), due to the lack of general recharge during the drought. In support of this contention, it is worth mentioning a study of induced infiltration from the River Skerne into the Magnesian Limestone aquifer in County Durham described by Hamill (1980). During the installation and testing of 23 abstraction boreholes near the River Skerne in the period 1967 - 69, the recharge rate and the water table elevation in the Magnesian Limestone aquifer were well above their long - term averages. Pumping test results indicated no interaction between the wells and the River Skerne. However, when the boreholes began to be continuously pumped for supply purposes in the period 1974 - 76 (when recharge rates and water table elevations were much lower than average), significant components of leakage from the River Skerne (up to 50% of site yield) were detected at the wells. In 1978, when recharge had increased again, the river - derived component of well yield fell to zero once more (Hamill, 1980, p. 169). If such a pattern affected Dorney also, the 2% river - derived component predicted by the 'average' steady-state site model would not be at all unreasonable.

The solute transport runs gave more detailed insights into the flow regime at Dorney, and these are discussed in Chapter 8.

7.4 -- SENSITIVITY ANALYSES.

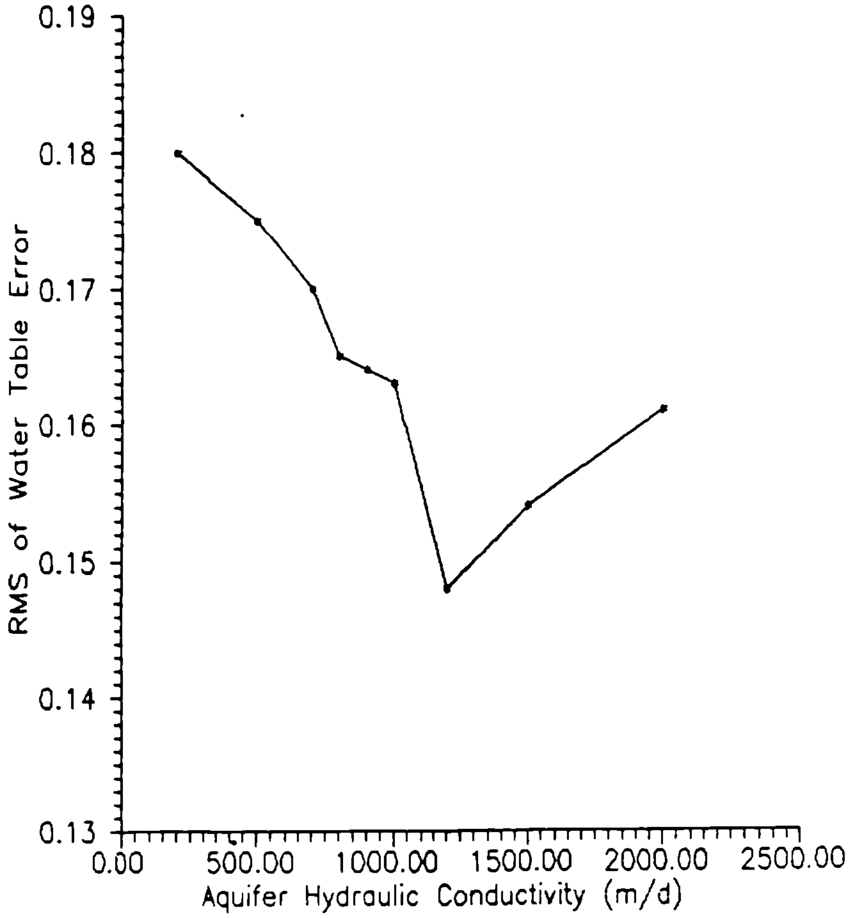
7.4.1 -- Introduction.

The term 'sensitivity analysis' may be defined as an investigation of the changes in model output caused by variations in the value of a given input parameter. Sensitivity analyses are usually included in deterministic groundwater modelling projects because:

(i) They shed light on the degree of uncertainty associated with 'calibrated' input data, and
(ii) They indicate which model parameters have the most influence on model predictions. This information is very valuable as an aid to the collection of further data.

In this study, the main purpose of the flow model sensitivity analyses is to illustrate the experiences gained during calibration with regard to the relative importance of the streambed parameters (thickness and hydraulic conductivity) in controlling model output. The sensitivity analyses discussed below were conducted as follows. Having obtained a steady - state calibration for each field site, multiple runs of the models were made in which one parameter (the analyte parameter) was varied at a time, while all other parameters were held constant. The

Figure 7.10 -- Variation in RMSE with Aquifer Hydraulic Conductivity.



root mean square error (RMSE; equation 7.1) in water table elevation across each domain was taken as the objective function for the purposes of assessing model sensitivity to variations in the analyte parameter. However, the RMSE proved insufficient in itself to describe model sensitivity in some cases (particularly in the analysis of sensitivity to streambed thickness), and other measures of sensitivity had to be used in tandem.

Numerous sensitivity analyses for groundwater models have been reported in the literature, but most of these do not include consideration of streambed parameters. Many studies have indicated the low sensitivity of flow models to fairly wide variations in hydraulic conductivity and/or transmissivity (eg Wang and Anderson, 1979; Lerner, 1985; Freyberg, 1988). This lack of sensitivity is fairly damaging to water resource predictions, and even more damaging where solute transport is modelled, because of the wide variations in groundwater velocities which are implied by subjectively choosing different values for hydraulic conductivity. However, since the impact of variations in transmissivity on model predictions has been widely discussed elsewhere, the author felt it would be more beneficial to concentrate on sensitivity analyses of stream - aquifer parameters in this study.

The few published studies which do report sensitivity analyses for stream - aquifer models are unanimous in concluding that output is far more sensitive to variations in stream parameters (in particular streambed thickness and hydraulic conductivity, and channel roughness), than to variations in the transmissivity and storage properties of the aquifer (eg Pogge and Chiang, 1977; Cunningham and Sinclair, 1979; Dillon, 1983; Bathurst, 1986; Prince et al, 1989).

7.4.2 -- Results and Discussion.

Three main analyte parameters were assessed in this study,

Figure 7.11 -- Model Sensitivity to Streambed Thickness.

(a) Effects on RMSE.

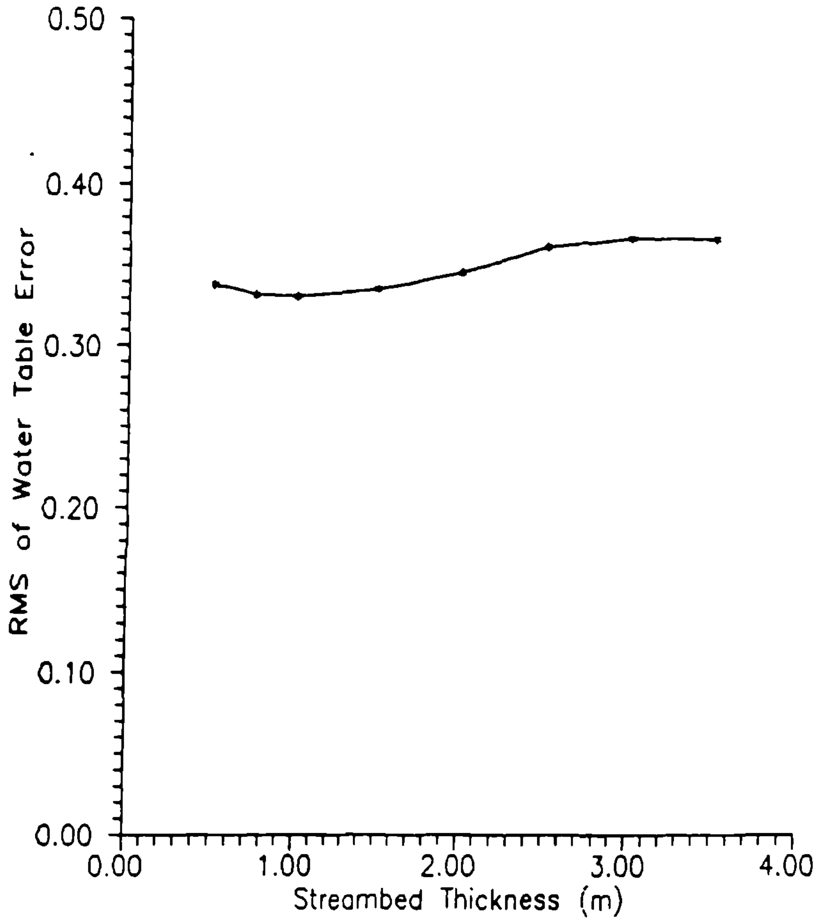


Figure 7.11 -- Model Sensitivity to Streambed Thickness (Continued).

(b) Effects on Water Table Error at a Stream Node.

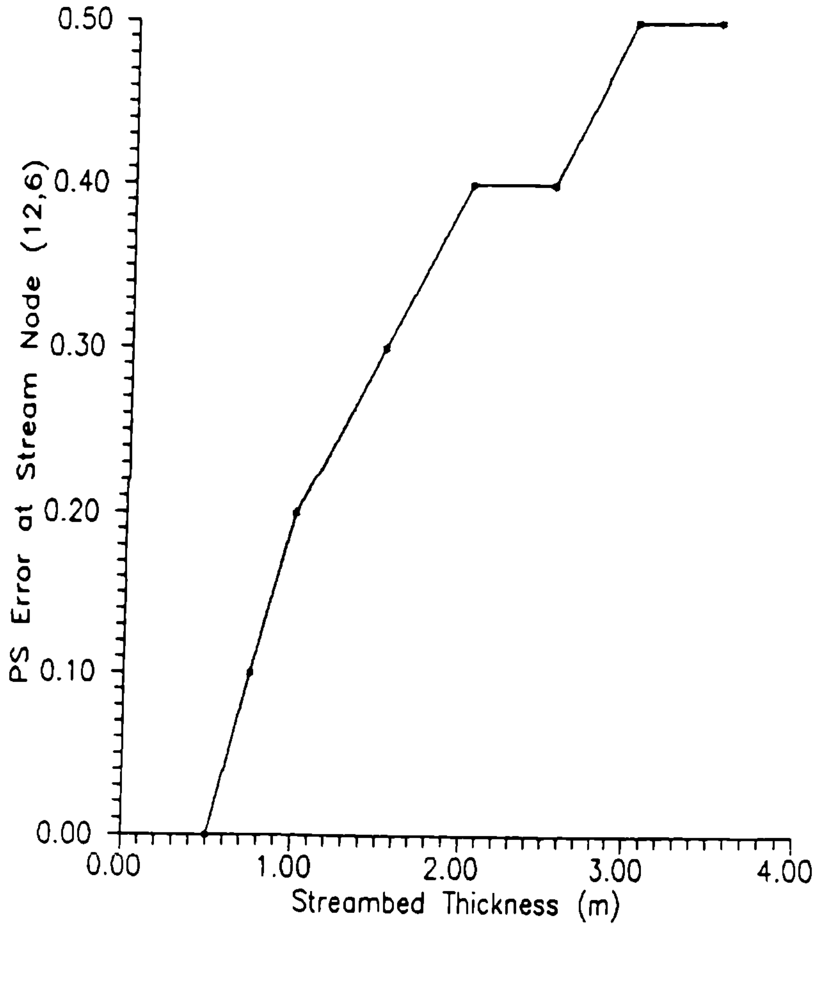
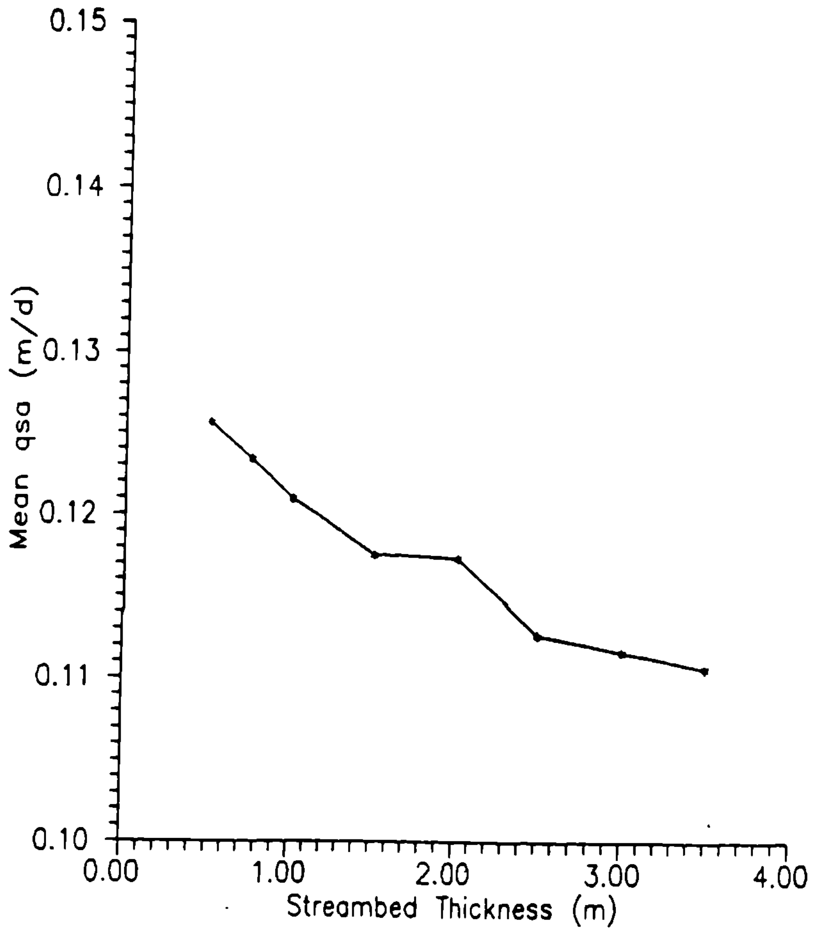


Figure 7.11 -- Model Sensitivity to Streambed Thickness (Continued).

(c) Effects on Mean Stream - Aquifer Exchange flux (qsa).



namely aquifer hydraulic conductivity (K_{aq}), streambed thickness (t_s) and streambed hydraulic conductivity (K_s). Model performance with respect to each of these analyte parameters is illustrated in Figures 7.10 through 7.12, and these results are summarised in Table 7.3. The sensitivity factor (F_s) in Table 7.3 is introduced to facilitate comparisons between variables. It is hereby defined as:

$$F_s = \frac{(\%\ \text{Variation in Objective Function})}{(\%\ \text{Variation in Analyte})} \quad . . . . (7.6)$$

In this case, the objective function is the RMSE in water table elevation, as stated above. The higher the value of F_s, the greater is the model sensitivity to that parameter. By assessing the values for F_s given in Table 7.3, it is clear that model sensitivity increases roughly in the order:

$$K_{aq} < t_s < K_s$$

These results conform closely to the findings of earlier authors mentioned above.

During calibration, the relative importance of these three parameters in controlling model output was experienced time and time again. It is not surprising therefore that a delicate balancing act was required to find combinations of all three parameters which would yield minimal RMSE values and 'correct' baseflows.

With reference to Figure 7.11 (a), it is clear that the RMSE in water table elevation for the domain as a whole is not particularly sensitive to rather large changes in streambed thickness. However, it cannot be concluded from this that all values of thickness are equally satisfactory. As shown in Figure 7.11 (b), the variation in the error in the piezometric surface in the gravels immediately below the streambed (at model node i = 13, j = 2) is quite marked

Table 7.3 -- Flow Model Sensitivity Analyses: Summary of Results.

Analyte	% Variation in Analyte	%Variation in RMSE	Sensitivity Factor (F_s)
K_{aq}	900	22	0.024
t_s (D)	127	13	0.102
t_s (G)	250	11	0.044
K_s (D)	220	16	0.074
K_s (G)	1000	640	0.640

Notes: (D) denotes Dorney, (G) denotes Gatehampton. K_{aq} = Aquifer hydraulic conductivity; t_s = Streambed thickness; K_s = Streambed hydraulic conductivity.

over the same interval in streambed thickness values. Furthermore, since acceptance of a calibration depended not only on minimisation of RMSE, but on matching observed baseflows also (Section 7.1.3 above), the variation in the mean value of the stream - aquifer exchange flux for the domain (qsa) with streambed thickness is also important. As shown in Figure 7.11 (c), qsa is inversely proportional to streambed thickness, and a correct match between observed and modelled baseflow at Gatehampton was obtained when qsa was maximised. In reality, streambed thicknesses are highly unlikely to exhibit values as high as those which produced the lowest qsa values, and thus the uncertainty involved in estimating streambed thickness is not as great as it is for streambed hydraulic conductivity estimation.

Streambed hydraulic conductivity has a far less ambiguous effect on model output than streambed thickness, exerting strong controls on both RMSE (Figure 7.12 (a)) and mean qsa (Figure 7.12 (b)). Given the paucity of data on the

Figure 7.12 -- Model Sensitivity to Streambed Hydraulic Conductivity.

(a) Effects on RMSE.

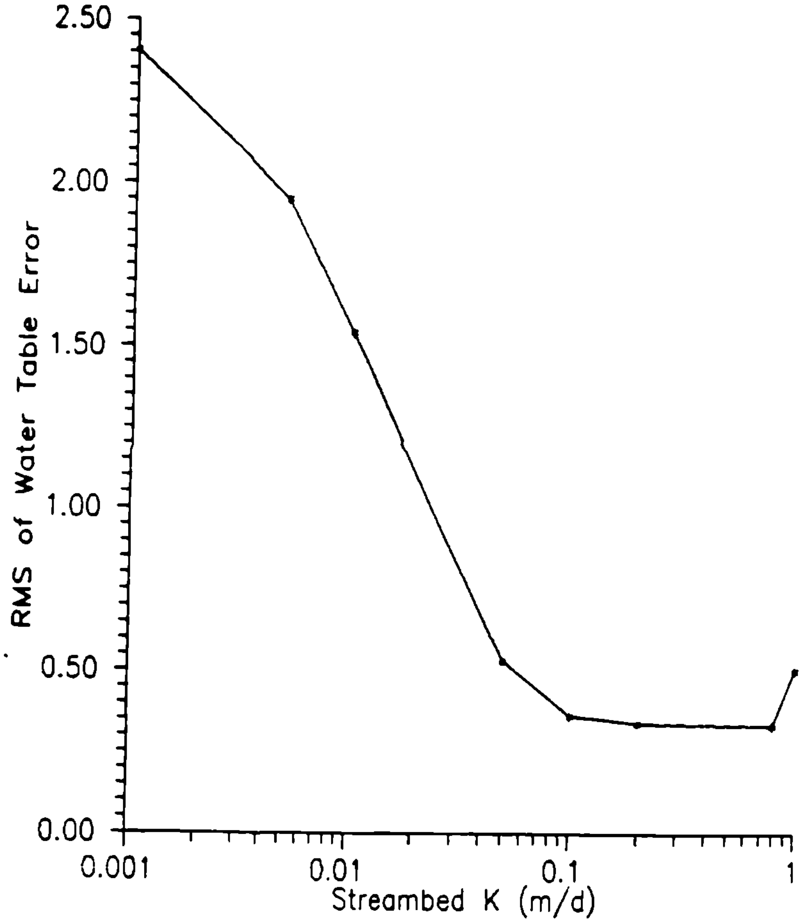
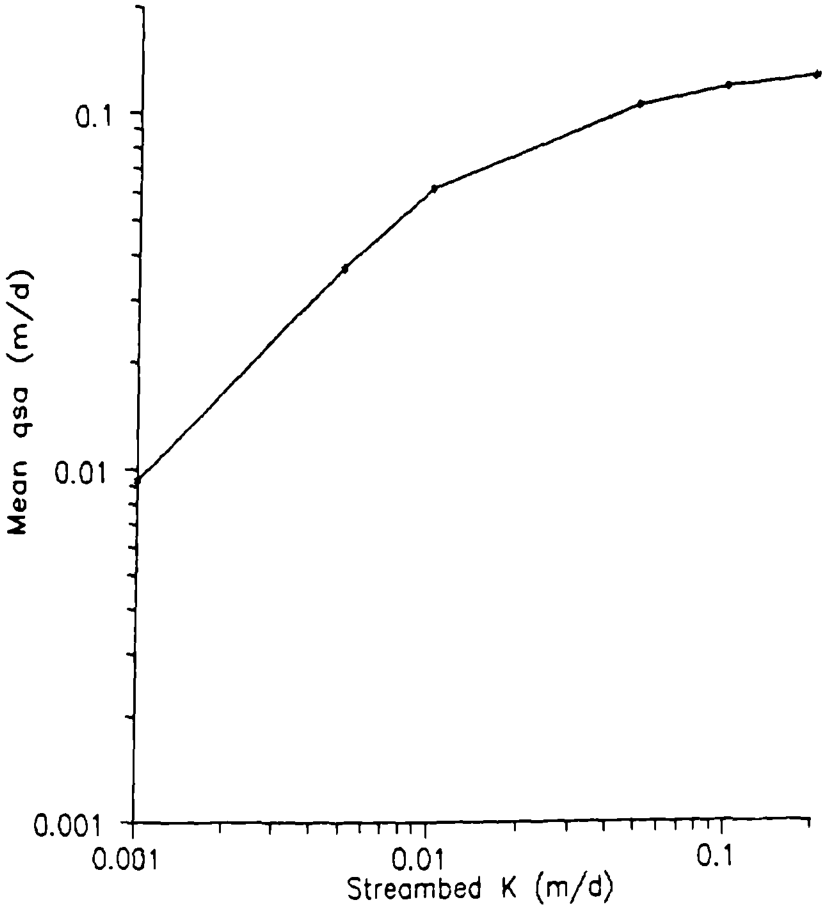


Figure 7.12 -- Model Sensitivity to Streambed Hydraulic Conductivity (Cont.).

(b) Effects on Mean Stream - Aquifer Exchange Flux (qsa).



hydrogeology of the streambed sediment, however, these results indicate that uncertainty in estimates of streambed hydraulic conductivity may cause substantial modelling errors.

7.5 -- SUMMARY AND CONCLUSION.

Flow models for two stream - aquifer systems with contrasting hydrogeological configurations have been succesfully developed and tested using the US-FLOW finite difference code described in Chapter 6. The performances of steady - state and transient models for both sites suggest that the conceptual model for flow in Thames Basin stream - aquifer systems (Section 5.2) is substantially correct. Sensitivity analyses performed on the calibrated models indicate that the hydraulic conductivity of the streambed sediment exerts the strongest control on model performance, with streambed thickness and aquifer hydraulic conductivity having less important effects. Output from steady - state flow simulations of wellfields at both sites formed the basis for the solute transport models described in Chapter 8.

CHAPTER EIGHT

SOLUTE TRANSPORT MODELLING OF FIELD SITES

8.1 -- INTRODUCTION

8.1.1 -- The Questions to be Addressed.

Assessing the vulnerability of riverside wells to pollution by the ingress of contaminated river water was one of the principal aims of this project. In Chapter 1 (Section 1.1.2), various questions which arise out of concern for this vulnerability were identified. In essence, all of these questions may be summarised in two main questions:

(a) How long must pollution in the river persist before the accumulated input of pollutants to the aquifer results in the abstraction of water of unacceptable quality from any of the riverside wells?

(b) How long will pollutants entering from the river persist in the aquifer?

8.1.2 -- Formulating Answers.

The two questions posed above implicitly include numerous questions about *advection, dispersion and retardation* processes in riverside aquifers. It hardly needs restating that knowledge of these processes in riverside aquifers of the Thames Basin is rather limited (Chapters 3, 5 and 7). Compounding this lack of knowledge, the mathematical modelling of dispersion is fraught with difficulties. Two interrelated issues are still debated with vigour; firstly the so-called 'scale - dependence' or 'time - dependence' of dispersion, and secondly the validity of representing mechanical mixing by a description borrowed from Fick's Law of diffusion (Matheron and Marsily, 1980; Anderson, 1984; Marsily, 1986, pp. 247-251).

Given these difficulties, it is clear that simple one-line answers to the two main questions posed above are not possible. Rather, it is necessary to define a range of answers which is feasible given various combinations of imperfectly - known input parameters. Therefore, in the simulations performed in this study, the sensitivity of model answers to variations in input parameters was assessed, and further runs were made using median values of parameters. The amount of variation allowed in input parameters was limited according to estimated minimum and maximum values, which were estimated from field data or from analogous studies reported in the literature.

A further question arises as to what is meant by the phrase 'water of unacceptable quality' in question (a) above. In the present context, the European Community Limit (EC Limit) for a given species in drinking water is taken as the dividing line between acceptable and unacceptable water quality.

8.1.3 -- Modelling Scenarios.

An infinite array of hypothetical pollution incidents could be proposed for the purposes of assessing the vulnerability of riverside wells. Any one of thousands of pollutant species could be chosen, and combined with numerous permutations of river regime, aquifer stresses and the thickness and permeability of the streambed sediment. To avoid embarking on such an endless path, three restrictions were introduced into the definition of test problems:

(i) It was decided that only pollutants which pose a real threat to riverside wells would be considered.

(ii) It was decided that only two pollutants would be considered for each site; the first would be a highly soluble conservative pollutant, and the second would be a persistent organic contaminant which is subject to retardation by sorption.

(iii) It was decided that the steady - state flow fields for Dorney and Gatehampton (obtained at the end of the modelling exercises described in Chapter 7) would be used exclusively, and no further flow modelling would be pursued at this stage. In line with this decision, the river flow regime would be kept constant for all simulations.

In Section 1.1.3, where the risk of river pollution was discussed, it was noted that the present quality of the Thames in the vicinity of Gatehampton and Dorney is very high, so that the major threat to riverside wells is posed by accidental spills. Accidental inputs to the river may be of different duration, depending on circumstances. For the purposes of argument, three scenarios are envisaged. Consider first the crash of a tanker containing hazardous chemicals on the M4 motorway or on Goring Bridge. Such a spill would have a very short duration, with all the pollutants entering the river within about 20 minutes. On the other hand, suppose a serious accident at a power station or factory prevented emergency services from entering the plant for a week, and that runoff of contaminated water occurred throughout this period. What impact would this have on riverside wells? Finally, if unforeseen circumstances forced an upstream water treatment works to release poor quality water into the river for a month, what impact might this have?

To reflect these three possibilities, the effects of spills of both the conservative and reactive contaminants were assessed for both field sites using 20 - minute, 7 - day and 28 - day inputs of pollutants into the river.

8.1.4 -- Selection of 'Test Pollutants'.

As mentioned above (restriction (i)), the selection of 'test pollutants' for the simulations was governed by a desire to predict the consequences of realistic problems. For instance, there would be no point in choosing chemical species which have extremely low mobility in groundwater systems (eg PCBs; Gay and Frimpter, 1985), or pollutants which are highly susceptible to biodegradation. Furthermore, it makes sense to choose species which might feasibly be found in the Middle Thames Valley. Obviously, banned chemicals or exotic poisons do not pose as high a threat as readily available toxic substances.

The two pollutants chosen in the end were chloride and lindane. Chloride is an obvious choice, since it is highly soluble, and is widely acknowledged to be a conservative ion. The pollution threat posed by chloride lies in its detrimental effect on taste, rather than in any toxicity, and its EC limit in drinking water is 250mg/l. The most likely source of chloride pollution in the Thames is the failure of a sewage treatment works. In addition, waste effluents from a number of industrial processes are very high in chloride, and a short - term input of chloride from a road accident involving a tanker containing such effluent can also be imagined.

Lindane is an optical isomer of hexachlorocyclohexane (HCH), and is a member of a group of toxic compounds known as chlorinated pesticides. With a solubility of 7 mg/l (Freeze and Cherry, 1979, p. 425), lindane is one of the more soluble chlorinated pesticides, and it also has a lower volatilisation rate and a greater resistance to biodegradation than most related compounds (Moore and Ramamoorthy, 1984, pp. 88 - 114). The toxicity of lindane to human beings has been widely investigated, and the list of conditions which it is known or suspected to cause or induce is disturbingly long: cancers, cardiovascular disease, hypertension, diabetes, hypoplastic anaemia, muscle damage, epilepsy, bone marrow disease, kidney failure and gastric disorders (Moore and Ramamoorthy, 1984, p. 109). The EC limit for lindane in drinking water is 0.001 mg/l. While lindane is banned in many countries, it is still readily available in Britain, where it is used in crop sprays and in 'do-it-yourself' timber treatment mixtures. Press reports have documented about 40 recent cases of injury and death caused by DIY lindane mixtures in Britain (see The Observer, 11-9-88, p. 4). The prospect of lindane pollution in the Thames seems quite realistic when it is remembered that a tributary of the Thames in Surrey suffered from a major spill of lindane in February 1989 (Section 1.1.3). Furthermore, a number of chemical plants in the Middle Thames valley produce wood treatment mixtures which are thought to contain lindane.

Although lindane is more persistent than many organic pollutants, it is metabolised by soil micro-organisms to form chlorobenzene compounds, many of which are themselves toxic (Moore and Ramamoorthy, 1984, pp. 97 - 98). However, the main control on the transport of lindane in groundwater would appear to be sorption onto organic matter. Measured values of the organic carbon partition coefficient (Koc) for lindane vary from 1300 (McCall et al, 1983) to 1995 (Marsily, 1986). Now Koc is related to the distribution coefficient (K_d; introduced in Section 6.3.2) by the simple identity:

$$K_d = Koc.Foc \quad . . . . \quad (8.1)$$

where Foc is the fraction of the solids composed of organic carbon.

Values of Foc for the gravels and the streambed sediment were obtained during the streambed sediment investigation (Appendix C), and thus values of Kd for lindane in both media can be easily obtained. Substitution of these values into equation (6.49) yielded a range of possible values of the retardation factor (Rd) for lindane. These are listed in Table 8.1 below. It is clear that very long residence times can be expected for lindane in the streambed sediment. Even the gravels will cause lindane to migrate at a rate almost 100 times slower than the bulk advection rate.

For both sites, it was assumed that chloride and lindane were mixed throughout the river water. Given that both of the modelled sites lie immediately downstream of weirs, this is not as unlikely as it may at first seem. The concentrations which the pollutants reached in the river

Table 8.1 -- Values of the Retardation Factor for Lindane in Clastic Sediments of the Middle Thames Valley.

Sediment	Foc	Retardation Factor
Shepperton Gravels	0.014	94
Streambed Sediment:		
(i) Gatehampton	0.016	206
	0.056	316
(ii) Dorney Silt	0.059	442
	0.079	677
(iii) Dorney Peat	0.574	1446

was prescribed in order to make sure that serious pollution was implied. For chloride, a concentration of 10,000 mg/l was adopted for all simulations, while a concentration of 7 mg/l was assumed for lindane (which is equal to its solubility).

8.1.5 -- Provision of Input Data.

The head and hydraulic conductivity distributions derived from the flow models (Chapter 7) were the basis of the advection calculations in the solute transport models for both sites. Nonetheless, to fully describe solute transport, parameters describing retardation (by sorption and matrix diffusion) and dispersion were also required. Direct determination of these parameters involves tracer tests and laboratory batch experiments (Freeze and Cherry, 1979, pp. 430 - 434) which are both expensive and difficult, and for this reason these parameters are frequently estimated by analogy with published data for hydrogeologically similar sites (cf Mackay et al, 1988).

Sorption and Matrix Diffusion Parameters. Values for retardation parameters in the stream - aquifer systems of the Thames Basin are few and far between. Many studies have been made of solute transport in the Chalk, and estimates of important retardation parameters can be made with reference to these. Since the Chalk at the field sites is assumed to be non - sorbing (Section 5.3.2), the only retardation process for which information is required is matrix diffusion. The value for the diffusion coefficient within the matrix blocks (3 x 10^{-5} m^2/d) was taken from the values compiled by Müller (1987). While this value strictly applies only to chloride, it was also used for lindane, in lieu of any other information. This is fairly reasonable, given the restricted range of possible values for this parameter (10^{-5} to 10^{-6} m^2/d; Gillham and Cherry, 1982). The new data on the Chalk fracture system presented in Appendix B were used to provide a value of fissure spacing (0.1m) for use in equation (6.67). Porosity values for the fissure system (0.01) and the matrix blocks (0.35) were assumed to be constant throughout the domain. The matrix block porosity was adopted from published values (Price, 1985), and the fissure system porosity was set equal to the calibrated specific yield of the Chalk at Gatehampton (Section 7.2.3), which is in close agreement with published values.

No published data on the sorption parameters of the Shepperton Gravels and the modern streambed sediment are known to exist, but the new data given in Table 8.1 above shed considerable light on the sorptive capacity of these units. Median retardation factor values of 500 (Dorney) and 250 (Gatehampton) were used for the majority of runs.

Dispersion Parameters. If chemical analyses from a number of observation wells are available to illustrate the spreading of a slug of contaminants in an aquifer, then values for dispersivity can be obtained by inverse calibration of a solute transport model. However, the chemical data available for the two field sites are not suitable for this purpose. Thus estimation of dispersivity is inevitable. Since the selection of too high a value for this parameter could lead to underestimation of break-through concentrations at wells, all estimates were conservative.

Earlier studies of dispersion in the Chalk fissure system are a valuable source of information. Chief amongst these is the paper by Black and Kipp (1983), which includes a review of other work on this topic. A log-linear relationship between fissure spacing and longitudinal dispersivity was derived by these authors, based on all available data. For the spacing used in this study (0.1m) a longitudinal dispersivity of about 20m is predicted by this relationship. This same value was obtained by Müller (1987) when he calibrated a model of Chalk pollution in Cambridgeshire, where fissure spacings are slightly larger (0.3m). Other values of longitudinal dispersivity for the Chalk have been compiled by Anderson (1979, p. 126). Perusal of these values, together with data from Jurassic carbonate aquifers in West Germany (Seiler et al, 1989, p. 245), suggested that values as low as 3m may be more suitable for the present study. The ratio of transverse to longitudinal dispersivity was assumed to be 0.05, following Müller's (1987) calibration.

Values for longitudinal dispersivity in the gravels do not exist, and were therefore estimated from published data for similar unconsolidated sand and gravel aquifers (Anderson, 1979, p. 126). A range of 12 to 30m was finally adopted. The ratio of transverse to longitudinal dispersivity was assumed to be 0.05 (Freeze and Cherry, 1979, p. 400).

For both the Chalk and the gravels, the ratio of vertical to longitudinal dispersivity was arbitrarily set at 0.01, since it was felt that vertical dispersivity is probably of the same order of magnitude as transverse dispersivity, if slightly smaller.

Definition of dispersion parameters for the streambed sediment was based entirely upon estimation. Because groundwater velocities in the streambed sediment are low, it is possible that molecular diffusion is an important component of dispersion (Section 6.3.4.4), and it was therefore necessary to estimate the value of the coefficient of molecular diffusion in the pore system of the streambed sediment (D_D). Freeze and Cherry (1979, p. 393) quote the range of possible values for this parameter in 'clayey geological deposits' as 10^{-5} to 10^{-6} m^2/d. With regard to mechanical dispersion in the streambed sediments, a very low value of dispersivity might reasonably be expected. In view of this, a value of 0.0001m (the minimum value for this parameter quoted by Freeze and Cherry, 1979, p. 400) was adopted.

Because of the uncertainty associated with all the estimates given above, the sensitivity of the models to the full range of values was tested whenever possible (Section 8.5).

8.1.6 -- Processing and Interpretation of Output.

Because the particle tracking method deals in masses of solutes rather than in concentrations, it is only possible to assess concentrations by considering the volume of water in which particles occur. In the case of solute breakthrough at wells, this is accomplished by dividing the number of particles arriving at a well in a given time interval by the volume of water discharged from the well in that same time interval. To produce curves of concentration versus time for a given well, therefore, it is necessary to group particle arrivals into equal time intervals (eg daily or ten-day intervals etc) and calculate the mean concentration for that interval. To produce a 'breakthrough curve' from this data, a plot of concentration versus time is produced. It is one of the operational hazards of the particle tracking method that the curves constructed in this manner are necessarily rather 'noisy' when compared with the output from solution techniques which deal directly in concentrations (Prickett et al, 1981). Nonetheless, the essential features of the breakthrough curves are still readily discernible.

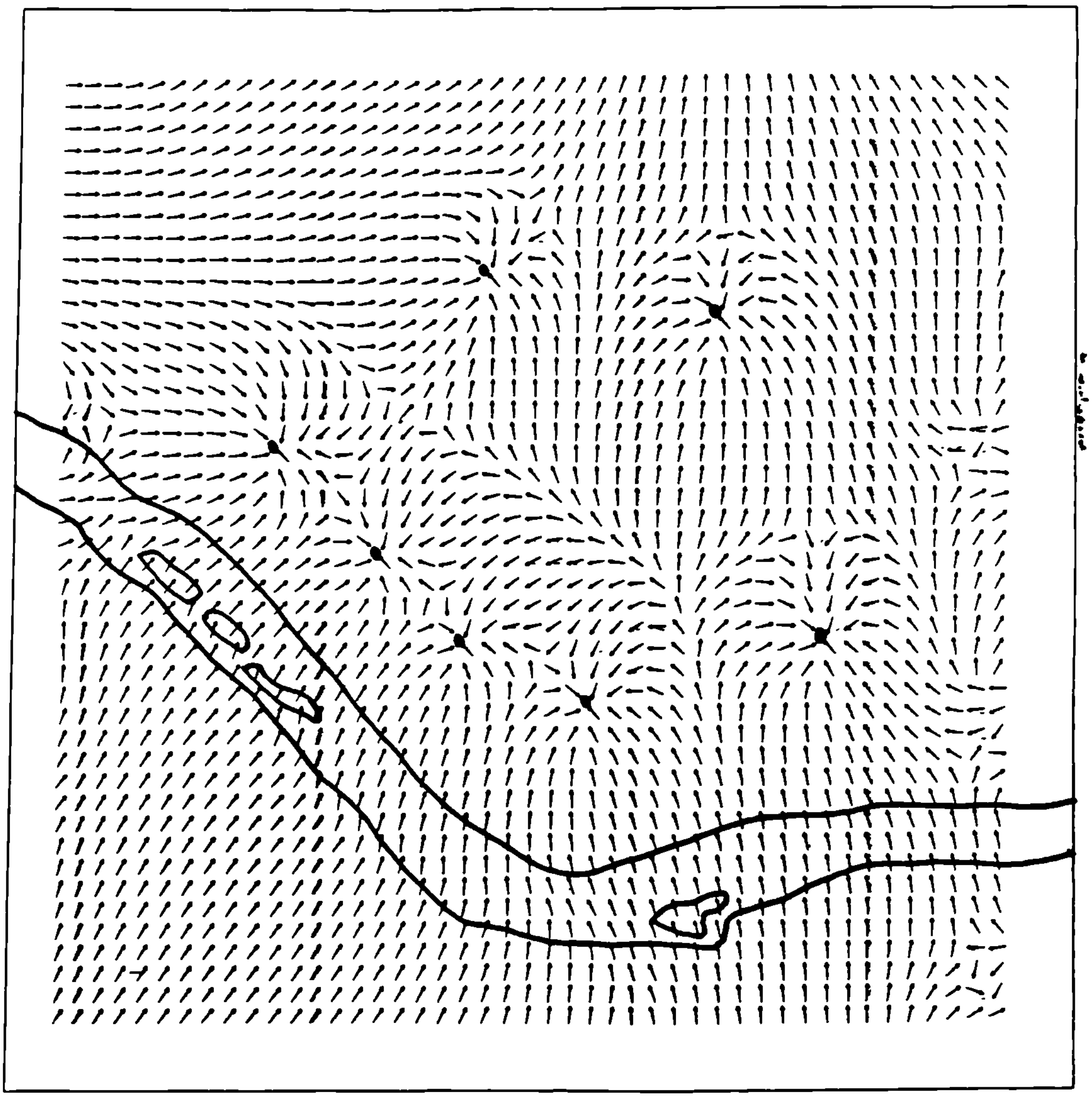
8.2 -- THE GATEHAMPTON POLLUTION SIMULATIONS.

8.2.1 -- The Gatehampton Velocity Field.

8.2.1.1 -- Determination of Velocities. The nested Gatehampton finite difference grid (50 x 50, with a uniform grid spacing of 10m), with its associated head and 3 - D hydraulic conductivity distributions, was used as the basis for the velocity calculations performed by US-VEL. Porosity values used in these calculations were 0.01 for the Chalk (see Section 8.1.5 above) and 0.25 for the gravels (set equal to the calibrated specific yield; Section 7.2.3). Horizontal velocities across cell boundaries were obtained for all the layers within the Chalk, as well as for the monolayer gravels. Vertical velocities for the streambed sediment and for all the interfaces between vertically stacked Chalk and gravel layers were also obtained. Figure 8.1 shows the directions of the resultant horizontal velocities in the chalk which were obtained from the x and y velocity components. The software which was written to produce these plots included an option which would scale the length of each arrow according to the magnitude of the velocity resultant at that cell, relative to the maximum velocity in the domain. However, the velocities in the immediate vicinity of the pumping wells were so large that all other arrows were virtually invisible when a plot was produced. Therefore it was decided to plot directions only.

Having obtained values for x - y - z velocity components at the boundaries of all cells in the domain, the way was open to perform particle tracking for each test problem.

Figure 8.1 -- Modelled Velocity Directions in the Chalk at Gatehampton.



However, before embarking upon this task, the new velocity data were used to perform two checks on the flow domain. Firstly, a check was made to see whether the computed velocities imply turbulent flow, since Darcy's Law is invalid in turbulent flow regimes (cf Section 5.2.1). Secondly, the validity of different solution techniques for matrix diffusion in the Chalk at Gatehampton (discussed in Section 6.3.4.4) was assessed.

8.2.1.2 -- Checking for Turbulent and Laminar Flow. The test for turbulent conditions involves the calculation of Reynolds Number (R_E), which, for flow through porous media is usually written (Freeze and Cherry, 1979, p.72):

$$R_E = \frac{\rho V d}{\mu} \quad . \; . \; . \; . \; (8.2)$$

where

$$\left.\begin{array}{l}\rho = \text{fluid density} \quad (999.7\ \text{kg/m}^3) \\ \mu = \text{fluid viscosity} \ (1.306\ \text{Pa s})\end{array}\right\} \text{(water at } 10^{\circ}\text{C; Marsily, 1986)}$$

d = a 'characteristic length' of the pore system (eg a mean pore dimension)

V = average linear groundwater velocity

Because of the difficulty in measuring pore sizes in unconsolidated media (such as the gravels), the definition of d in (8.2) is usually taken as some representative grain diameter. The most appropriate value to use for a fissure continuum is the mean fissure aperture. Using the above formulation, the critical value above which turbulent flow is indicated lies somewhere between 1 and 10 (Freeze and Cherry, 1979, p. 73).

Reynolds Number for the Gravels. If medium sand (2×10^{-4} m grain diameter) is used for d (since this comprises the matrix in Gm facies units of the Shepperton Gravels), and one of the higher gravel velocities from the US-VEL output is used for V (eg 60 m/d = 6.944×10^{-4} m/s), then a Reynolds number of 0.0001 is obtained for the gravels. If, for the sake of argument, the diameter of a flint clast (about 0.05m) was used for d, which would only be reasonable in matrix - free clast - supported gravel horizons, then the value of R_E would still only be 0.03. Both of these values are well below the critical limit, indicating that flow in the gravels is laminar even at the higher velocities.

Reynolds Number for the Chalk. To determine the Reynolds Number for the Chalk fissure continuum, it is necessary to have an estimate of fissure aperture. While fracture apertures up to 1 cm were observed at outcrop, frost action may have opened these to a greater extent than subsurface fissures. It is possible to estimate fissure aperture for a system of equally spaced horizontal fissures if hydraulic conductivity is known. This is accomplished by the application of the following equation (Freeze and Cherry, 1979, p. 74):

$$Kh = \left[\frac{\rho g}{\mu}\right]\left[\frac{F_f b^3}{12}\right] \quad \ldots\ldots\ldots\ldots (8.3)$$

where

Kh = horizontal hydraulic conductivity (m/s)

F_f = fracture frequency per metre along a vertical scan-line (m^{-1})

g = acceleration due to gravity (9.80665 m^2/s)

b = fissure aperture (m)

μ = fluid viscosity

Since the hydraulic conductivity in the upper layers of the Chalk at Gatehampton was calibrated at 170 m/d (1.968 m/s), and the value of F_f is about 10 m^{-1} (Appendix B, Table B.1), solution of (8.3) for b yields a value of 0.0068m (6.8mm). This is a rather wide fissure aperture, but it is on the order of magnitude observed in highly permeable Chalk of the Thames Valley using borehole television

(Price, 1985; Tate et al, 1971). With a velocity of 60m/d (among the higher values calculated by US-VEL for the upper layer of the Chalk), the Reynolds Number for the Chalk is about 0.0036, which again is well within the laminar flow range.

8.2.1.3 -- Validity of Matrix Diffusion Solutions. Using the new velocity information, it was possible to use equations (6.64) and (6.69) to calculate the approximate distances from entry into the Chalk at which the boundaries between the regions in the solution for matrix diffusion occur (cf Section 6.3.4.4). A velocity of 60m/d and values of 3 and 20m for the longitudinal dispersivity (α_l) of the Chalk were used, and the results obtained may be summarised as follows:

(1) The progress of the solute mass is fully described by advection and dispersion alone when it has travelled less than a distance (L_i) of 9m (α_l = 3) to 16m (α_l = 20) in the Chalk.

(2) Between the distance L_i and a distance (L_d) of 900m, a complete description of the distribution is only possible if a full solution of equation (6.63) is obtained.

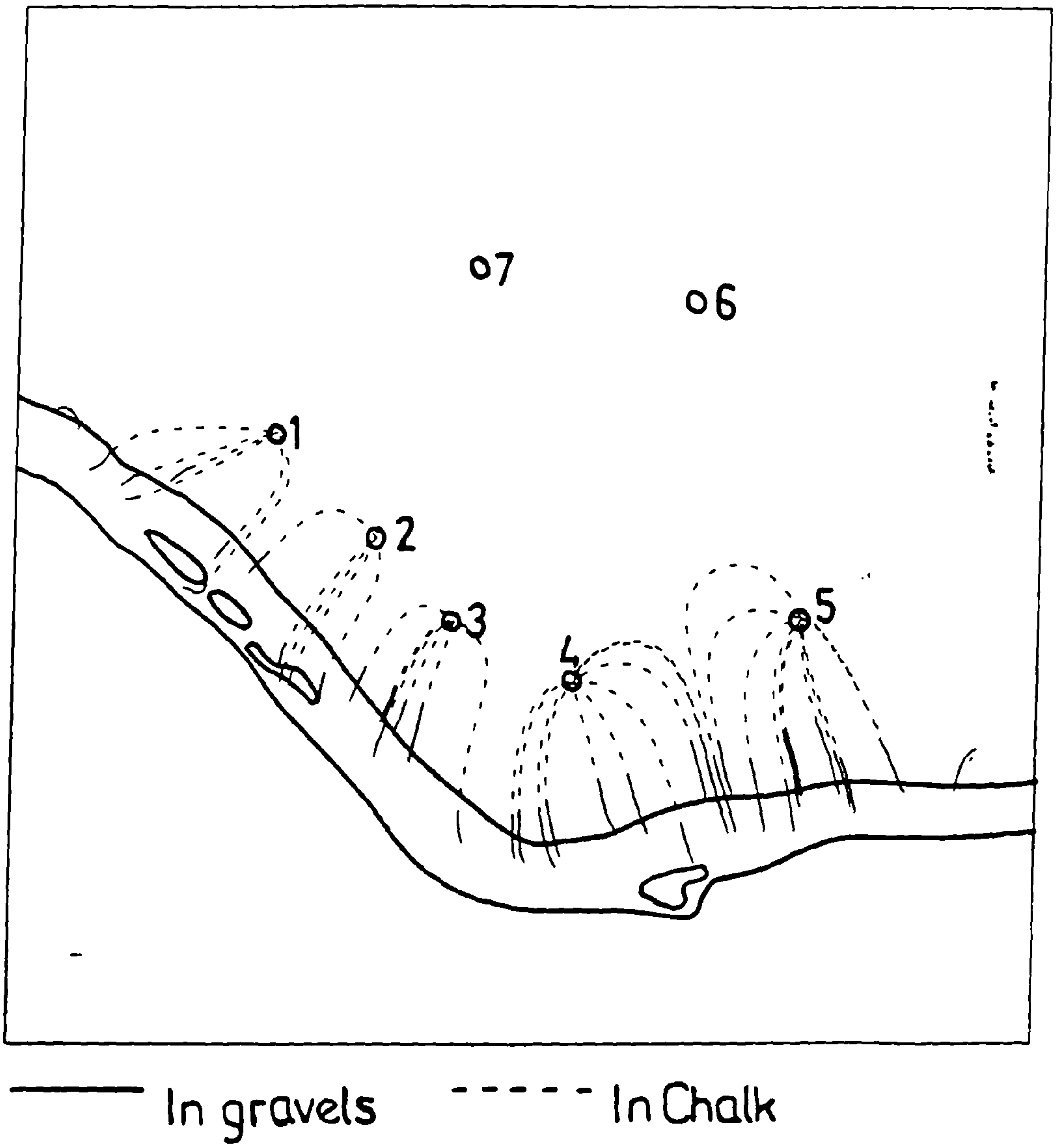
(3) Beyond 900m, the effective dispersion and apparent retardation approach (equations 6.65 to 6.68) is valid.

The significance of these results will be considered further, when details of particle trajectories are discussed.

8.2.2 -- Particle Tracking.

8.2.2.1 -- Application of US-TRACK. As outlined in Sections 8.1.3 and 8.1.4 above, three different input times were used for both chloride and lindane simulations. Additionally, duplicate runs for each case were conducted to allow assessment of matrix diffusion effects using the MDRA method outlined in Section 6.3.4.4. Several sensitivity runs were also made.

Figure 8.2 -- Gatehampton Particle Trajectories.



All in all, about 30 runs were made for the Gatehampton site, each using up to 10000 particles to represent the dissolved solute mass. Tracking through the three dimensional Gatehampton domain was expensive, however, with up to 2 cpu seconds being required per particle on the Amdahl 580/162 mainframe computer. Because of this, advantage was taken of one of the peculiarities of the particle tracking method: Runs with large numbers of particles were divided into smaller jobs, and the results aggregated after execution. This additive nature of results is one of the main advantages of the particle tracking method (Prickett et al, 1981, p. 3).

8.2.2.2 -- Results. A qualitative appreciation of the performance of US-TRACK in modelling solute transport at Gatehampton is afforded by Figure 8.2, in which trajectories for a few particles are plotted. However, quantitative evaluation of the model results requires a rather more rigorous approach. Perhaps the most effective way to assess the variable modelled response of the Gatehampton field site to different input conditions is to compare a few parameters which describe solute arrival at the pumping wells. The parameters chosen for comparison are those which define the maxima and minima of the breakthrough curves for each well, namely:

(i) The time of the earliest pollutant arrival.

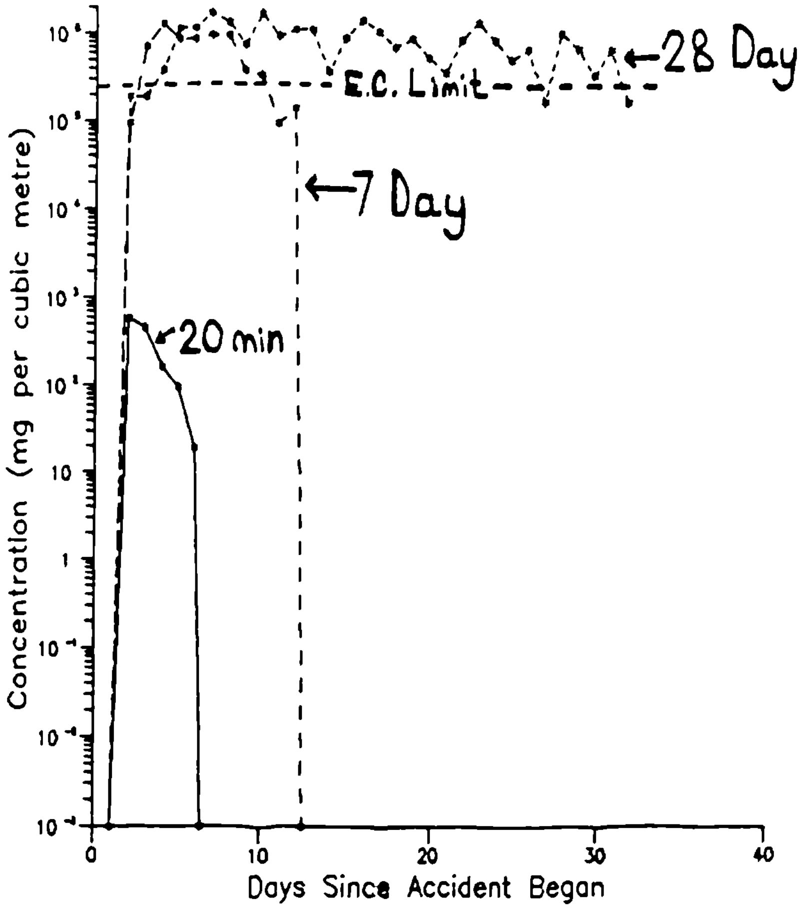
(ii) The peak arrival time.

(iii) The rate of pollutant arrival (or the pollutant concentration) at the peak time.

(iv) The time the last particle arrived.

Now there are seven wells at Gatehampton and all of these received particles during the simulations, so that the total volume of results in terms of the four parameters above is quite large. However, the results are amenable to summary in terms of the mean response of those wells which, because of their similar positions, displayed similar behaviour. Thus Tables 8.2 and 8.3 summarise the responses

Figure 8.3 -- Chloride Breakthrough at Gatehampton Well 5 for River Events of Different Durations.



of wells 1 - 5, since these wells are all disposed close to the river (Figure 3.11) and behaved in a similar manner. Wells 6 and 7, which are remote from the river, showed different breakthrough behaviour, which is contrasted with that of wells 1 - 5 in the discussion below.

To facilitate discussion, two important abbreviations are introduced here. ADO signifies 'advection - dispersion only', while ADMDR indicates 'advection - dispersion with matrix diffusion retardation'. These two phrases refer, of course, to the two options in the MDRA method (Section 6.3.4.4).

Chloride Simulations. Chloride breakthrough at the Gatehampton wells is summarised in Table 8.2. Two main facets of the chloride results for Gatehampton warrant attention; the effects of input duration, and the effects of matrix diffusion.

(i) Effects of variable input duration. When the input of pollutants into the river continued for only 20 minutes, the EC limit was not breached at any of the wells. After a 7 - day input, however, wells 1 - 5 returned concentrations in breach of the EC limit, though wells 6 and 7 were still below it. After a 28 - day input event, all of the wells save well 7 returned concentrations in excess of the EC limit.

The effects of variable input duration on chloride breakthrough are exemplified by the plots for well 5 given in Figure 8.3, where the breach of the EC limit by the 7-day and 28 - day events is clearly shown.

(ii) Effects of Matrix Diffusion. The general effect of matrix diffusion, which is revealed by comparing ADO and ADMDR results, is to cause greater retardation and dispersion of pollutants, so that peak arrival times are delayed, peak concentrations are reduced, and the total

Table 8.2 -- Mean Gatehampton Chloride Results (Wells 1 - 5)

	Earliest Arrival (days)	Latest Arrival (days)	Peak Arrival (days)	Concentration at Peak Arrival (mg/l)
(a) 20 - Minute Input				
ADO	0.7	5.6	2	6
ADMDR	1.0	160.0	9	0.1
(b) 7 - Day Input				
ADO	1.1	10.9	6	1105
ADMDR	3.1	160.1	14	334
(c) 28 - Day Input				
ADO	1.5	31.0	7	1825
ADMDR	5.0	170.0	27	1300

duration of pollutant breakthrough is greatly increased.

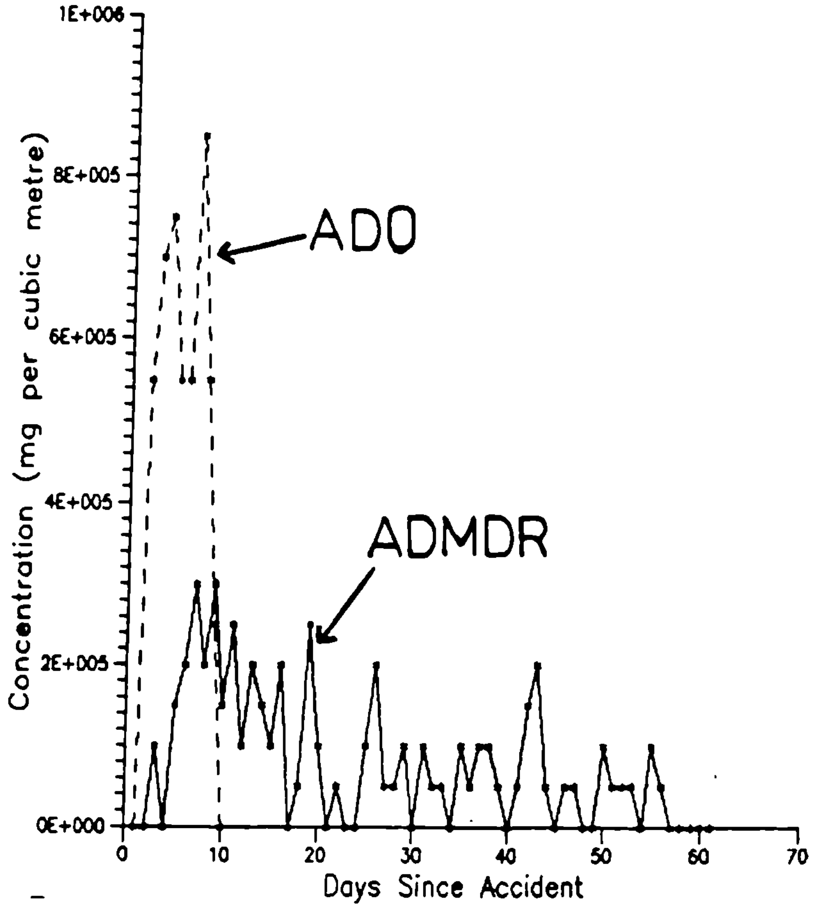
The validity of the representation of matrix diffusion in this model can be assessed using the results of the ADO and ADMDR runs. Using a special subroutine to log particle trajectories, it was found that, between entering the Chalk and arriving at a well, all of the particles travel further than 9m (L_i) but less than 900m (L_d). Because of this, neither the ADO runs nor the ADMDR runs give a full description of solute transport. However, since a solution to the 'full' description of the problem would yield values which lie between those given by the ADO and ADMDR solutions, the range of possible values is fully defined by the ADO and ADMDR limits given in the present discussion.

The reduction of peak concentrations is well illustrated by the data given in Table 8.2, where the introduction of ADMDR is always accompanied by a reduction in peak concentration. However, the increased spreading of pollutants caused by matrix diffusion resulted in an increase in chloride concentration at well 7 from zero to 197 mg/l during the 28 - day input. While well 6 had shown an increased chloride concentration when input rose from 20 minutes to 7 days, a reduction occurred during the 28 - day input, apparently due to the dispersion of the solute mass in the interior of the aquifer towards well 7.

Delayed arrival times were evident at wells 1 - 6 when ADMDR was included. For a 28 - day input, the mean earliest arrival time at wells 1 - 5 was 1.5 days with ADO (Table 8.2). On the other hand, the mean earliest arrival time was 5 days when ADMDR was used. Latest arrivals were also retarded. After a 28 - day spill, ADO runs predicted that all particles would leave the domain within 32 days (last arrival at well 5). With ADMDR, the latest arrival at well 5 occurred after 126 days (4.5 months), and the final particle left the domain at well 7 after 550 days (1.5 years). The mean time of peak arrival at wells 1 - 5 was increased from 7.2 days (ADO) to 37 days when the full effects of matrix diffusion were included. In general, particle arrivals were found to be delayed by a factor of 5 with ADMDR.

To illustrate some of the effects described above, the ADO and ADMDR breakthrough curves for well 2 after a 7 - day input are shown in Figure 8.4. The ADO run predicted a total cessation of pollution within 10 days of the onset of river pollution, while the ADMDR run predicted that particles would continue to arrive for more than two months after the accident. Nonetheless, ADO and ADMDR results both indicated that peak arrival concentrations at well 2

Figure 8.4 -- The Effects of Matrix Diffusion at Well 2.



could be expected within ten days of the onset of river pollution.

To summarise the model predictions, there is no risk of unacceptable chloride concentrations at any of the Gatehampton wells when input durations are very short (20 minutes). After longer inputs (7 and 28 days), unacceptable concentrations are highly probable at wells 1 - 5 within 1 to 4 weeks of the onset of river pollution. Well 6 may show unacceptable levels, if matrix diffusion processes prove to be slight. There is never any real chance of pollution at well 7, however, for any of the scenarios modelled.

Lindane Simulations. The results of lindane runs for wells 1 - 5 are shown in Table 8.3. There is little difference between the chloride and lindane simulations in terms of the ultimate sensitivity of wells to pollution. Just as in the chloride runs, no concentrations in excess of the EC limit for lindane were found after an input of only 20 minutes duration, but wells 1 - 6 returned concentrations in excess of the limit for durations of 7 and 28 days. Well 7 only breached the EC limit when ADMDR runs were performed for 7 - day and 28 - day inputs. As a whole, the sensitivity of wells to lindane pollution is higher than for chloride, probably because the ratio of input concentration (in the river) to the EC limit is 7000 for the lindane runs, but only 40 for the chloride runs.

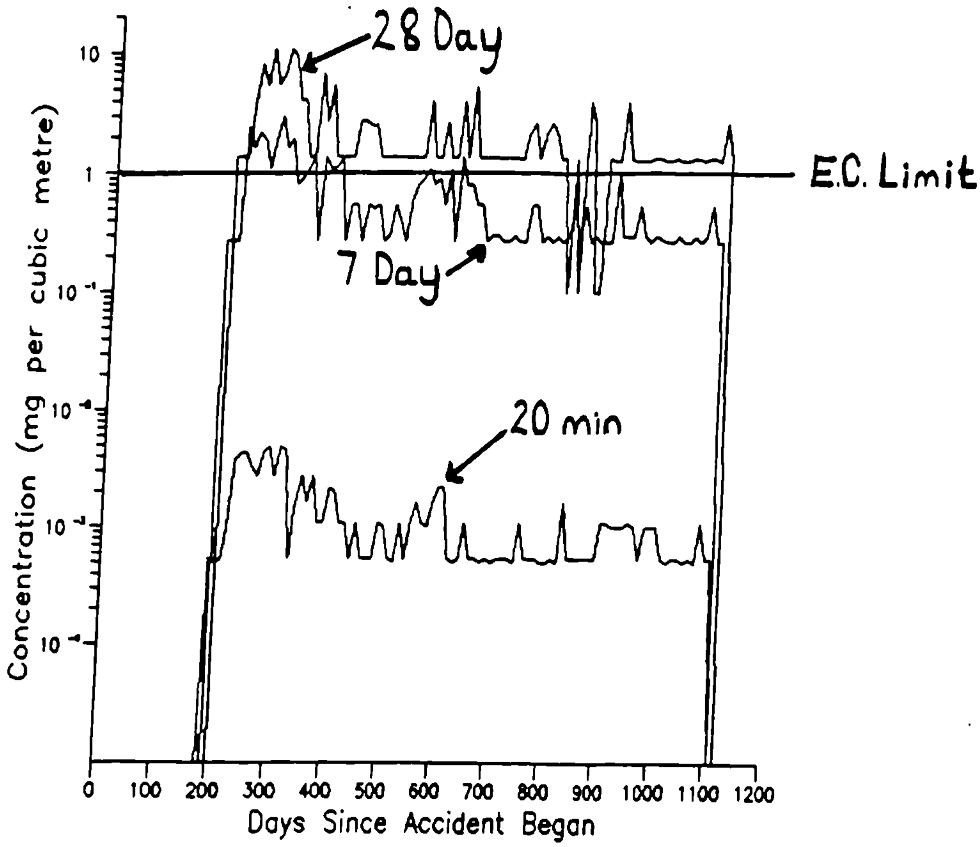
Figure 8.5 shows the 20 - minute, 7 - day and 28 - day lindane ADO breakthrough curves for well 3. In terms of general shape, the rising limbs on Figure 8.5 are very similar to the analogous curves for chloride shown in Figure 8.3. The falling limbs are dissimilar however, due to the difference in time scale along the abscissae of Figures 8.3 and 8.5. This difference in time - scale is due to the effects of retardation by sorption, and it constitutes the most important distinction between the

Table 8.3 -- Mean Gatehampton Lindane Results (Wells 1 - 5)				
(a) 20 - Minute Input				
	Earliest Arrival (days)	Latest Arrival (days)	Peak Arrival (days)	Concentration at Peak Arrival (mg/l)
ADO	199	2102	298	9.8×10^{-5}
ADMDR	293	2572	334	8.3×10^{-5}
(b) 7 - Day Input				
	Earliest Arrival (days)	Latest Arrival (days)	Peak Arrival (days)	Concentration at Peak Arrival (mg/l)
ADO	203	2107	300	0.034
ADMDR	225	2574	326	0.027
(c) 28 - Day Input				
	Earliest Arrival (days)	Latest Arrival (days)	Peak Arrival (days)	Concentration at Peak Arrival (mg/l)
ADO	210	1935	302	0.121
ADMDR	232	2392	338	0.117

lindane and chloride results.

The earliest arrival time recorded for lindane was 185 days (6.6 months; well 3, 20 - minute input), and the latest was 3526 days (9.7 years; well 3, 28 - day input). Mean values for earliest and latest arrivals at wells 1 - 5 were 210 days (7.5 months) and 2392 days (6.5 years) respectively. After a 28 - day input, peak arrival times averaged 302 days (ADO) to 338 days (ADMDR) (Table 8.3). At 36 days, the difference between arrival times with and without ADMDR is similar to what it was for the chloride runs (30 days). This is to be expected, since US-TRACK is based on the reasonable assumption that matrix diffusion affects all

Figure 8.5 -- Lindane Breakthrough at Gatehampton Well 3 for Three Different Input Durations.



chemical species equally. In practical terms, a difference of 30 days is more significant when the final solute arrival occurs only 126 days after the onset of river pollution (chloride, well 5) than it is when 2295 days must elapse before the cessation of pollution (lindane, well 5). In the first case, the error introduced by ignoring matrix diffusion would be on the order of 25%, whereas, in the second case, the error would be about 1%.

These results clearly indicate that sorption in the streambed sediment exerts far more control than matrix diffusion on the breakthrough of lindane. Comparison of Figure 8.6 with Figure 8.4, which are both plots of well response with and without ADMDR, illustrates this point. In Figure 8.6, where lindane breakthrough at well 3 is shown, there is little difference between the ADO and ADMDR plots. On the other hand the ADO and ADMDR plots for chloride breakthrough at well 2 are markedly different (Figure 8.4). Further illustration of the primacy of sorption in describing the lindane breakthrough curves is furnished by the proportion of run time which a given particle spends in the different parts of the Gatehampton stream - aquifer system. Analysis of run-time output from US-TRACK revealed that, on average, the migration time of a given particle was roughly divided between the different media as follows:

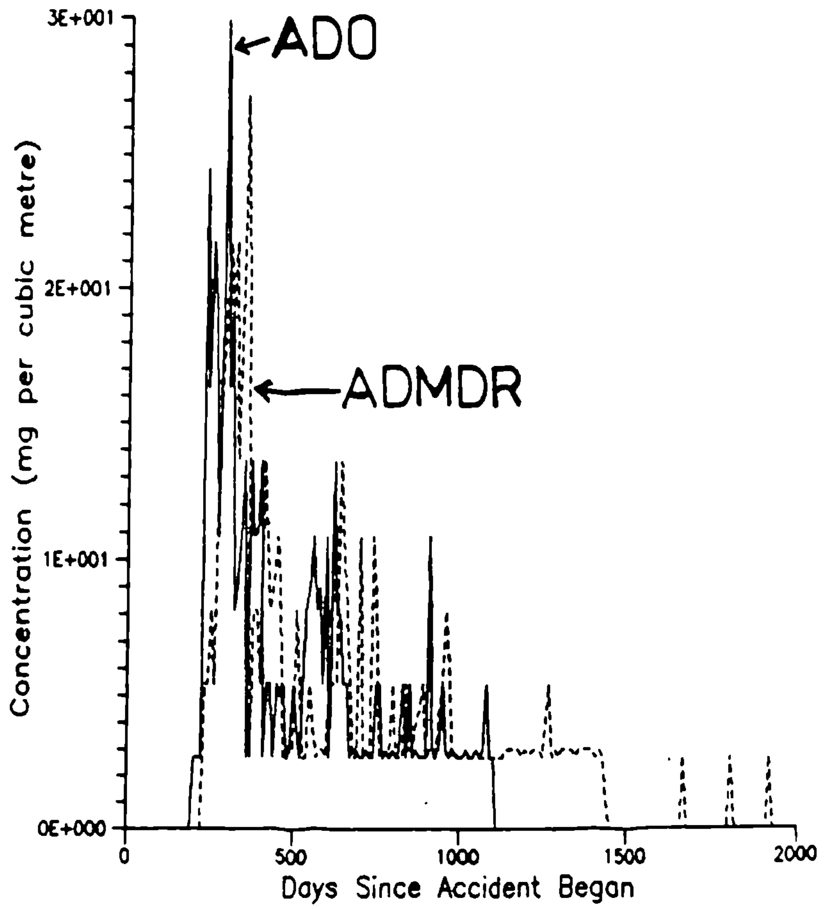
Streambed sediment (90%) : Gravels (7%) : Chalk (3%)

Apart from reflecting the low velocities in the silty streambed sediment, this distribution of residence times correlates well with the organic matter content of the three media at Gatehampton (Appendix C; Chapter 5):

Streambed sediment (3.4%) : Gravels (1.4%) : Chalk (0%)

<u>8.2.2.3 -- Summary and Conclusion.</u> The results of the Gatehampton pollution simulations allow various properties

Figure 8.6 -- The Effects of Matrix Diffusion on Lindane Breakthrough at Gatehampton Well 3.



of the site (which were identified on the basis of field evidence) to be quantified for the first time.

The chloride simulations indicate that advection at Gatehampton is very rapid. Conservative pollutants would begin to arrive at wells 1 - 5 within 1.5 days of the onset of pollution in the River Thames, with peak concentrations occurring after a week. As would be expected, the two wells which lie furthest from the river (wells 6 and 7) show less vulnerability to pollution, but even at these wells, pollutants may begin to arrive after only 5 days.

The slowest responses to conservative pollutants will occur if matrix diffusion processes are at their most efficient. Nonetheless, early arrivals would still be expected after no more than 5 days, with peaks occurring within 5 weeks of the start of the river pollution event. Background pollution may well persist for up to 6 months.

Non-conservative pollutants entering the Gatehampton stream - aquifer system will be greatly retarded by sorption in the streambed sediment. Lindane would take 6 months or more to reach the wells closest to the river, and peak breakthroughs would be unlikely to occur before 10 months. At the worst, trace amounts of lindane could continue to arrive at the wells for almost ten years.

On the basis of the simulation results, the three dominating geochemical processes at Gatehampton are felt to be rapid advection, matrix diffusion in the Chalk, and sorption in the streambed sediment and the gravels. For those solutes which are non-sorptive, matrix diffusion effects will be very marked. On the other hand, for most trace metals and organic pollutants, breakthrough will be chiefly governed by sorption, and the effects of matrix diffusion on the timing of pollution will be slight by comparison.

8.3 -- THE DORNEY POLLUTION SIMULATIONS.

8.3.1 -- Calculation of Velocity Field.

The final head and hydraulic conductivity distributions from the central 30 x 30 portion of the Dorney finite difference grid (Figure 7.7) were used as input to the US-VEL component of UNCLESAM. Because the geology of the Dorney site is much simpler than that at Gatehampton (Section 3.5.2), velocity components were only required for one aquifer layer (the gravels). The directions of the resultant horizontal velocities for the Dorney gravels are shown in Figure 8.7.

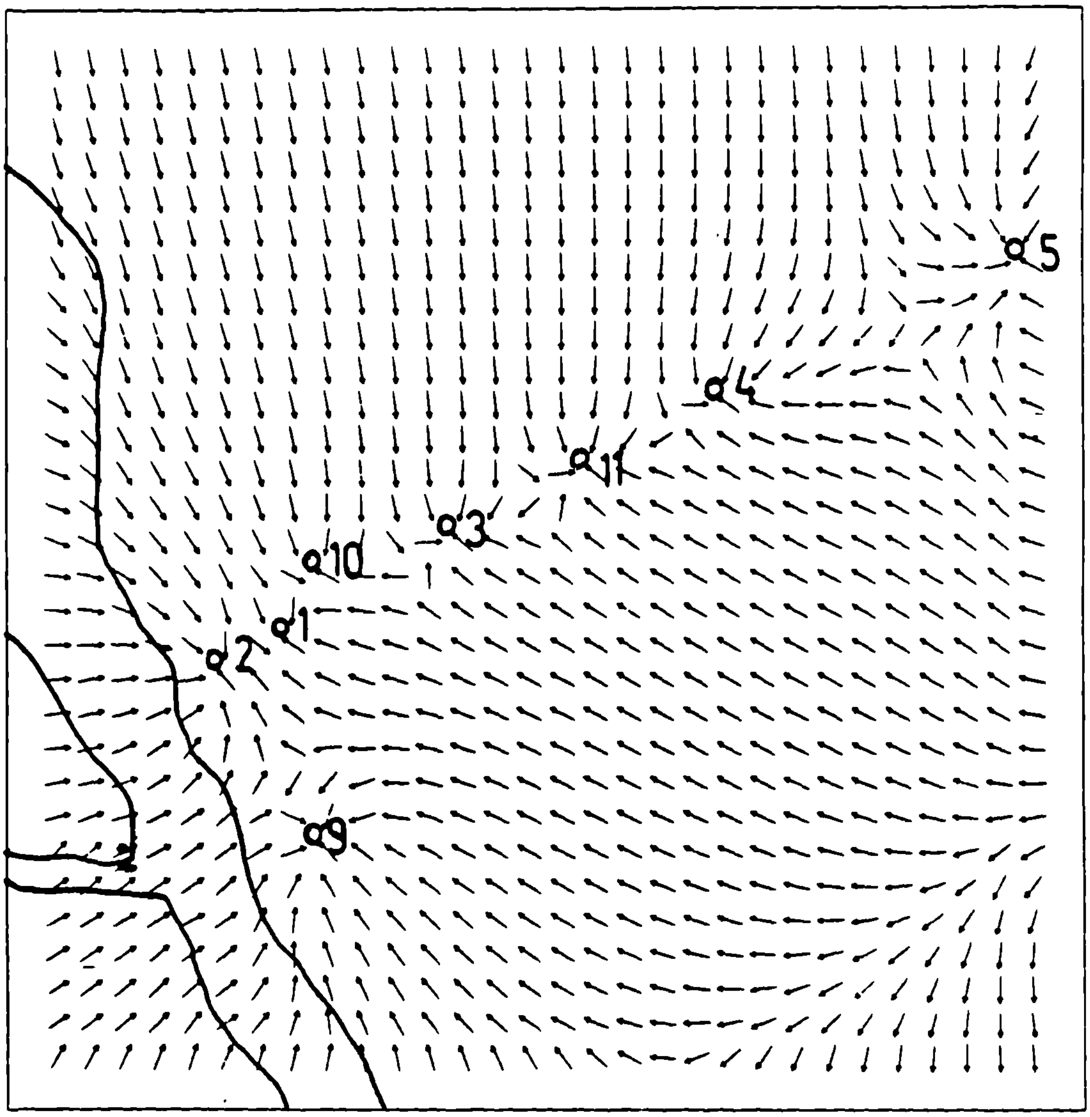
A uniform porosity value of 0.25 was used to obtain these values. This porosity value was set equal to the calibrated value of specific yield for the site (Section 7.3.3). To investigate the sensitivity of the model to this parameter, however, a duplicate run of US-VEL was performed with porosity set at 0.05 (a lower limit suggested by the calibrated model for the Upper Thames Gravels described by Dixon et al, 1989). Taking model node (3,4) as an example, the calculated velocity with a porosity of 0.25 was 33m/d, whereas this increased to 165 m/d when the porosity was changed to 0.05. Given that the most productive Dorney wells lie less than 100m from the Thames, the implications of such a variation in the velocity estimate are obvious.

As for the Gatehampton site, the new velocity field was subjected to the test for turbulent flow prior to commencing particle tracking. Once again, the Reynolds Number was well below the critical range, indicating that the flow model results are mathematically reasonable.

8.3.2 -- Particle Tracking.

8.3.2.1 -- Application of US-TRACK. Because of the relative simplicity of the Dorney model domain, many runs required as little as 0.05 cpu seconds per particle, and

Figure 8.7 -- Modelled Velocity Directions for the Gravels at Dorney.



therefore each run could be completed in a single batch job. Between 5000 and 11000 particles were used for each run. Furthermore, since the Chalk is not present in the Dorney model domain, there was no need to model matrix diffusion, and this halved the number of runs required. Because of these savings, more resources were available for sensitivity analyses, and the results of these are given in Section 8.5.

8.3.2.2 -- Results. Analysis of model results was easier for Dorney than for Gatehampton because only 3 of the 8 wells at Dorney showed any vulnerability to pollution from the river. The three vulnerable wells are, not surprisingly, the three closest to the river (well numbers 1, 2 and 9; Figure 3.14). Experimental runs with advection as the sole transport process (Figure 8.8) indicated that well 1 only experienced river contributions on account of dispersion. For this reason, the breakthrough of solutes at this well is not as simple to describe as for wells 2 and 9. In the discussions which follow, it is assumed that longitudinal dispersivity in the gravels is set at 12m, and that the retardation factor for lindane in the streambed sediment is set at 500 (cf Table 8.1). The effects of variations in these input parameters are discussed separately, in the sensitivity analysis section (8.4).

Chloride Simulations. The results of the chloride runs for Dorney are summarised in Table 8.4 below. It is clear that, even after a 28 - day input, only well 2 ever exceeded the EC limit for chloride (250 mg/l) at peak arrival. The breakthrough plots for the 7 - day and 28-day inputs at well 2 are shown in Figure 8.9. This contrasts quite markedly with the analogous plot for Gatehampton well 5 (Figure 8.3), where the EC limit for chloride is shown to be exceeded after both 7 and 28 - day inputs.

Two other characteristics of the Dorney results are worthy

Figure 8.8 -- Sample Particle Trajectories for Dorney.

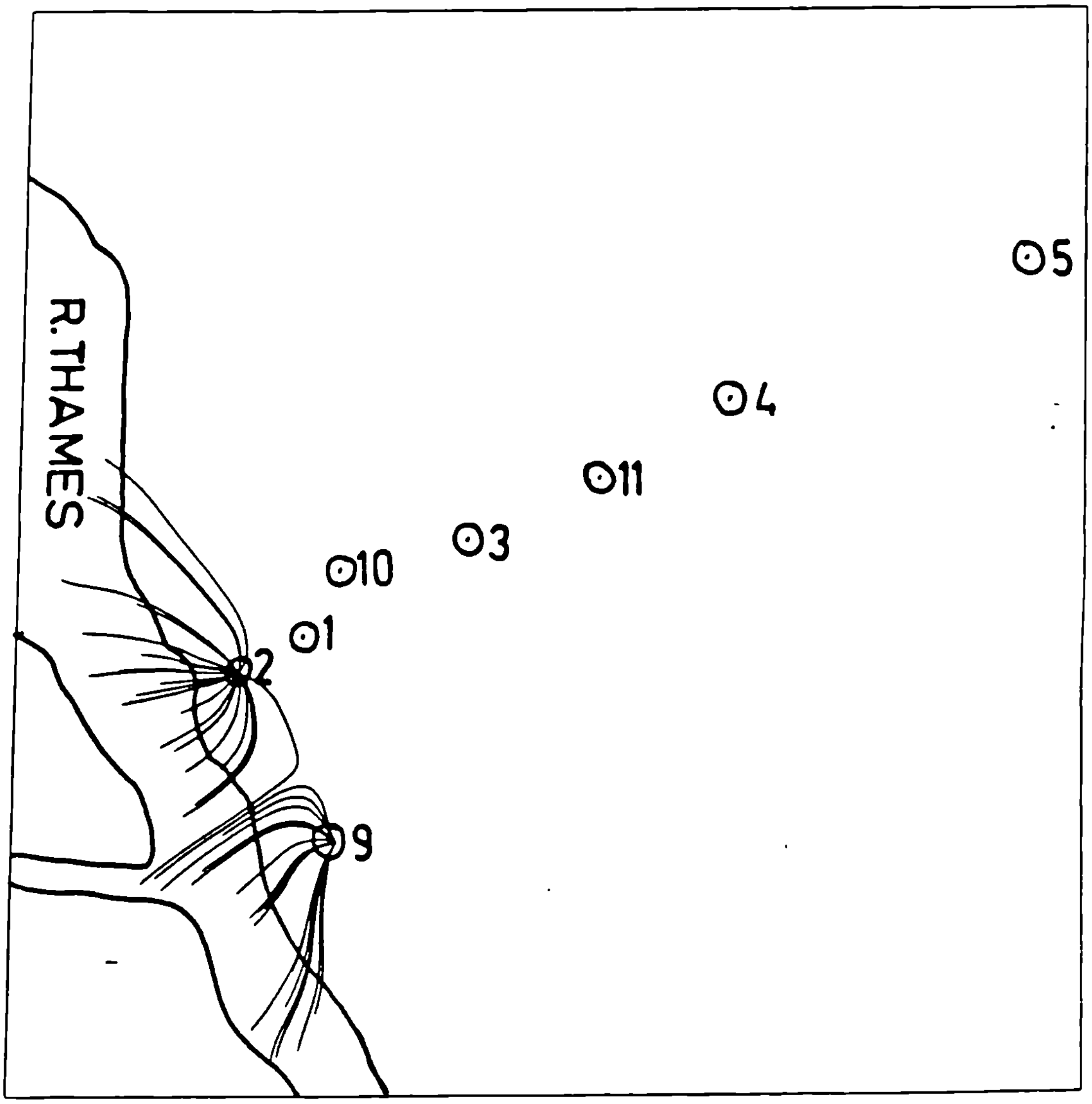


Figure 8.9 -- Chloride Breakthrough at Dorney Well 2 After Inputs of Variable Duration.

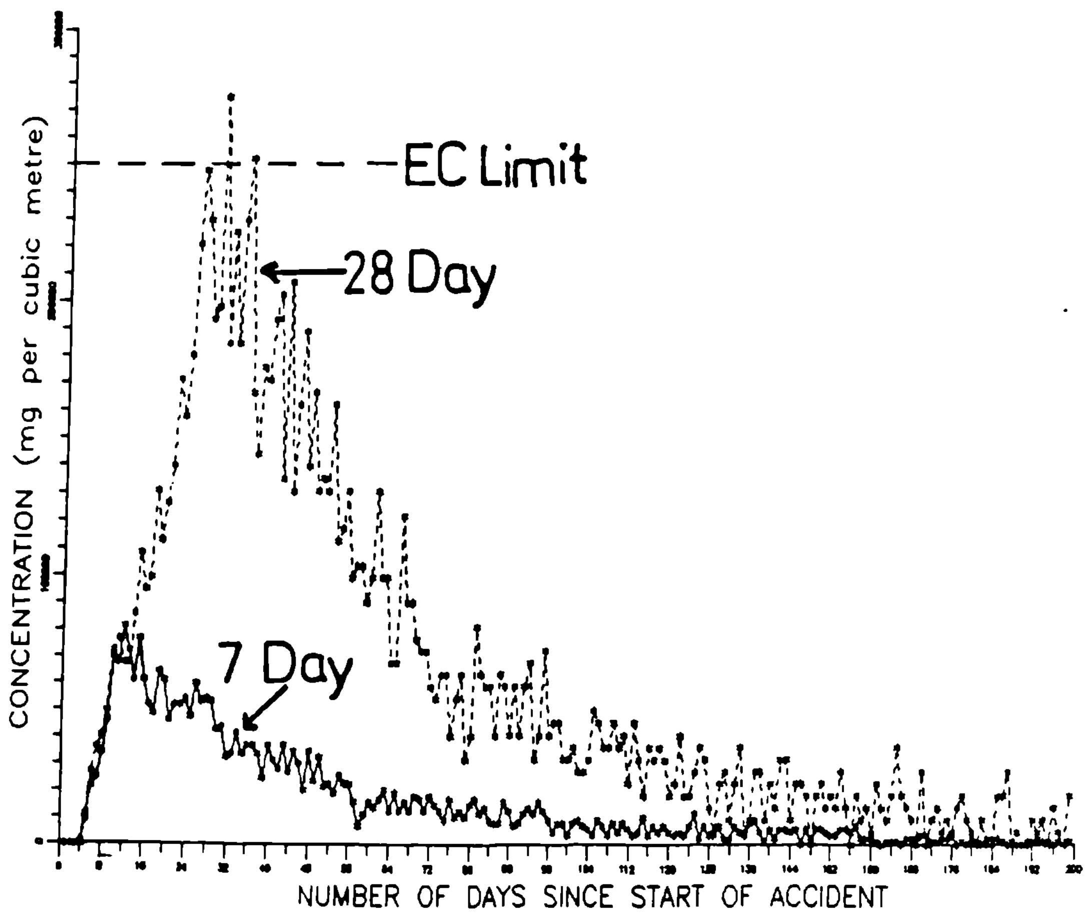


Table 8.4 -- Summary of Results for Dorney Chloride Runs

(a) 20 - Minute Input

Well No.	Earliest Arrival (days)	Latest Arrival (days)	Peak Arrival (days)	Concentration at Peak Arrival (mg/l)
1	28	562	168	0.01
2	4	698	9	0.17
9	6	1661	23	0.08

(b) 7 - Day Input

Well No.	Earliest Arrival (days)	Latest Arrival (days)	Peak Arrival (days)	Concentration at Peak Arrival (mg/l)
1	63	568	63	3.0
2	4	701	12	81.2
9	7	1186	19	37.2

(c) 28 - Day Input

Well No.	Earliest Arrival (days)	Latest Arrival (days)	Peak Arrival (days)	Concentration at Peak Arrival (mg/l)
1	66	583	66	12.0
2	5	712	30	275.2
9	7	1205	43	126.0

of note. Firstly, the earliest particles to arrive at the Dorney wells took 4 days to get there (which is much later than at Gatehampton, where the earliest arrival at well 1 occurred within half a day). Secondly, the latest arrivals took between 563 and 1661 days (4.5 years) to arrive at the Dorney wells (compared with the latest Gatehampton arrival of 500 days at well 7).

Lindane Simulations. The results of the Dorney lindane simulations are summarised in Table 8.5 below. In terms of vulnerability to pollution, only wells 2 and 9 ever showed

Table 8.5 -- Summary of Results for Dorney Lindane Runs

(a) 20 - Minute Input

Well No.	Earliest Arrival (days)	Latest Arrival (days)	Peak Arrival (days)	Concentration at Peak Arrival (mg/l)
1	6149	36501 *	13479	2.3×10^{-8}
2	878	36501 *	6200	3.8×10^{-7}
9	1315	36501 *	15844	7.3×10^{-8}

(b) 7 - Day Input

Well No.	Earliest Arrival (days)	Latest Arrival (days)	Peak Arrival (days)	Concentration at Peak Arrival (mg/l)
1	6156	36500 *	12879	1.2×10^{-5}
2	877	36502 *	6200	1.9×10^{-4}
9	1295	36501 *	14934	5.3×10^{-5}

(c) 28 - Day Input

Well No.	Earliest Arrival (days)	Latest Arrival (days)	Peak Arrival (days)	Concentration at Peak Arrival (mg/l)
1	4871	33795 *	12900	9.6×10^{-4}
2	879	36502 *	6400	1.6×10^{-3}
9	1189	36506 *	12400	1.2×10^{-3}

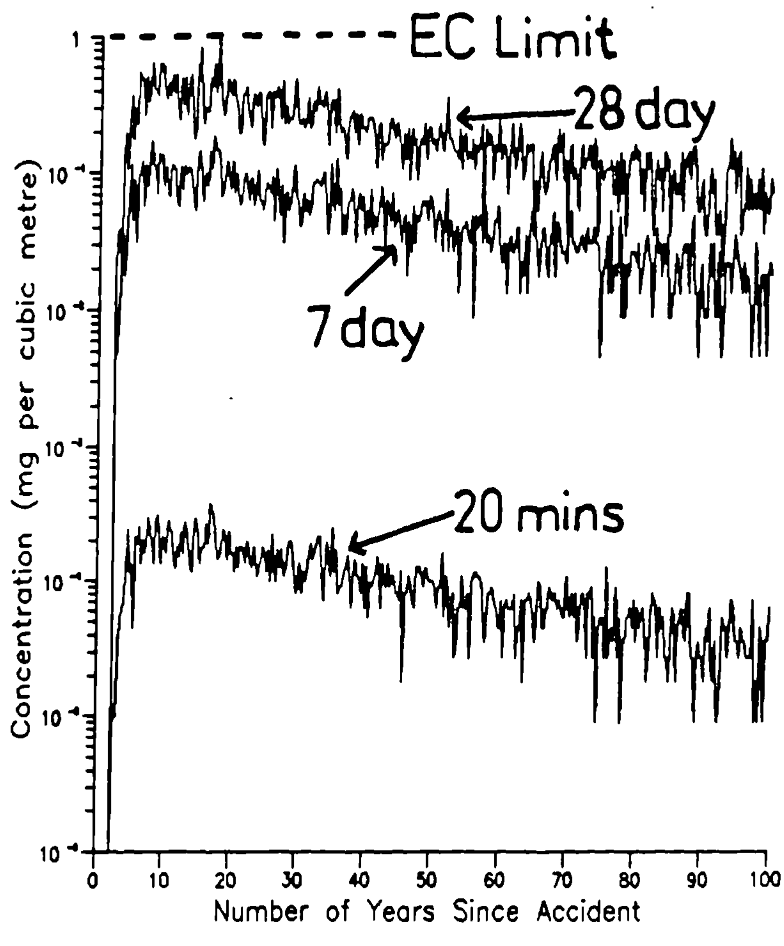
Notes: EC limit for lindane = 1×10^{-3} mg/l

* Maximum time allowed for particle movement was 100 years (ie 36500 days. 23% of particles were still in the streambed sediment after 100 years.

concentrations in excess of the EC limit, and this was only after a 28 - day input.

Lindane breakthroughs at well 2 after events of three different durations are shown in Figure 8.10. Comparison of this figure with the plots for the same problem at Gatehampton (Figure 8.5) reveal one of the most remarkable features of the Dorney results: Retention of particles in

Figure 8.10 -- Lindane Breakthrough at Dorney Well 2 After Inputs of Variable Duration.



the system for more than a hundred years. The results of the Dorney lindane runs showed that, irrespective of the length of input time, 23% of the solute mass remained in the streambed sediment even after simulation times of 100 years. This did not occur at Gatehampton, where even the most tenacious particles had exited the domain within 10 years, and it can only be attributed to the higher value of the organic carbon partition coefficient (Koc) at Dorney (Table 8.1), coupled with the lower groundwater velocity in the streambed sediment at this site. Not surprisingly, peak arrival times were also greatly affected by retardation, varying between 17 and 43 years. In the unlikely event that the streambed sediment lay undisturbed for many decades, these results suggest, for example, that a month - long event in 1990 could cause lindane concentrations in excess of the EC limit at the Dorney wells as late as the year 2040. In the more likely event that the sediment is dredged away, however, these results raise questions about the environmental effects of disposing of such lindane - rich silt either at sea or on land. In particular, the practice of agricultural spreading of dredged sediment could well lead to health problems.

<u>8.3.2.3 -- Summary and Conclusions.</u> On the basis of the modelling results presented above, it can be concluded that the Dorney wells are safe from pollution above the EC limits by chloride or lindane for all but the longest river pollution events (28 days). Even where a 28 - day input occurred, it would seem that only wells 2 and 9 are likely to yield water of unsatisfactory quality; mixing of this water with 'clean' water from the other six wells at the site would no doubt solve even this problem. However, since the chronic toxicity of lindane may be quite high, the persistence of this pollutant in the system for periods in excess of 100 years (as predicted by the model) could give cause for concern.

Two main conclusions emerge from the results of the Dorney pollution simulations. Firstly, the chloride results indicate that the dispersion processes in the gravels may be far more significant than has hitherto been appreciated. The latest arrival times for chloride (1.5 to 4.5 years; Table 8.4) indicate that dispersion results in considerable attenuation of the pollutant plume, suggesting that low concentrations of hazardous pollutants could be supplied to wells 1, 2 and 9 for many years after a short river pollution event.

The second conclusion concerns the role of the streambed sediment. The chloride runs revealed that the low permeability of the sediment at Dorney (as calibrated in the flow model) resulted in delayed arrivals of conservative solutes. Where reactive solutes are concerned, the highly sorptive nature of the sediment (due to its high organic carbon content), which was modelled in the lindane runs, suggests that up to 25% of the solute may remain bound in the streambed sediment for as long as 100 years.

8.4 -- COMPARISON OF THE DORNEY AND GATEHAMPTON RESULTS.

8.4.1 -- Introduction.

By comparing and contrasting the breakthrough parameters for the two simulated sites it was possible to isolate some of the properties of the gravels and the Chalk which were not obvious when the sites were considered in isolation.

8.4.2 -- Earliest Arrival Times.

For both chloride and lindane runs, the earliest arrival times at Gatehampton were far shorter than at Dorney. While the hydraulic conductivity of the gravels at Dorney was calibrated at 1200 m/d (cf 1500 m/d at Gatehampton), it is felt that the difference in earliest arrival times between the two sites was more strongly influenced by the lower hydraulic conductivity of the streambed sediment in the Dorney model (0.015 m/d compared with 0.2 m/d at Gatehampton). For lindane, the effect of greater retardation at Dorney (Rd = 500, compared with 250 at Gatehampton; Section 8.1.5) must also have made a significant contribution, although the effects of the latter were more clearly seen when latest arrival times were compared.

8.4.3 -- Latest Arrival Times.

By comparing the latest chloride arrival times in Table 8.4 with those for the Gatehampton chloride runs (Table 8.2), another contrast between the Gatehampton and Dorney sites can be easily recognised. Even with full matrix diffusion, the latest arrival time recorded from Gatehampton was 500 days (well 7). By contrast, the latest arrival times recorded for Dorney varied from 562 to 1661 days. Comparison of the trajectory plots for the two sites (Figures 8.2 and 8.8) suggests why; at Dorney, the distance travelled by any particle in the gravels was far greater than it was at Gatehampton. Therefore, there was far more opportunity for the effects of dispersion in the gravels to influence particle travel times at Dorney. The full effects of gravel dispersion were not discernible in the Gatehampton results, even though the evidence from Dorney suggests that these effects were possibly more profound than the retardation and dispersion effects due to matrix diffusion in the Chalk which dominate at Gatehampton.

The extreme tardity of the latest lindane arrivals at Dorney are due to the highly sorptive nature of the streambed sediment at that site, as discussed in Section 8.3.2.2 above.

8.4.4 -- Well Vulnerability.

Results of both lindane and chloride runs show that the Dorney wells are far less vulnerable to pollution entering from the river than are the Gatehampton wells. This finding no doubt reflects the fact that the total modelled river contribution at Dorney was only 2% of the site yield (Section 7.3.4), compared to about 10% at Gatehampton (Section 7.2.4).

8.5 -- SENSITIVITY ANALYSES.

8.5.1 -- Introduction.

A few runs were performed to test the sensitivity of the solute transport models to variations in input parameters. In particular, attention was paid to parameters describing dispersion in the gravels and Chalk and retardation in the streambed sediment. Because of the expense of particle tracking runs (cf Section 8.2.2.1 above), the number of analyses which could be performed was very limited, and hence the results quoted here are not as extensive as might be hoped. Nonetheless, they do serve to indicate broad trends which may be useful in further studies. In all of the analyses, the objective function used to evaluate model sensitivity was mean concentration at peak breakthrough.

8.5.2 -- Dispersivity in the Gravels and Chalk.

Since the dispersivity values used in these modelling exercises were wholly based upon estimates from the literature, it seemed worthwhile identifying the amount of error associated with the range of values suggested in Section 8.1.5.

(i) The Gravels. The range of 'possible' values for the dispersivity of the gravels identified in Section 8.1.5 was 12 to 30m. Figure 8.11 shows the change in breakthrough for Dorney well 2 which resulted when the longitudinal dispersivity was changed from 12m to 30m. With the lower dispersivity, the peak concentration at breakthrough was 0.17 mg/l, whereas with the higher dispersivity this was reduced to 0.13 mg/l. This corresponds to a 30% change in concentration for a 150% change in dispersivity, which yields a sensitivity factor (F_S; see equation 7.6) of 0.2.

(ii) The Chalk. When the dispersivity of the Chalk was varied from the minimum (3m) to the maximum value (20m) identified in Section 8.1.5, the mean concentration at peak breakthrough (for Gatehampton wells 1 - 5 after a 28 - day input) declined from 1825 mg/l (Table 8.2) to 1780 mg/l. These changes yield a sensitivity factor of only 0.004.

The difference between the sensitivity factors for the gravels and the Chalk strongly supports the contention made in Section 8.4.3 that dispersion in the gravels has a more profound influence on solute breakthrough than dispersion in the Chalk. Furthermore, this result suggests that the characterisation of dispersion parameters for the gravels is a more pressing need than the further assessment of dispersion parameters for the Chalk. By the same token, the relative insensitivity of the model to variations in Chalk dispersivity is encouraging, and bolsters confidence in the predictions made for the Gatehampton site.

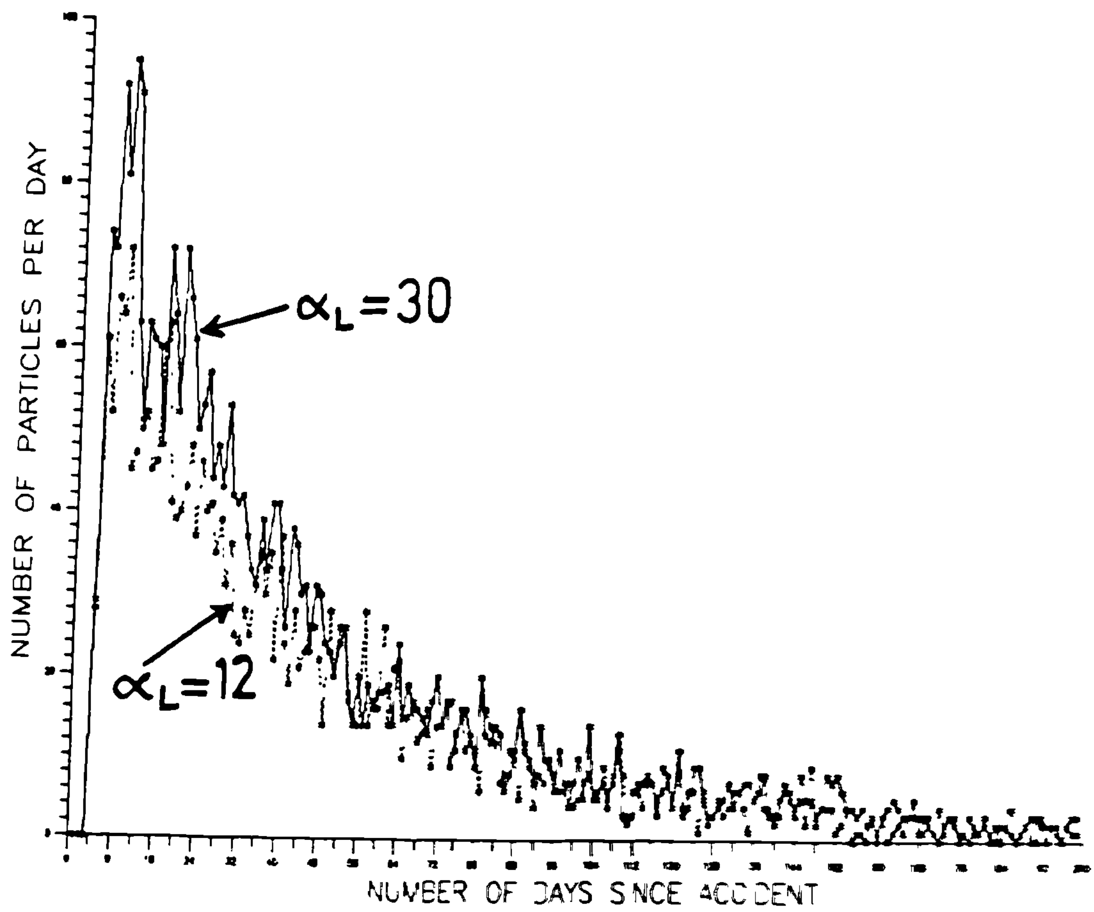
8.5.3 -- Streambed Retardation Factor.

The range of possible retardation factors for the streambed sediment at Dorney is exceptionally wide, due to the occurrence of peats at that locality. When the retardation factor was increased from 500 to 1500, the mean concentration of lindane arriving at well 2 during peak breakthrough was found to decrease from 3.80×10^{-7} mg/l to 1.98×10^{-7} mg/l. These figures yield a sensitivity factor of 0.45, which indicates a high degree of model sensitivity to variation in the streambed retardation factor.

8.5.4 -- Discussion.

Of the three parameters investigated, the streambed retardation factor ($F_s = 0.45$) proved to have the most influence on model performance, followed by gravel dispersivity ($F_s = 0.2$), with Chalk dispersivity having little effect on model output ($F_s = 0.004$). These results

Figure 8.11 -- The Effects of Varying Gravel Dispersivity on Chloride Breakthrough at Dorney Well 2.



mirror the findings of the flow model sensitivity analyses (Section 7.4), in which the streambed parameters (particularly hydraulic conductivity; see Table 7.3) were also found to have more influence than aquifer parameters on model performance. In the light of these findings, it is suggested that further field studies of the stream-aquifer systems of the Thames Basin should give priority to the characterisation of the processes discussed here in the order of their importance for model performance.

8.6 -- SUMMARY AND CONCLUSION.

In this chapter, the successful development of models to predict the response of wells to river pollution at two sites in the Middle Thames Valley has been described. Variations in geology between the two sites allowed the behaviour of the Chalk and the Shepperton Gravels to be assessed separately.

Model predictions suggest that conservative pollutants could reach wells at both sites within four days. While such pollutants would be unlikely to persist in the Gatehampton aquifer after about 1.5 years, dispersion in the gravels may cause background levels of contamination over periods up to 4.5 years at Dorney.

Reactive pollutants, such as lindane, would be strongly retarded by sorption onto organic matter in the streambed sediment, and peak concentrations at wells may not occur until 10 months (Gatehampton) or 17 years (Dorney) after the onset of pollution in the river. Preliminary results show the streambed sediment at Dorney to be more sorptive than that at Gatehampton, however, and this is reflected in the fact that 23% of the solute mass was predicted to be still within the Dorney sediment after 100 years, whereas all the solute was predicted to have left the Gatehampton domain within 7 years.

For both conservative and reactive pollutants, short - term pollution events (20 minutes duration) seem incapable of causing pollution levels in excess of EC limits at the wells. If river pollution persists for 7 days, however, samples from most of the Gatehampton wells could exceed EC limits. At Dorney, it is more likely that pollution in the river would have to persist at a high level for 28 days before EC limits would be exceeded at any of the wells.

Limited sensitivity analyses indicate that model sensitivity to the following parameters increases in the order stated below:

Sensitivity to Chalk Dispersivity $<$ Sensitivity to Gravel Dispersivity $<$ Sensitivity to Streambed Retardation Factor

CHAPTER NINE
DISCUSSION AND CONCLUSIONS

9.1 -- INTRODUCTION.

In this, the final chapter of this thesis, an attempt is made to draw the different strands of the study together. To do this, it is necessary to discuss the more important new results which have arisen out of this study, and note whether these have any wider significance (Section 9.2). Proposals for further work in this field of study can then be made (Section 9.3), and the narrative thus brought to a close (Section 9.4).

9.2 -- NEW RESULTS AND THEIR CONTEXT.

9.2.1 -- Introduction.

As the scope of this study broadly embraced the fields of geology and hydrological modelling, the more important results which arose from it are somewhat diverse. For the purposes of discussion, therefore, it is necessary to divide this summary into two sections. The first deals with the hydrogeological results, and the second with the results of conceptual and mathematical modelling.

9.2.2 -- Hydrogeology.

9.2.2.1 -- New Results. New hydrogeological information will be described in stratigraphic order.

(i) The Chalk. The main contribution to the hydrogeology of the Chalk arising out of this study is the new geological model for the development of the permeability of the Chalk which was proffered in Chapter 4. In essence, this new model argues that the lateral variations in Chalk permeability which are manifest in stream - aquifer systems of the Thames Basin can be explained in terms of Devensian palaeohydrogeology. Permafrost was present beneath the interfluves, acting as an aquitard which prevented the flow of water through, and therefore the dissolution of, the

Chalk. Beneath major rivers, such as the proto-Thames, taliks (unfrozen zones) were present. Because the proto-Thames was braided, the taliks beneath minor anabranch channels were probably seasonal, whereas beneath major channels the taliks would be perennial. In the seasonal taliks, freeze - thaw action would pulverise the Chalk, leading to the development of putty chalk at what is now the gravel / Chalk interface. In the perennial taliks, on the other hand, dissolution would continue all year, leading to the development of zones of high fissure permeability.

A few less important results were offered in support of this new model. In particular, the field data presented in Appendix B are important inasmuch as they illustrate that the fissure permeability of the Chalk does not vary with fracture frequency (which was shown to be fairly homogeneous over wide areas of southern England), but rather with fissure aperture.

(ii) The Gravels. Field study of the Middle Thames Gravels brought three benefits to this study:

(a) It inspired the formulation of the Chalk permeability model (Chapter 4), which is dependent on the palaeo-environmental interpretation of the Gravels.

(b) The determination of organic matter content on samples of Shepperton Gravels from Gatehampton and Kingsmead (Appendix C) furnished useful data on the sorptive nature of the gravels (Section 8.1.5). At about 1%, the organic matter content is much higher than was anticipated, and is indeed much higher than the value of 0.1% quoted for similar glacial outwash gravels in Switzerland (Schwarzenbach et al, 1983).

(c) The measurement of the relative abundances of sand and gravel sub-facies in quarry faces allowed the calculation of average hydraulic conductivities for large volumes (1000 m^3) of gravel (Section 5.2.3). These values provided a useful benchmark with which 'calibrated' values for gravel hydraulic conductivity could be compared (Section 7.2).

(iii) **The Streambed Sediment.** The new data on the hydrogeological and geochemical properties of the Thames streambed sediment (presented in Appendix C and Section 3.4.4) are the only known data on this subject. Briefly, they proved the sediments to be predominantly grey - brown silts and clays, with localised peats. Organic matter contents vary from 1.6% (silts) to 57.4% (peat), about a mean of 15.6%. Lab permeameter measurements yielded a lower limit for hydraulic conductivity in the gravels as 0.002 m/d. All of these data proved invaluable in the modelling exercises described in Chapters 7 and 8.

9.2.2.2 -- The Wider Context. There is an increasing appreciation of the value of basic geological information in the formulation of hydrogeological models. For a few years, the geological aspects of groundwater studies seem to have been somewhat eclipsed by mathematical aspects. However, it is now widely appreciated that mathematical modelling capabilities are far ahead of data provision capabilities (Abriola, 1987; Anderson, 1987; Rushton, 1989).

Previous models for the development of the Chalk as an aquifer were thoroughly reviewed in Section 4.4.1, and therefore nothing more need be said about the place of the new model in the specific context of Chalk hydrogeology. However, the wider context of the model may still be explored.

In the development of the Chalk permeability model (Chapter 4) and in the use of facies abundances to estimate gravel permeabilities (Section 5.2.3), attempts were made to integrate geological facies models with hydrogeological characterisation. These attempts may be viewed as part of a growing trend towards the maximisation of geological input in hydrogeological studies.

As mentioned in Section 5.2.3, efforts to integrate facies models with hydraulic parameters have recently been made in the USA (Anderson, 1989), Switzerland (Jussel, 1989), and southern England (Dixon, personal communication, 1989). However, these efforts were by no means the first in this direction. For instance, Pettyjohn and Randich (1966) used lithofacies maps of glaciogenic Quaternary sediments to define aquifer boundaries and 'hydrofacies' (ie lithological units which have distinctive hydraulic properties). Sharp (1977) used facies data to evaluate the validity of some common assumptions made in the numerical modelling of alluvial aquifers. In particular, Sharp (1977) noted the pronounced increase in grain size (and therefore permeability) with depth which is common in alluvial aquifers of the central USA, and the fact that no major rivers in that area fully penetrate their alluvial aquifers. Both of these invariable geological characteristics have been frequently ignored by numerical modellers. Hydrochemical studies and evaluations of aquifer history frequently involve the application of petrological and geochemical techniques; for examples, the papers by Sharp and McBride (1989), Kreitler (1989) and Back and Baedecker (1989) should be consulted.

Despite this increasing trend towards the maximisation of geological input in groundwater studies, however, very few investigators have presented data on the hydrogeological and geochemical properties of streambed sediments. Indeed, for all of the literature examined in the course of this study, only fleeting mentions of streambed properties could be found. Karickhoff (1984) and Schwarzenbach et al (1983), for instance, briefly quote some compositional data (% organic matter, silt and clay contents etc) for streambed sediments in the USA and Switzerland respectively. While numerous authors have estimated streambed hydraulic conductivity in the course of model calibration, an extensive literature review failed to reveal any published examples of lab or field measured values for this parameter.

Until recently, in-situ measurement of the permeability of channel beds was restricted to studies of canal linings. In these studies, measurements were made using 'seepage meters', which are essentially falling head permeameters connected to a 'bell' on the canal bed (Bouwer and Rice, 1963). Lerner et al (1989; Chapter 14) have reviewed a few examples of these canal studies. The use of conventional seepage meters in many natural rivers is precluded by the strong waves and currents and the depths of water encountered. However, in the last few years, two techniques have been developed to overcome these difficulties. Cherkauer and McBride (1988) have described a large seepage meter which is claimed to be suitable for use in large rivers, although it has so far only been tested in large lakes. Welch and Lee (1989) have devised a method for installing and monitoring piezometers in the beds of rivers. These piezometers have been used in rivers up to 8m deep, penetrating the bed sediment to depths of 2.5m below the sediment surface. Flexible tubing can be used to connect these piezometers to permanent monitoring cylinders on the river bank. Using this method, water samples may be obtained and head measurements taken at any position in the stream - aquifer interface. Both of the above techniques are limited in scope at their present level of development, and (according to their designers), neither would be suitable for measurements in unconsolidated silt (such as the Thames bed sediment). To date, no values for streambed parameters measured with these techniques have yet been published.

Viewed against this background, the new data on the streambed sediment of the Thames, meagre though they are, represent a significant increase in the store of knowledge on this subject. Given the importance of streambed properties in controlling flow and transport in stream-aquifer systems, and also the sensitivity of both flow and transport models to streambed parameters describing them (Sections 7.4.2 and 8.5), it is clear that much would be gained by more detailed field and laboratory studies of streambed sediment.

9.2.3 -- Modelling.

9.2.3.1 -- New Results. In discussing the results of the modelling component of this study, it is convenient to divide the presentation into three sections; conceptual modelling, mathematical modelling, and the results of model application.

(i) Conceptual Modelling. Conceptual modelling is a process of summary and simplification, and for this very reason, it cannot add new data to mankind's store of knowledge, although it can greatly enhance our understanding of existing data.

To summarise the main points of the conceptual model briefly, the assumed properties of the three hydrostratigraphic units will be stated in list form:

Chalk -- Flow: Heterogeneous (laterally and vertically), vertical K not equal to horizontal K. Flow occurs in a fissure - continuum.

-- Transport: Advection, matrix diffusion and mechanical mixing in the fissure system dominate solute distribution.

Gravels -- Flow: Regularly heterogeneous (may be regarded as homogeneous on the scale of modelling). Isotropic. Flow intergranular.

-- Transport: Advection, mechanical mixing and sorption are the dominant processes.

Streambed Sediment -- Flow: Heterogeneous (lack of data compels use of homogeneous data set), flow in vertical direction only. Flow intergranular.

-- Transport: Advection, slight mechanical mixing, molecular diffusion, strong sorption.

(ii) Mathematical Modelling. A number of unusual or innovative features were included in the formulation of UNCLESAM. These are listed below.

Coupling of flow in the two hydraulically continuous aquifer layers (gravels and Chalk) was accomplished by using a simple Darcian equation (equation 6.19), in which the distance over which the hydraulic gradient is calculated was set equal to half the sum of the thicknesses of the upper and lower layers. The permeability used in this equation is the harmonic mean of the upper and lower layer hydraulic conductivities, weighted according to layer thickness.

Within the Chalk layer, stratification into sub-layers of varying hydraulic conductivity is explicitly included, and is used in the calculation of transmissivities according to the latest position of the water table. In the solute transport module, this structure is used as the basis for calculating vertical velocity components in the Chalk according to a simple interpolation algorithm.

Allowance is made for the gravel layer to 'pinch - out' against the Chalk, and the flow of groundwater across this boundary is accounted for by a simple mass balance calculation.

Simple extensions of the particle tracking method were made to allow:

(a) the introduction of vertical velocity components

(b) the solution of the equation describing distal transport through a dual - porosity system in terms of an enhanced dispersion coefficient and an apparent retardation due to solute exchange between the fissures and the porous matrix blocks

(c) the representation of molecular diffusion in the streambed sediment

(d) efficient modelling of transport through homogeneous low permeability zones by the temporary use of a large timestep for tracking in such zones.

(iii) Results of Model Application. Although great uncertainty surrounds model predictions, particularly those for solute transport, a number of interesting results emerged when UNCLESAM was applied to the field sites at Gatehampton and Dorney.

In water resource terms, the flow models suggested that the river - derived components of total site yields are rather small (10% at Gatehampton, and only 2% at Dorney). Solute transport simulations suggested that neither site is likely to yield water of unacceptable quality (measured against EC limits) after a short river pollution event, such as a tanker spill. After more sustained river pollution events (1 week at Gatehampton, 1 month at Dorney) the quality of water from the wells closest to the river could deteriorate below EC standards. While conservative pollutants could reach the wells rapidly (0.5 days at Gatehampton, 4 days at Dorney), retarded species may take many months (Gatehampton) or even years (Dorney) to reach peak breakthrough at the wells.

Sensitivity analyses of both flow and solute transport models indicated that streambed parameters (especially hydraulic conductivity and sorption parameters) exert a far stronger influence on model performance than any of the parameters describing flow and transport in the aquifers. Where conservative contaminants enter highly permeable Chalk, a full description of solute arrival at wells is only possible if a full solution of the equations for matrix diffusion is obtained. Nonetheless, advection-dispersion calculations will give a worst case estimate of peak breakthrough. Dispersion in the gravels is thought to be quite marked, and the modelling results suggest that where a flowline stays in the gravels for a substantial distance, the effects of gravel dispersion in modifying solute distributions are likely to be more profound than the effects of matrix diffusion during subsequent flow in the Chalk.

9.2.3.2 -- The Wider Context. Numerous models of flow and transport in the Chalk have been described in the literature (eg Connorton and Reed, 1978; Morel, 1979; Oakes, 1981; Black and Kipp, 1983; Müller, 1987; Retrowski et al, 1988), and therefore the conceptualisation of the Chalk is not a new task. Virtually all of the assumptions made about the Chalk in this study have been made in earlier studies, and found to be trustworthy. A minor exception to this may be noted, however; on the basis of the new model for Chalk permeability development (Chapter 4) two additional assumptions were made:

(a) It was assumed that the hydraulic conductivity of the Chalk at Gatehampton is at its highest wherever it is overlain by the Shepperton Gravels.

(b) It was assumed that the structured variation in Chalk permeability with depth need only be represented where the Chalk is overlain by the Shepperton Gravels.

The second of the above assumptions allowed simplifications in transmissivity calculations in areas where the Chalk forms the surficial aquifer. These simplifications produced valuable savings in run time and storage.

Few modelling studies of the Thames Gravels have been made to date, and those which have (eg WRC, 1988; Dixon et al, 1989) are for flow only (though a solute transport model for the Upper Thames Gravels is under development at the Institute of Hydrology). No models have so far included any detailed representation of the streambed sediment. Therefore the assumptions proffered for the gravels and the streambed sediment in the conceptual model have greater novelty value than those proffered for the Chalk. At present the only way to assess the validity of the conceptualisations for these two media is to monitor the performance of the mathematical models which enshrine them. Given the good agreement between the observed and modelled drawdown behaviour (especially for the Gatehampton site; Section 7.2.3 and Figures 7.5 and 7.6), confidence in the validity of the conceptual model seems to be justified.

There is one assumption in the conceptual model which could have an adverse effect on model output if the UNCLESAM code were applied to certain field sites. This is the assumption that the Staines Alluvium operates as an impermeable 'seal' on the banks of the river, so that all stream - aquifer exchanges must occur across the streambed sediment. For Gatehampton and Dorney, the alluvium is sufficiently widespread that this assumption seems to be perfectly reasonable. However, at some other sites in the Thames Basin, the Staines Alluvium is locally absent and the river banks are cut into Shepperton Gravels. In such sites, more exchange would occur through the banks than through the streambed, and the above assumption would no longer be valid.

Many of the unusual features in the UNCLESAM code have subsequently been discovered to have a precedent in the work of other authors. For instance, while the coupling technique for the gravel and Chalk layers was developed from first principles, it was later discovered that the same formulation had been independently derived by McDonald and Harbaugh (1984) and the Water Research Centre (WRC, 1988) for application in a finite element model. The calculation of an overall transmissivity for a superposed system of layers is well established (Rushton and Redshaw, 1979), and the interfacing of one- and two-layer model segments to represent the pinch - out of strata has previously been described by Rovey (1975). In the solute transport module, the introduction of vertical flows and molecular diffusion into the particle tracking formulation have been previously accomplished by Ahlstrom et al (1977) and Mackay et al (1988). Three of the particle tracking features are new, however:

(a) The temporary use of a large timestep to speed execution where a homogeneous low - permeability layer (eg the streambed sediment) is being traversed by a particle.

(b) The adaptation of the particle tracking scheme to include enhanced dispersion and apparent retardation due to distal matrix diffusion effects.

(c) The vertical interpolation algorithm which represents the details of vertical flows in the layered Chalk.

Since the first two of the above features are simply logical extensions of the original formulation of the particle tracking method (Prickett et al, 1981), there can be little doubt that they perform adequately. Nonetheless, the enhanced dispersion technique was checked against published results, and was found to be performing just as expected (Figure 6.16). The third new feature, the vertical velocity interpolation algorithm, performed well when it was compared with finite difference solutions to test problems (Figures 6.23 through 6.25), but the range of flow conditions for which it is valid is as yet unknown. All that can be said at this stage is that the results it produced in the Gatehampton simulations seem reasonable and logical.

Modelling errors can be greatly increased if vertical components of flow and transport are ignored, and the efforts made in this study to include vertical variations in permeability and vertical velocity components are very much in line with recent trends in flow and transport modelling (Connorton, 1985; Konikow and Mercer, 1988; Rushton, 1989).

Because of the uncertainty surrounding the definition of input data, the model predictions summarised in the previous section can only be accepted with a great deal of caution. Nonetheless, this is the first time quantification of pollutant travel times and well vulnerability for stream - aquifer systems in the Thames Basin has been attempted, and if the model results serve no other purpose they will still be valuable as 'conversation pieces' for resource managers. However, the good agreement between observed and modelled drawdowns in the flow models does lead one to suppose that the solute transport results have a little more value than this.

To place these modelling efforts in context, it is instructive to compare them with recently published case-studies of similar efforts. In this way, the strengths and weaknesses of the new models become more apparent, and the standing of the new results in the wider context may be evaluated. Table 9.1 gives a comparison of the new models with published case studies by Kovar and Grakist (1989) and Zipfel and Horalek (1989), who both modelled stream-aquifer systems in the Rhine Basin. At both of the study sites, single - layer clastic aquifers are partially penetrated by the Rhine.

It is clear from Table 9.1 that the new models compare very favourably with the two recently published models in scope and depth of coverage. In particular, the new models include nine features which were omitted from the model of Kovar and Grakist (1989), and four which were not considered in the much more thorough study by Zipfel and Horalek (1989). While it could be argued that the breadth of coverage says more about the optimism of the researcher than about the quality of the results, this comparative study certainly suggests that the new models are in line with modern trends in stream - aquifer modelling.

Table 9.1 -- A Comparison of Stream-Aquifer Pollution Models			
Model --> / Feature	Present Study	Kovar & Grakist (1989)	Zipfel & Horalek (1989)
More than One Aquifer Layer?	Yes	No	No
Rapid Groundwater Velocities?	Yes	No	No
Calibrated Flow Model Tested For Transient Run?	Yes	No	Yes
Dispersion Included?	Yes	No	Yes
Modelling of Vertical Flow and Transport?	Yes	No	Yes
History Matching With Water Quality Data?	No	Yes	No
Nested Grids Used for Small - Scale Simulations?	Yes	No	Yes
Predictions of Future Conditions Attempted?	Yes	No	Yes
Detailed Modelling of Streambed Sediment?	Yes	No	No
Non - Conservative Pollutants Simulated?	Yes	No	No

9.3 -- PROPOSALS FOR FURTHER WORK.

9.3.1 -- Introduction.

It is often the case that detailed studies such as this raise more questions than they answer. Indeed, the scientific stature of any such project would be dubious if it did not, in reaching one horizon, open up a vista over unexplored territory. Thus, before closing the present discussion, it is appropriate to outline some of the prospects for further work which arise out of this project.

9.3.2 -- Hydrogeology.

Three main aspects of the hydrogeology of Thames Basin stream - aquifer systems are obvious candidates for further study; in order of decreasing importance these are the properties of the streambed sediment, the hydraulic characterisation of the Shepperton Gravels, and the expansion of the database for the Chalk.

(i) The Hydrogeology of the Streambed Sediment. All of the foregoing work has demonstrated the importance of the modern streambed sediment in controlling flow and transport in stream - aquifer systems. The sensitivity of flow and transport models to streambed parameters was also noted. In the light of these findings, it is suggested that a major program of sampling and in - situ testing of the streambed sediment should be a scientific priority in any further studies of stream - aquifer interactions in the Thames Basin. In particular, the following information should be sought:

(a) Spatial and temporal variations in the thickness of the streambed sediment. Direct measurement of sediment thickness may not always be easy. For example, unless the sediment thickness is measured by digging from within a diving bell, it might be difficult to decide the exact location of the streambed / gravel interface for the purposes of 'remote sensing' from a boat (using either geophysical means or some sort of physical probe). On the other hand, the estimation of thicknesses from information on sedimentation rates and dredging frequency (as in the present study) is subject to great uncertainty.

(b) The hydraulic conductivity of the sediment. It is highly desirable that this be determined in - situ, perhaps using a seepage meter (Cherkauer and McBride, 1988) or specially installed piezometers (Welch and Lee, 1989). Whichever method was used, some modifications to existing designs would be inevitable.

(c) Spatial variations in the composition and geochemical properties of the sediment. Sampling of the streambed sediment at many points would be necessary to characterise these properties. Ideally, sampling would be best undertaken using a specially designed bed sediment coring device mounted on a boat (eg Golterman et al, 1983; Munch and Killey, 1985). It may be that several sampling programmes would be necessary to delineate temporal trends.

The techniques described in Appendix C could be applied to these samples, but it would also be very useful if laboratory batch - column experiments were also performed to assess bio-degradation and other processes which are as yet unquantified for the Thames sediment. It may be possible that the different 'facies' within the sediment (grey silt, brown mud, peat etc) could be mapped as a result of this exercise, and linked to data on hydraulic conductivity and geochemical properties, so that predictions of well vulnerability could be improved.

If the above programme of characterisation were carried out, predictive models based on the UNCLESAM code could be developed for all riverside wellfields with considerable confidence.

(ii) Gravel Hydrofacies. The possibility of defining 'hydrofacies' by combining information on hydraulic properties with information on the distribution of lithofacies (Pettyjohn and Randich, 1966) has been mentioned at several points in the preceding text (Sections 5.2.3, 9.2.2.1), and efforts in this regard at other sites were reviewed in Section 9.2.2.2. Taking these efforts as a guide, the definition of hydrofacies for the Shepperton Gravels would seem to be feasible, and there is no doubt that the statistical information which such an exercise would produce could be used to derive much more meaningful models of advection and dispersion in the gravels. In view of the relative importance of gravel dispersivity in controlling pollutant breakthrough at wells (Section 8.5), any improvement in the description of dispersion in the gravels must be welcomed.

(iii) The Hydrogeology of the Chalk. Because of its general importance in the water supply of England, the Chalk will continue to be the focus of much research. With regard to the findings of the present study, it is simply proposed that the new model for the development of Chalk permeability be borne in mind during future studies of the Chalk, so that due attention is given to data which may be used to further test and refine this model. In particular, further observations on the following would be very useful:

(a) Fracture and fissure frequency, the latter particularly in boreholes.

(b) Palaeohydrogeology of the Chalk. A study of the age and composition of sediments infilling ice - wedge casts and subterranean openings in the Chalk may yield valuable information on this topic.

(c) Features which give further clues about the Devensian history of the Thames Basin (gelifluction lobes, fossilised patterned ground etc).

(d) The distribution of fissures and permeability in Chalk beneath gravel trains which mark previous courses of the Thames during earlier cold stages of the Quaternary.

None of the four items above would require the establishment of special studies; all could be observed during the course of routine field work.

9.3.3 -- Modelling.

9.3.3.1 -- Introduction. Reflecting upon the modelling efforts and results described in Chapters 5 through 8, a number of ideas for further work arise. These proposals are classified into those dealing with model formulation and those dealing with model use.

9.3.3.2 -- Further Work on Model Formulation. Four possibilities spring to mind:

(i) Modelling Flow through River Banks. In evaluating the conceptual model (Section 9.2.3.2), it was noted that the assumption that the Staines Alluvium operates as an impermeable 'seal' on the banks of the river may not be valid for some of the field sites in the Thames Basin. Thus it is proposed that it would be useful to develop UNCLESAM further so that this particular assumption may be relaxed. Quite how the formulation of the mathematical model could be changed to incorporate this feature is not immediately obvious, but it is probable that a suitable methodology could be derived. This facility would considerably increase the generality of the UNCLESAM code, allowing very complex hydrostratigraphies to be modelled easily.

(ii) Further Evaluation of the Vertical Velocity Interpolator. The limited tests performed on the simple vertical interpolation algorithm in this study are insufficient to indicate the full range of conditions for which it is valid. Therefore it would be valuable to return to first principles, and compare the approximations inherent in the interpolator with the full three-dimensional case. In the process of deriving the approximate expression from the 'exact' expression, the limiting assumptions which are implicitly included in the formulation of the simple interpolation algorithm would be revealed. This exercise would allow the validity of the algorithm to be defined.

(iii) A General Representation for Matrix Diffusion. It was noted in Section 6.3.4.4 that the solution of the equation describing solute transport with matrix diffusion can be divided into three 'regions' (Lever et al, 1983). Two of these regions (the proximal and distal regions) produce solutions which are identical to the solutions of simpler expressions, both of which have particle tracking analogues. There is as yet no particle tracking representation for the intermediate region, which, at Gatehampton, is approximately defined by the zone where a solute is more than 9m and less than 900m into the Chalk along its particular path of motion. Since this region envelopes most solute travel paths from the river to the wells, it is obviously desirable that a technique be found to fully represent the intermediate region within a particle tracking code. If concentration - dependent calculations are rejected (as they must be if the particle tracking method is not to be robbed of its main advantages over other methods), then an alternative formulation must be sought. It is possible that some sort of random retardation procedure could be introduced to represent the delay in solute movement caused by matrix diffusion (the author has heard that research in this direction is under way at Lancaster University). The fundamental problem with such an approach would be to define the basis on which these random retardations could be assigned. What physically meaningful criterion could be used?

Another possibility would be to abandon the particle tracking method altogether, and re-develop the solute transport module of UNCLESAM using a finite element representation incorporating matrix diffusion (as used by Müller, 1987, for example). However, this alternative would re-introduce the problem of numerical dispersion, which has been avoided in the present study.

(iv) Improve the Representation of Time - Dependent Dispersion. Given the importance of dispersion in the gravels in controlling breakthroughs, it would be useful to represent the time - dependence of dispersion as faithfully as possible. Marsily (1986, pp. 247 - 251) gives an excellent review of research to date on this interesting subject. However, there is as yet no generally agreed method for modelling the time - dependence of dispersion, and therefore the proposal that more work be done on this problem is no more than a pious benediction at this stage.

9.3.3.3 -- Further Work on Model Use. Apart from stating the obvious, such as a proposal that UNCLESAM be applied to more sites and that the models presented here be updated in the light of future experience, two more particular suggestions are made:

(i) **Variations in Streambed Thickness.** It would be interesting to take one of the site models and assess well vulnerability to river pollution in the event that the streambed sediment is completely removed by dredging. Obviously, this would require the generation of several new velocity fields for the site, which would require quite a lot of time and effort. For this reason no attempt was made to address this problem in the present project. In some ways, the effects of complete removal of the streambed sediment are obvious; well pollution will get worse. The question to be addressed, of course, is 'how much worse?'.

(ii) **Nested Models.** In the Gatehampton model, slight distortions in the flow field were found to result from the effects of the fixed head boundaries around the perimeter of the nested grid. To avoid this problem recurring, it is suggested that nested grids are given known - flow (Neumann) boundaries instead of fixed head boundaries in future.

9.3.4 -- Operational Suggestions.

As a result of the assessment of well vulnerability at Gatehampton and Dorney, a few operational suggestions are proffered.

(i) **Liaison with Dredging Department.** In view of the critical role of the streambed sediment in preventing or attenuating groundwater pollution, it is suggested that those concerned with groundwater resources and quality should make sure that they have ready access to future schedules and past records for dredging operations for those river reaches adjacent to major wellfields. In this way, the risk of contamination from *past and future river* pollution events can be more readily assessed.

(ii) **Liaison with River Quality Officers.** It is suggested that an arrangement is made such that groundwater managers can be automatically informed of any river pollution event which takes river quality above EC limits. Along with the dredging timetables, this information could be used to make a rapid assessment of whether there is any threat to riverside well sources.

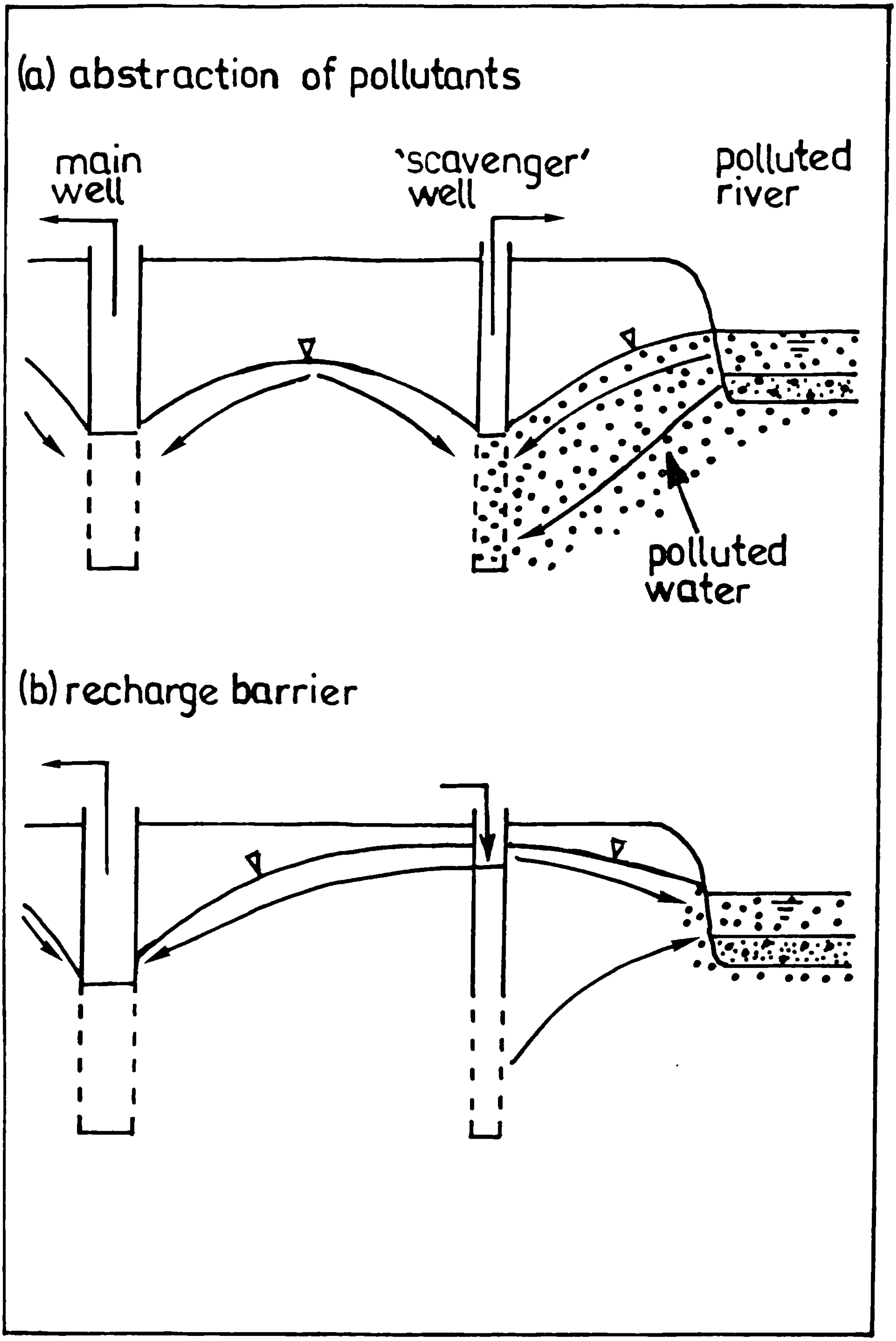
(iii) **Response to the Threat of Pollution.** If the information coming from river quality officers and dredging operators suggests that impingement of pollution on a riverside aquifer is imminent, contingency plans for dealing with the emergency must be brought into effect. Of course, from an utterly pragmatic point of view, the water supply undertaking concerned (Thames Water plc, Mid-Southern Water Company etc) could simply arrange for water from the riverside wells to be given more water treatment than usual. From the point of view of a regulatory authority (such as the National Rivers Authority), however, the prevention or minimisation of aquifer pollution would be a more desirable object of any contingency plans.

Any such contingency plans must acknowledge the main difference between river pollution and groundwater pollution, which has been highlighted by the modelling results presented in Chapter 8: The time scale over which pollutants may persist in the subsurface is many times greater than the time it will take for river pollution to cease. On the other hand, pollutants may begin to arrive at the Gatehampton wells within half a day (with peak arrivals as soon as 1.5 days after the onset of river pollution), so the implementation of emergency plans must not be delayed. In preventing or ameliorating groundwater pollution from river spills, therefore, steps must be taken to minimise the ingress of pollutants into the aquifer, since restoration of the aquifer may be virtually impossible once pollution is established. Even if a pollution event in the river is short in duration (like the 20 minute spills in the modelling runs), so that it is unlikely to cause a breach of EC limits at the wells, it is still worth attempting to prevent ingress of pollutants, for any subsequent events combining with the first may cause a breach of EC limits.

Obviously, merely switching the pumps off for a few days is not a suitable response. The most rapid recovery rates (eg 14 days at Gatehampton; Robinson et al, 1987) are still so slow that pollution would be well established before the groundwater gradient reversed and began to cause transport of pollutants back to the river. Another approach is necessary.

If 'scavenger wells' had been installed immediately adjacent to the river before the pollution crisis arose, then a number of alternative strategies would be possible. In the first strategy (Figure 9.1a), these wells could be pumped so that all of the polluted groundwater would be interdicted before it had travelled far into the aquifer. The second option (Figure 9.1b) would be to use these scavenger wells as recharge wells, and create a recharge boundary which would locally reverse the hydraulic gradient and prevent the flow of any contaminated water into the subsurface until such time as the river pollution subsided and the contaminated streambed sediment could be dredged

Figure 9.1 -- Stream - Aquifer Pollution Prevention Using Scavenger Wells.



away. Unpolluted water from the main pumping wells could be used for this artificial recharge. Of these two options, the second is the more attractive since it renders the ingress of pollutants virtually impossible, and also provides a cordon for the supply wells during the potentially hazardous operation of dredging away the streambed sediment. A third option, which would reverse the hydraulic gradient within the aquifer and also minimise the total loss of water, would be to simultaneously recharge the main wells and pump the scavenger wells. Depending on the circumstances, the total pollutant load in the mixed water emerging from the scavenger wells might be diluted below danger levels.

It is suggested that some consideration be given to the construction of 'scavenger wells' at riverside well fields in the Thames valley, and to their operation according to one or other of the above strategies. UNCLESAM could be used to model the various management options, thereby aiding the optimal design of such wells. This proposal for further modelling work can be added in retrospect to the list of modelling proposals in Section 9.3.3.3 above.

9.4 -- SUMMARY AND CONCLUSION.

9.4.1 -- Summary.

Stream - aquifer systems in the Thames Basin have been investigated and modelled, and an assessment of the vulnerability of wells to pollution by the ingress of polluted river water has been made. Flow and solute transport in these stream - aquifer systems were found to be primarily controlled by the varied hydraulic and geochemical properties of three hydrostratigraphic units, namely; the Cretaceous Chalk, the Devensian Shepperton Gravels, and the modern streambed sediment.

The Chalk is a very pure limestone aquifer in which flow and solute advection occur mainly in major bedding - plane fissures, which have been widened by dissolution. In between these fissures, saturated 'matrix blocks' of highly porous but relatively impermeable Chalk act as solute reservoirs. Solutes are exchanged between these matrix blocks and the water in the fissures by molecular diffusion, in response to concentration gradients. This two - way exchange, which is known as 'matrix diffusion', is the primary attenuation mechanism affecting solutes in the Chalk, and it affects conservative and reactive solutes alike.

The Shepperton Gravels (Devensian) comprise a member of the Middle Thames Gravel Formation (Quaternary). They are predominantly composed of massive, coarse pebbly gravels with interbedded channel - fill lenses of well sorted medium grained sand. Although generally unconsolidated, the Shepperton Gravels are locally cemented by goethite and other iron compounds, which are currently precipitating at the water table in many sites. Fines are rare in the gravels, but organic matter may be present in quantities up to 1.5% by mass. The hydraulic conductivity of the gravels is high ($\leqslant$ 2000 m/d), and their specific yield is variously estimated at 0.05 to 0.25. Flow and transport are intergranular, and mechanical dispersion is quite marked. Adsorption onto organic matter and iron hydroxides causes retardation of reactive contaminants relative to conservative species by as much as a factor of 100.

The modern streambed sediments are predominantly grey silts and brown muds (with some peat locally), and they are very rich in organic matter ($\leqslant$ 57.4%). They are of variable thickness, but seem to be about 0.5m thick at the study sites. Hydraulic conductivity is very low (0.001 - 1.0 m/d), and molecular diffusion probably makes a significant contribution to the movement of solutes. Reactive solutes are strongly retarded (by a factor $\sim$ 1500) by sorption onto organic matter and clay minerals.

The hydrogeological framework of the Middle Thames stream-aquifer systems is largely a product of Devensian processes of erosion (dissolution and cryoturbation of the Chalk) and deposition (the aggradation of the Shepperton Gravels in a braided river system). Lateral variations in the permeability of the Chalk seem to be a function of the distribution of permafrost during the Devensian and other cold stages of the Quaternary. In particular, dissolution in perennial sub-river taliks (unfrozen zones) would appear to account for the high permeability of the Chalk in river valleys, with cryoturbation in seasonal taliks beneath minor river channels leading to the development of a confining layer of 'putty chalk' between the Chalk and the gravels at some sites.

A mathematical model for flow and solute transport in stream - aquifer systems has been developed. In this model, an implicit finite difference formulation for flow is used, and line - successive over - relaxation is used to solve the difference equations. Coupled equations for up to three layers (Chalk, gravels and streambed sediment) are solved simultaneously to obtain values of head throughout the modelled domain. Groundwater velocities are calculated from these head distributions, and used as input to the solute transport module, which routes 'particles' (representing discrete masses of solute) through the model domain. This particle tracking is accomplished by simple 3 - D advection calculations coupled with a 'random walk' representation of dispersion.

Application of the model to two riverside wellfields (Dorney and Gatehampton) produced interesting results. The percentage river contributions to total yield at the two wellfields were found to be only 2% (Dorney) to 10% (Gatehampton). Predictions of pollutant movement for river spills of variable duration were made. Spills of chloride and lindane (a chlorinated pesticide) over periods of 20 minutes, 1 week and 1 month were modelled. It was found that none of the wells are likely to experience pollutant concentrations in excess of EC limits after a 20 - minute river spill. The Gatehampton wells would probably succumb after a 7 - day river spill, though it would take a 28-day spill before even one of the Dorney wells showed pollutant concentrations in excess of EC limits. Travel times to the wells were predicted to be as fast as 0.5 days (chloride at Gatehampton), but retardation of lindane by the streambed sediment could cause background pollution to persist for more than 100 years (Dorney). Studies of model response and sensitivity analyses both showed that the most important controls on flow, transport and model performance were the hydraulic conductivity and sorptive capacity of the streambed sediments. Mechanical dispersion in the gravels was next in importance.

On the basis of these results, it is suggested that further studies be made of the hydrogeology of the streambed sediments, preferably including in - situ measurement of hydraulic conductivity. Studies relating the lithofacies of the gravels to their hydraulic properties may also be useful in improving the description of dispersion in the gravels.

Finally, it is proposed that 'scavenger wells' be installed at major riverside wellfields. Injection of unpolluted water into these wells during river pollution events would reverse the hydraulic gradient and thus prevent the ingress of pollutants to the aquifers.

9.4.2 -- Conclusion.

When the results of this study are compared with the aims stated in 1.1.2, it is clear that the objectives identified at the outset of this project have been largely satisfied. Of course, many questions remain to be addressed, and some of these have been identified in Section 9.3. However, it is hoped that this project will be seen as a valuable contribution towards the understanding of stream - aquifer interactions. In particular, it is hoped that both groundwater managers and research hydrologists may find something of value in these pages.

Appendix A

FIELD SITE SUMMARY FOR THAMES WATER/NEWCASTLE UNIVERSITY STREAM - AQUIFER INTERACTION PROJECT

SITE NAME	DATE OF COMPLETION	OPERATOR/ OWNER	LICENCE NO.	WELL CATALOGUE NO.(s)	GRID REF.	LICENCED ABSTRACT'N	AQUIFER	GEOLOGICAL SUCCESSION	COMMENTS
Gatehampton Pumping Station Oxon	23.1.1987	TWA(S&W)	23/159	SU57-212 SU67-219 A-G SU68-75 A-O	SU59957987 SU60057978 SU60157970 SU60447973 SU60417994 SU60128007	60 TCMD	Chalk (Middle & lower)	River Gravels (3m - 13.5m) Chalk (M&L)	Reports available (1984, 1987) SU57-212 E Logs,caliper Pumping test: 81/8
Hedsenham Pumping Station Bucks	14.10.1968	TWA(E&N)	23/110	SU78-8 A-E	SU792842	55 TCMD	Chalk	River Gravels (2m - 10m) Chalk	Originally 5 sources. No. increased to 6 on 5.7.1976 Pumping tests: 65/4,84/5
Hurley Pumping Station Berks	8.5.1967 12.2.1973	Mid-Southern Water Co.	26/60 26/76	SU88-15 A-C SU88-16 A-B	SU83528410 SU83178393 SU83218415	38.6 TCMD	Chalk	River Gravels (5m) Chalk	1 source 'A' to 'B' from 1967. Source 'C' added 1976 (SU83218415) Pumping tests: 70/34, 72/13
Taplow Court and Cliveden Pumping Station Bucks	14.2.1966 8.5.1972	TWA(E&N)	26/9 26/75	SU98-72 SU98-70 SU98-31 A-C	A,B,C,E re-spectively SU90568295 SU90528269 SU90478225 SU90638324	40.5 TCMD	Chalk	Taplow Chalk Cliveden Gravel (4m) Chalk	A,B,C Taplow Sites lettered N to S E, Cliveden (most northerly site) Pumping tests: 65/2 68/23, 69/28, 69/33, 69/34 Licencer 26/9 (1966) is for station at SU904821 2.25 mgd. Note licences, 26/20, 26/2 for 0.5 mgd at paper mill for indu-strial processes and cooling
Dorney Reach Bucks	14.5.1973	TWA(E&N)	27/97	SU97-77 A-P	SU918789	27.3 TCMD	Gravels	River Gravels (5-11.7m) Reading Beds (6m)	8 sources, less than 25 feet deep Reports available Pumping tests: 74/33, 70/21, 71/29
Bray Berks	12.12.1977	Mid-Southern Water Co.	26/87	SU97-78	SU914787	27.3 TCMD	Gravels	Sandy Clay(3m) Gravel & Sand (5m) Clay (0.3m) FineSand(3.3m) Clay (0.3m)	Same abstraction rate as Dorney from half as many wells (4). Pumping test: 73/10
Eton School Pumping Station Bucks	5.4.1971	TWA(E&N)	27/92	SU97-13	SU968777	8.6 TCMD	Gravels & Chalk	No details	5 wells, 250 feet deep 1 each, 35', 26', 23' deep
Chertsey Pumping Station Surrey	10.10.1966	North Surrey Water Co.	27/33	TQ06-42 A-O	TQ048676	68.2 TCMD	Gravel	Made (1m) Gravels (8m) Bargate Beds (0.7m)	3 wells with sumps at depth of 21'
Broadmead Herts	20.9.1966	TWA(E&N)	7/37	TL31-7	TL353139	6.8 TCMD	Chalk	Alluvium & Gravels (5.5m) Chalk (190m)	
Amwell End Herts	20.9.1966	TWA(E&N)	7/34	TL31-10	TL361638	5.7 TCMD	Chalk	Gravels (12m) Chalk (130m)	

Amwell Hill Herts	20.9.1966	TWA(E&N)	7/35	TL31-65 A-B	TL367127	13.6 TCMD	Chalk	Soil (0.5m) Chalk	
Amwell Marsh Herts	20.9.1966	TWA(E&N)	7/36	TL31-66	TL375123	32.7 TCMD	Chalk	Gravels (5m) Chalk	
Rye Common Herts	20.9.1966	TWA(E&N)	7/43	TL31-95	TL379111	16.4 TCMD	Chalk	Gravels (6m) Chalk	Varied 20.1.1984 to current abstraction levels
Hoddesdon Herts	20.9.1966	TWA(E&N)	8/173	TL30-14	TL378090	16 TCMD	Chalk	Gravels (4.5m) Reading Beds (11m) Chalk	Confined
Broxbourne Herts	20.9.1966	TWA(E&N)	8/170	TL30-9	TL373074	16 TCMD	Chalk	Gravels (3m) London Clay (6.1m) Reading Beds (18.3m) Chalk	Confined
Turnford Herts	20.9.1966	TWA(E&N)	8/178	TL30-7	TL360044	11.4 TCMD	Chalk	Gravels (7.5m) London Clay (10m) Reading Beds (12m) Thanet Beds Chalk (4m)	Confined beneath Tertiary

Appendix B

An Analysis of the Chalk Fracture System.

Knowledge of the fracture system of the Chalk is the key to understanding the hydraulic properties of this unusual aquifer. As illustrated in Figure 3.3, fractures in the Chalk are generally developed in three mutually perpendicular sets, with one set roughly parallel to bedding. The bedding - plane parallel set shows the greatest lateral persistence of the three sets, and previous workers have stated that this set also has the highest frequency (Scholle, 1977; Connorton, 1987, Personal Communication), although they have failed to present any field data to support this contention. Despite the absence of fracture frequency data, the most widely accepted model for the development of Chalk permeability (Ineson, 1962) asserts that the association of high fissure permeabilities with river valleys can be explained by an increased frequency of fracturing in the valleys. This assumed increase in fracture frequency (which has never been established) is attributed to tectonic effects, so that the rivers within the Thames Basin are claimed to follow 'zones of structural weakness'. These supposed 'zones' are further postulated to be either tectonic disturbances of Alpine age, or shatter zones associated with relief of overburden pressure consequent upon erosion by the rivers (Ineson, 1962).

To move beyond conjecture, the present author decided to conduct a field survey to establish the broad features of the Chalk fracture system in south east England. At 13 Chalk exposures, therefore, simple scanline surveys were conducted. Figure B.1 shows the location of the sites of the scanline surveys, and grid references for these are included in Table B.1. The exposures studied fall into two main groups; namely the Kent group (comprising two in the Medway Valley and three coastal exposures) and the Thames-Cambridge group (comprising three sites in the Middle Thames Valley, one in the Lea Valley and two near Cambridge).

The scanline method used in this study was a simplification of the method advocated by La Pointe and Hudson (1985). Two mutually perpendicular straight lines (each 2m long) were imposed on each outcrop, and the points of intersection of fracture traces on these scanlines were recorded. In this study, all outcrops studied showed dips of less than 5^{o}, and it was thus possible to ensure that the 'horizontal' scanline was always disposed parallel to bedding. Measurements of the lengths of traces and their angles of intersection with the scanline were also made at most of the sites.

Trace Lengths. With regard to trace lengths, the following generalisations may be made:

Table B.1 The Chalk Fracture System: Summary Statistics.

Location	Grid Ref.	Unit of Chalk	Fracture Frequency F_f (no./m) BPP	BPN	Dist. from river (km)	Mean BPN trace length (cm)
Thames - Cambridge Samples:						
Hindhay	SU868828	U	9.0	5.5	3.1	75.7
Playhatch	SU742765	U	9.0	6.0	1.5	17.7
Pangbourne Station	SU632767	U	7.0	5.0	0.1	12.7
Chadwell Spring	TL348135	U	8.5	8.0	0.5	60.5
Melbourn	TL380439	M	13.3	9.0	3.7	231.0
"	"	M	10.0	6.5	3.7	282.0
Harlton	TL391520	L	12.1	4.2	2.1	50.4
"	"	L	6.0	6.0	2.1	34.6
Kent Samples:						
Pegwell Bay	TR355644	U	6.5	5.5	-	33.6
Stone Bay	TR399687	U	1.5	4.0	-	54.6
Folkestone Warren	TR242374	L	2.5	2.5	-	88.0
Blue Bell Hill	TQ742622	U	1.0	0.5	2.7	-
Kit's Coty	TQ750610	M	1.0	3.5	2.5	273.3

Notes: BPP = bedding plane parallel fractures; BPN = bedding plane normal fractures. Chalk Units: U = Upper, M = Middle L = Lower.

(i) The bedding plane parallel (BPP) set invariably display trace lengths which persist the full extent of the outcrop. This is true even where the outcrop is several kilometres long, as at Stone Bay (TR 399687) on the Isle of Thanet. Trace lengths were thus recorded as infinity for all fractures of this set.

(ii) The bedding plane normal (BPN) sets (ie the 'vertical' fractures) show a wide variability in trace length, but all save one measurement are less than three metres long, and most are less than one metre. Table B.1 includes the mean of BPN trace lengths at the exposures studied.

Orientation. As shown in Figure 3.3, the BPN fractures tend to be fairly smooth planar discontinuities, while the BPP fractures tend to be undulose, with an amplitude of around a centimetre either side of the mean plane of dip. This morphological difference is no doubt a reflection of differing genetic origins; the BPP set is clearly related in some way to depositional fabrics, while the BPN set are classic secondary joints which probably developed due to release of elastic strain from the compacted carbonate grains during Tertiary uplift. Interpretation of the angles of intersection of the fracture traces with the scanlines has to take these morphological factors into account. Since the 'horizontal' scanlines were set parallel to bedding, the BPN fracture trace intersections yield information about the true angular relationship between the BPP fractures and the BPN fractures. On the other hand, the local intersection of undulating BPP fractures with the 'vertical' scanlines do not convey very useful information about the overall disposition of these fractures, which can only really be assessed by observing a larger area of the outcrop. In the light, of these comments, the orientation data collected in the present survey may be simply summarised as follows:

(i) *No significant deviations of the BPP* fractures from the overall bedding plane parallel orientation were observed at any of the outcrops.

(ii) The BPN set were also remarkably consistent, with no fractures being recorded at angles of less than 65^{o} to bedding, and few at angles less than 85^{o}.

Frequency and Spacing. As mentioned above, unsupported assertions about the areal variation in Chalk fracture frequency are used to support important models for the development of the spatially variable Chalk permeability distribution. Furthermore, permeability in the Chalk is critically dependent on the hydraulic connectivity of the fracture sets, which can be assessed by combining fracture length data with information on fracture spacings. For these reasons, further analysis of the variation of fracture spacings in the Chalk is given here.

Fracture frequency (F_f; in units of number of fractures per metre of scanline) can be defined by:

$$F_f = N / L \quad . \; . \; . \; . \; . \; . \; . \; (B.1)$$

where N = number of traces intersected, and

L = length of scanline (m)

Mean fracture spacing (F_s) in metres is related to F_f by the following expression:

$$F_s = 1 / F_f \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; (B.2)$$

Equation (B.1) was applied to the raw data for each site to obtain the values for F_f given in Table B.1.

The division of the sample sites into two geographical 'provinces' (Kent and Thames - Cambridge), was observed to correspond to apparent differences in the absolute frequency of BPP and BPN fractures (Table B.1). To test whether these observed differences are statistically significant, a Mann - Whitney Test was applied to the data. In this test, which is described fully by Davis (1986; pp. 92 - 96), data from both provinces are pooled, and arranged in order of magnitude. Each observation is then assigned a rank number according to its position in the pooled list, and the sum of all these ranks is calculated. If the data from the two provinces are drawn from the same population, the ranks of data from one province would be expected to be spread evenly throughout the pooled set when compared with the ranks from the other province (allowing for differences in the size of the two samples). To test whether this is the case, the following test statistic is calculated:

$$T_{mw} = \sum_{i=1}^{n} R(Xi) - \frac{n(n+1)}{2} \quad . \; . \; . \; . \; . \; . \; . \; . \; (B.3)$$

where n = the number of observations of X in the first sample
Xi = ith observation of the variable X in the first sample
R(Xi) = the rank of this ith observation in the pooled set
T_{mw} = the Mann - Whitney test statistic

When the value of T_{mw} has been determined, the number of observations in the two original samples (designated m and n) are used to find the theoretical range of T_{mw} values which the pooled set would exhibit if the samples were from the same population (these values are tabulated in Davis, 1986). If the calculated value of T_{mw} lies outside this range of values, the two original samples are shown to be from different populations.

The results of the Mann - Whitney test for the Chalk fracture frequency data given above are shown in Table B.2. For both BPP and BPN fractures, the frequencies of Kent sets are shown to be significantly lower than those of the Thames - Cambridge sets.

Table B.2 -- Mann - Whitney Test Results for Definition of Provinces.

Fracture Set	T_{mw} (Calculated for Kent Set)	Limiting Values of T_{mw} Upper	Lower
BPP	1.0	31.0	9.0
BPN	2.5	31.0	9.0

This strongly suggests that the tectonics of the London Basin Synclinorium are *somewhat different from those of the* Kent area (roughly coincident with the Wealden Anticline). Variations in BPP and BPN frequencies within these two separate provinces may be assessed by comparing the mean values for each province (Table B.3) with the data for individual sites given in Table B.1. It may be readily seen that, within a single province, virtually all sites show frequencies which lie within one standard deviation either side of the mean frequency for that province. Thus it may be concluded that the Chalk fracture system is fairly homogeneous within a given tectonic province, but that significant heterogeneity can be expected between neighbouring tectonic areas.

The Mann - Whitney test was also used to test whether there really is a significant difference between BPP and BPN frequencies within a given province. Table B.4 gives the values obtained from this analysis. These demonstrate that, at the 99% level of confidence, the BPP and BPN frequencies do differ significantly from each other in the Thames - Cambridge province, but that there is no significant difference between them in the Kent province.

One last test of fracture frequencies was performed, in order to examine the hypothesis that there is an inverse relationship between fracture frequency and the distance of a Chalk site from the centre of a modern river valley (as postulated by Ineson, 1962). In Figure B.2, F_f values are cross-plotted against their corresponding distances from the nearest river (the Cam, Thames, Lea or Medway; Figure B.1), and the correlation coefficient (r_c) was calculated (cf. Davis, 1986, pp. 34 - 41). When all valley -side sites were included in the analysis, the values of r_c obtained were 0.0051 and 0.1476 for the BPN and BPP sets respectively. When the Kent sites were excluded, to be consistent with the definition of provinces outlined above, the r_c values obtained for BPN and BPP sets are 0.2596 and 0.5737 respectively. Out of all of these values for r_c,

Table B.3 -- Means and Standard Deviations for BPP and BPN Frequencies in the Separate Provinces.

Province	Fracture Set	Mean	Standard Deviation
Kent	BPP	2.5	2.3
	BPN	3.2	1.9
Thames - Cambridge	BPP	9.4	2.4
	BPN	6.3	1.6
Both Provinces Together	BPP	6.7	4.2
	BPN	5.1	2.2

only the last of them could possibly be argued to represent any kind of correlation, although such an argument would be highly tendentious. Even if the argument is accepted, however, the value obtained indicates a weak direct correlation, rather than an inverse correlation as postulated by Ineson (1962). Thus the available data are not in any way consistent with Ineson's (1962) assertion that the frequency of Chalk fracturing increases towards the centres of modern river valleys[1]. This conclusion is of importance to the new model for the areal variation in Chalk permeability proposed in Chapter Four.

Hydraulic Connectivity may be assessed in a number of ways, but a simple approach was adopted here. In this approach, it is assumed that to ensure connection of two BPP fractures by a BPN fracture, the BPN fracture must be a minimum of 2 times the mean spacing of the BPP fractures (Figure B.3). Using this assumption, the relative degree of connectivity at the various sites is represented by a "Connectivity Factor" (C) which is here defined as:

$$C = L_{BPN} \; / \; 2 \; (F_{sBPP}) \qquad \ldots\ldots\ldots\ldots \quad (B.4)$$

---

1. In passing, it should be noted that wide fissures also occur in interfluve areas above the present level of the water table (Robinson, Banks and Connorton, Personal Communication, 1989). Some of the larger fissures in this setting contain recent deposits of sand and mud washed in from the land surface. The origin of these fissures is considered in Chapter Four.

Table B.4 -- Mann - Whitney Test Results for Discriminating Between BPP and BPN Frequencies.

Province	T_{mw} (Calculated for BPP Sets)	Limiting Values of T_{mw} Upper	Lower
Kent	9.5	20.0	5.0
Thames - Cambridge	56.0	48.0	16.0

where L_{BPN} = mean trace length of BPN fractures
F_{sBPP} = mean spacing of BPP fractures

This connectivity factor may be verbally expressed as "the minimum number of pairs of neighbouring BPP fractures which are, on average, connected by each BPN fracture". Table B.5 gives the values of C for the various study sites. The results indicate that the differences in fracture geometry between the Thames - Cambridge and Kent provinces are reflected by a difference in hydraulic connectivity of the laterally persistent BPP fractures; while frequencies are higher in the Thames - Cambridge province, connectivity is higher in Kent. It would be interesting to perform a comparative study of Chalk flow mechanisms in the two areas to fully assess the hydraulic significance of this contrast.

Variation in fissure permeability with depth was investigated for a number of sites in the Middle Thames area as part of this study. The method used to make these investigations was formulated by Connorton and Reed (1978), who applied it to studies of Chalk permeability in the Kennet Valley, and a closely related methodology has also been described by Paillet et al (1987) from a field study in New Hampshire, USA. The essentials of the method are as follows:

Using impeller flowmeter data from uncased pumping wells, the percentages of the total well discharge which are contributed by discrete depth intervals within the borehole can be calculated. These percentage contributions are clearly related to the relative permeability (syn. hydraulic conductivity) of these depth intervals. Thus it follows that a 'relative permeability' factor can be defined for the various depth intervals within a pumping well. Application of this method to Chalk wells during the development of the Thames Groundwater Scheme revealed the non-linear decrease in fissure permeability with depth which is now regarded as typical of the Chalk in river valleys (Owen et al, 1977).

Table B.5 -- Connectivity Factors for the Study Sites.

Site	Connectivity Factor (C)
Hindhay	3.40
Playhatch	0.79
Pangbourne	0.44
Chadwell Spring	2.57
Melbourn 1	15.36
Melbourn 2	14.10
Harlton 1	2.08
Harlton 2	2.88
Pegwell Bay	2.59
Stone Bay	18.22
Folkestone	17.60
Kit's Coty	136.65

Using the few available flowmeter data from the Middle Thames Valley, the distribution of relative hydraulic conductivity with depth was derived for several sites. Table B.6 gives the results of these calculations, which are of great importance for the development of the conceptual and mathematical models in Chapters Five and Six. To obtain the actual hydraulic conductivity in any depth interval, the maximum possible hydraulic conductivity at each site is multiplied by the relative hydraulic conductivity for the given interval. This method is used in the subroutine TRNSM which calculates transmissivities in the flow module of UNCLESAM.

Table B.6 -- Relative Hydraulic Conductivities in the Middle Thames Area.

Site	Depth (m) 0-10	10-20	20-30	30-40	40-50	50-60	60-70	70-80	>80
Maddle Farm	1.00	1.00	1.00	1.00	0.72	0.46	0.03	0.03	0.00
Taplow ABH1	1.00	1.00	1.00	1.00	1.00	0.37	0.37	0.30	0.00
Taplow h	1.00	1.00	1.00	1.00	1.00	0.58	0.05	0.05	0.00
Taplow n	1.00	1.00	1.00	1.00	1.00	0.20	-	-	-
Gate-hampton ABH3	-	1.00	1.00	1.00	0.10	0.10	0.07	0.00	-

Notes: Flowmeter data was obtained from the following sources;
Maddle Farm - Connorton and Reed (1978); Taplow - Edmunds, Owen and Tate (1976); Gatehampton - Robinson et al (1987).

Figure B.1 - Locations of Scanline sites

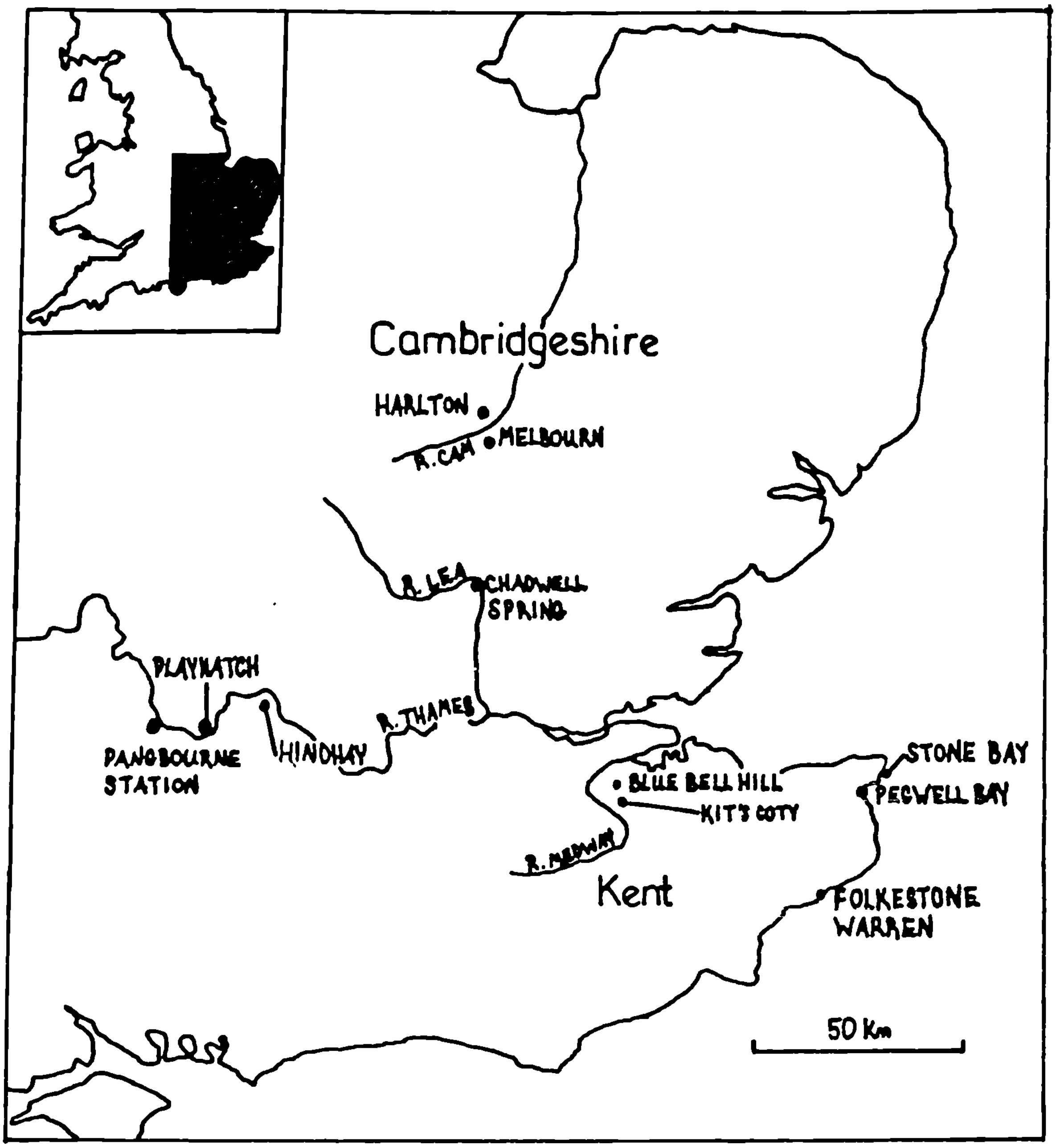
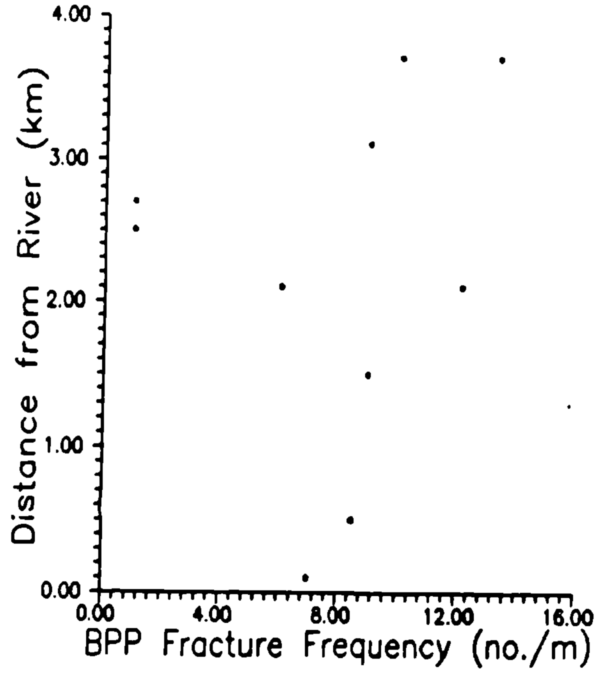


Figure B.2 -- Scatter Plots of Fracture Frequencies Against Distance from the Nearest Main River.

(a)



(b)

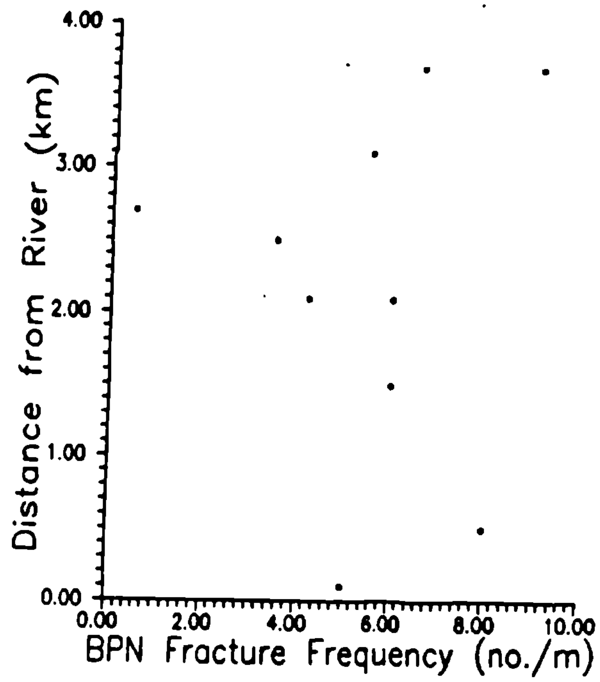
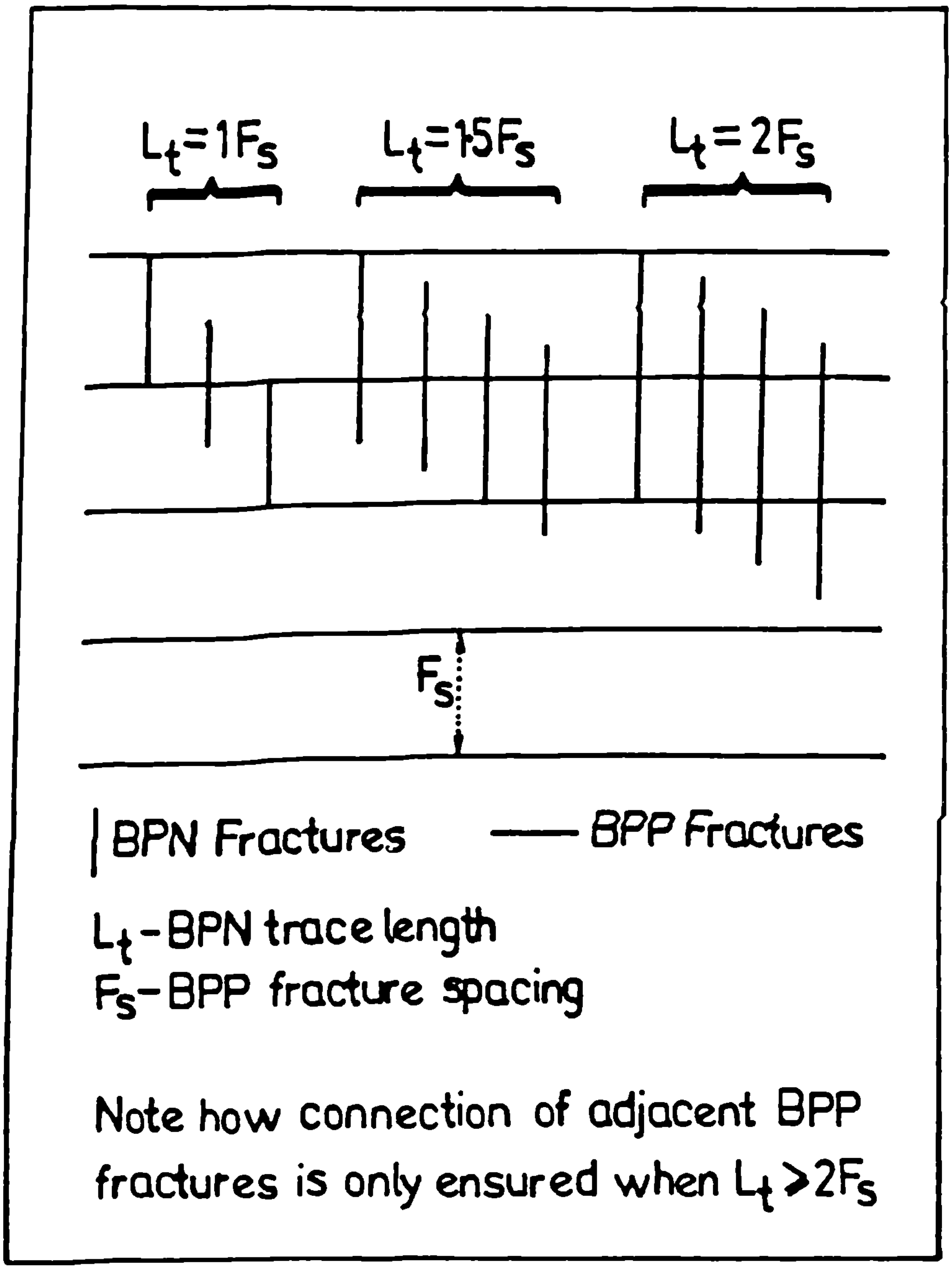


Figure B.3 -- Explanatory Sketch for the Definition of the Connectivity Factor.



Appendix C

Methods and Results of the Streambed Sediment Investigation.

METHODS

Sampling. Two sample sites were selected, with the selection being governed by a balance between the desire to sample as close as possible to the two well fields at Gatehampton and Dorney/Bray and the availability of facilities and assistance from the Rivers Division of the Thames Water Authority. The two sites selected were:
1. Basildon Stockyard (SU 608795), near Gatehampton, and
2. Ruddles Pool (SU 937772), near Dorney/Bray.

At Basildon (on 18-7-1988) a large crane with an automatic bucket sampler was used to retrieve six samples at random from a 15 metre reach of the river, within 5 metres of the south-west bank. The samples were taken from the bucket sampler immediately upon reaching the bank, and placed in 500 ml wide-mouthed PVC flasks, which were then labelled (G1 - G6) with indelible ink and stored for transit back to Newcastle. At Ruddles Pool (on 20-7-1988) samples were taken from piles of streambed sediment which had been recently dredged from the Pool, then left to dry in the sun on the haugh near Eton (SU 955778). Again, six sample bottles were filled and labelled (D1 - D6) prior to transit.

Sample Description. All of the samples (plus two samples from the Middle Thames Gravel Formation for the purposes of comparison) were examined with the naked eye and a hand lens, and then certain sub-samples were further examined in polished blocks using reflected - light petrological microscopy, under the guidance of Dr. J.M. Jones, (Organic Geochemistry Unit, University of Newcastle Upon Tyne), who also undertook a point - count analysis on seven of the samples to determine the relative volumetric abundance of each of the components. Data on grain-size, mineralogy and the nature of the included organic matter were obtained, which have both hydraulic and geochemical significance.

X-Ray Diffractometry (XRD). This standard method for determining the mineralogy of fine-grained sediments (see for example Battey, 1972) was used to investigate the mineralogy of the clay fraction of a sub-group of the samples. The XRD machine in the Department of Geology, University of Newcastle Upon Tyne, was used for the determinations. By recording the diffraction of X-rays when they are passed through a powdered sample of a mineral, the spacings of ionic layers in the crystal lattice (d-spacings) can be obtained. This information can be used to determine the mineralogy of the sample by comparison with standard listings of d-spacings given in JCPDS (1980).

Table C.1 -- Sample Descriptions.

Basildon (Gatehampton) Samples.

Sample No.	Description
G1	Grey muddy silt with small angular clasts of flint (up to 8 mm diameter), abundant aragonitic shell fragments, and entire bivalve tests.
G2	Dark grey muddy silt with small angular clasts of flint (up to 8 mm diameter), abundant aragonitic shell fragments, and entire bivalve tests.
G3	A matrix of grey muddy silt with shell fragments supporting angular pebbles of flint (up to 2 cm in their largest dimension).
G4	Identical to G2.
G5	Identical to G2.
G6	Identical to G2.

Middle Thames Gravels Samples.

Sample No.	Unit	Location	Description
KMG2	Shepperton Gravels	Wraysbury (TQ 013744)	Dark grey medium - grained compositionally and texturally mature quartz sand.
GHG2	Staines Alluvium and Shepperton Gravels Contact	Gatehampton Railway Embankment (SU 605797)	Coffee - brown medium - grained moderately well sorted quartz sand with scattered chalk grains (medium) and subrounded haematite grains up to 3 mm diam. Modest silt and clay content leads to crumbing when dry.

Table C.1 -- Sample Descriptions (Cont.).

Ruddles Pool (Dorney/Bray) Samples.

Sample No.	Description
D1	Brown silty clay with angular clasts of peat (up to 5 mm diameter) and flint (up to 2 mm diameter). Slightly carbonaceous (effervesces with 5% HCl), but no conspicuous shell fragments.
D2	Pitch - black fibrous homogeneous peat.
D3	Brown silty clay with angular flint clasts (up to 5 mm diameter) and scattered fine quartz grains.
D4	Grey - brown clayey silt. Extremely carbonaceous (violent effervescence with 5% HCl). Shell fragments (up to 5 mm diameter) and angular flint clasts (up to 3 mm diameter) present.
D5	Brown silty clay with angular clasts of peat (up to 5 mm diameter) and flint (up to 2 mm diameter). Slightly carbonaceous (effervesces with 5% HCl), but no conspicuous shell fragments.
D6	Brown silty clay, with angular flint clasts (up to 5 mm diameter) and scattered fine quartz grains, supporting large angular flint pebbles (up to 2 cm longest dimension).

Determination of Organic Matter Content. A simple method for determining the total organic matter content of a solid sample is given in the "Standard Methods" handbook edited by Franson et al (1985, pp. 99 -100, [Method 209(f)]). The procedure is as follows: The weight of a refractory dish was recorded (weight 'B'), and 25 to 50g of wet sample was added to this dish, and the new weight recorded (C). The sample was now dried by placing the dish in an oven at 103°C to 105°C overnight. Cooling to weighing temperature was accomplished in a desiccator, and the dish and dry sample were re-weighed (A). Next the sample in the dish was placed in a muffle furnace and ignited to about 550°C for an hour to drive of all remaining volatiles. After cooling in the desiccator once more, the final weighing was made (D). With these weights, the following formulae were used to determine percentage total solids (%TS) in the original sample, and the percentage of these solids which were volatile solids, lost on ignition (%VS) (which are

Table C.2 -- Streambed Sediment Composition (Volume %) from Microscopic Point - Count Analyses.

Sample:	G1	G2	G4	G5	D2	D3	D5
Component							
Sand	27.0	26.0	29.4	32.6	1.2	6.6	8.2
Clay	27.8	36.8	49.0	35.4	31.6	83.6	67.6
Marl	31.8	22.5	9.4	20.4	--	2.4	1.0
Glauconite	0.6	1.3	0.6	0.6	--	--	--
Limestone	4.4	6.4	1.4	4.4	--	0.8	0.8
FeO	6.2	4.4	0.8	1.8	--	0.4	0.2
Shell Debris	0.6	1.2	3.4	2.2	--	0.2	0.4
Flint	0.2	1.2	0.0	0.4	--	0.2	1.4
"Char" (Burnt Coal)	0.2	0.2	1.0	Tr.	--	--	--
Peat	--	--	--	--	65.6	--	--
Wood	1.2	--	4.8	2.2	--	5.4	19.4
Pyrite	--	--	--	--	1.2	0.4	0.8
Coal	--	--	0.2	--	0.2	--	0.2

Notes: 500 points per analysis. Accuracy probably about +/- 3%

generally regarded as organic matter; Dr A. James, Public Health Engineering, University of Newcastle Upon Tyne, Personal Communication, 1988).

$$\%TS = ((A - B) \times 100) / (C - B) \quad . . . . (C.1)$$
$$\%VS = ((A - D) \times 100) / (A - B) \quad . . . . (C.2)$$

Portions of all of the streambed samples (plus two samples from the Middle Thames Gravel Formation for the purposes of comparison) were subjected to this test.

Table C.3 -- Crystal d-spacings for Clay Fractions in Streambed Sediment Samples.

Sample No.	d-spacings in Order of Decreasing Intensity 1	2	3	4	5
D1	3.26	4.12	2.97	4.34	
D2	3.26	3.41	4.12	4.35	2.79
D3	3.24	4.08	3.10	2.95	4.29
D4	3.25	4.10	2.95	4.30	
D6	3.26	2.97	4.12	4.34	
G2	3.24	2.95	4.09	3.15	4.32
G4	3.26	2.95	4.11	3.74	4.33

Permeameter Tests. To obtain estimates of the saturated hydraulic conductivity of the streambed sediment, falling-head permeameter tests were conducted on re-packed samples. The method is described by Freeze and Cherry (1979, p. 336), and the theory and application will not be detailed here, other than to say that the method involves measuring the time (t) it takes for the head in a standpipe feeding a cylindrical sample cell to fall from one level (Ho) to another (H1). A permeameter in the geotechnical engineering laboratories at the University of Newcastle Upon Tyne was used for the determinations. The expression used to calculate hydraulic conductivity (K) from the lab measurements is:

$$K = [(aL)/(At)].[\ln(Ho/H1) \quad . \; . \; . \; . \; . \quad (C.3)$$

where a = cross - sectional area of the standpipe
A = cross - sectional area of the sample cell
L = length of the sample cell
t = time taken for the head in the standpipe to decline from Ho to H1

RESULTS

Sample Descriptions. The 14 basic sample descriptions are given in Table C.1, and Table C.2 summarises the information gained by microscopic examination (from a point - count analysis by Dr. J.M. Jones, Organic Geochemistry Unit, University of Newcastle Upon Tyne). It is clear from the descriptions that a certain variety is exhibited by the streambed sediment, but that all the samples were predominantly fine grained (silts, clays, peats).

Table C.4 -- Results of Weight - Loss - on - Ignition Test for Organic Matter Content.

Sample No.	A	B	C	D	%TS	%VS
G1	106.48	84.42	112.97	106.13	77.3	1.6
G2	109.42	84.57	123.16	108.43	64.4	4.0
G3	107.18	74.80	117.66	106.45	75.5	2.2
G4	101.51	85.94	115.94	100.64	51.9	5.6
================> Mean for all *Gatehampton Samples:*						3.4
GHG2	121.06	86.86	122.12	120.57	97.0	1.4
KMG2	116.09	84.98	119.53	115.81	90.0	0.9
================> Mean for all Gravel Samples:						1.2
D1	108.77	84.00	120.00	106.94	68.8	7.4
D2	98.19	86.11	121.24	91.26	34.4	57.4
D3	94.46	67.39	107.22	92.37	68.0	7.7
D4	115.86	82.95	128.19	113.92	72.7	5.9
D5	70.69	45.99	81.89	68.84	68.8	7.5
D6	98.49	75.98	110.67	96.72	64.9	7.9
=============> Mean for all Dorney/Bray Samples:						15.6
=============> Overall Mean for Streambed Sediment:						10.7

Key: A = weight of dish + dry sample
B = weight of dish alone
C = weight of dish + wet sample
D = weight of residue and dish after ignition
%TS = weight - percent total solids
%VS = weight - percent volatile solids

XRD Results. The d-spacings of seven samples were obtained and these are tabulated below (Table C.3). When these d-spacings were compared with standard listings in JCPDS (1980) and in Brindley and Brown (1980, p. 351), the evidence suggested that all samples were dominated by a mixture of montmorillonite and palygorskite. A number of heated samples were also studied, and these returned peaks characteristic of meta-montmorillonite, confirming the interpretation of the peaks for unheated samples.

Organic Matter Content. The results of the ignition test are given in Table C.4. The same samples of Middle Thames Gravels were used in this test as in the descriptions (Table C.1) and are referred to by the same sample numbers. The results indicate that the mean organic matter content (expressed in weight percentage) of the streambed sediment is between 3 and 16 times that of the Middle Thames Gravels.

Permeameter Tests. The dimensions in the falling - head permeameter test were as follows (cf. the notes above):

$A = 8659\ mm^2$ $a = 11.7\ mm^2$ $L = 40\ mm$
$Ho = 1565\ mm$ $H1 = 1065\ mm$

Table C.5 lists the times taken for the head to decline from Ho to H1, and the hydraulic conductivities calculated using these times and the information listed above.

A Note on Experimental Accuracy. The test results reported above are subject to experimental error. If this investigation were the main focus of this study, rather than a small component of it, a more thorough sampling and testing programme could have been designed, with duplicate samples and blanks being included in the tests. Constraints of time, and a realisation that increased rigour would not be warranted by the use to which the data are to be put, led to a decision to maintain a rather simplistic approach to the investigation. When the inherent uncertainty of the methods themselves (discussed in the references cited above) is added to this, the data presented here must be regarded as approximations rather than exact statements. Nonetheless, these approximations represent a dramatic increase in the amount of information available on the streambed sediments.

Table C.5 -- Falling - Head Permeameter Results for the Streambed Sediment.

Sample No.	t (s)	K (m/s)	K (m/d)
G4	896	2.32×10^{-8}	0.0020
G3	738	2.82×10^{-8}	0.0024
D3	1065	1.95×10^{-8}	0.0017

APPENDIX D -- Table D.1 ICPMS Trace Element Analyses of Waters from Selected Riverside Wells and the River Lea (micrograms / ml)

Site	R. Lea (Ware)	R. Lea (Dobb's Weir)	Amwell Marsh	Amwell End	Rye Common
Al	1.04	1.04	1.04	0.52	1.04
Fe	< 0.3	< 0.3	< 0.3	< 0.3	< 0.3
Mg	4.20	5.40	7.20	4.80	8.40
Ca	132.0	126.0	136.0	121.0	137.0
Na	42.0	57.0	28.0	19.0	24.0
K	4.10	6.60	4.10	2.50	4.10
Ti	< 0.3	< 0.3	< 0.3	< 0.3	< 0.3
P	3.00	2.00	1.00	1.00	< 0.3
Mn	< 0.3	< 0.3	< 0.3	< 0.3	< 0.3
Ba	0.05	0.04	0.05	0.08	0.07
Ce	0.01	0.01	< 0.01	< 0.01	0.01
Co	0.04	0.04	0.03	0.04	0.03
Cr	0.10	0.14	0.21	0.16	0.22
Cu	0.04	0.04	0.07	0.01	0.04
La	0.05	0.04	0.05	0.04	0.04
Li	0.01	0.01	0.01	< 0.01	0.01
Mo	0.06	0.07	0.06	0.09	0.09
Nb	0.01	< 0.01	< 0.01	< 0.01	< 0.01
Ni	0.08	0.11	0.08	0.08	0.06
Sc	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
Sr	0.42	0.51	0.51	0.70	0.83
V	0.01	0.01	< 0.01	< 0.01	0.01
Y	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
Zn	< 0.01	0.09	< 0.01	< 0.01	0.09
Zr	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01

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