Predicting the applicability of Aquifer Storage Recovery (ASR) to the UK Chalk aquifer

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ABSTRACT

Aquifer Storage Recovery (ASR) is a cyclic form of artificial recharge where water is injected and abstracted from the same borehole. Widely utilised in the USA, there has been significant caution over the development of ASR as a method of artificial recharge in the UK. A primary concern has been double-porosity effects, especially for the Chalk aquifer.

The Chalk, characterised as a fractured rock with a double-porosity, forms one of the major aquifers within the UK. It is formed of blocks of a small-grained highly porous (30 - 50%) media, separated by fractures which contribute about 0.1 - 1% of the porosity. Within the chalk matrix blocks, groundwater flow is negligible due to the small pore throats, so fracture flow dominates. The primary difficulty in making ASR effective in a double-porosity aquifer is the diffusion of solutes from low-quality native water within the matrix into the recharge water stored within the fractures.

A novel form of double-porosity solute transport model, the DP-Pulse model, has been developed which discretises the flow velocity and fracture space while keeping time and space within the rock matrix as continuous variables. The aquifer is characterised by two parameters, a characteristic diffusion time, $t_{cb}$, and a porosity ratio, $\sigma$, and also by the shape of the blocks. The DP-Pulse model was calibrated to data obtained from an ASR test site within the Chalk of southern England.

Subsequently, the DP-Pulse model was incorporated into an Operational Research (OR) model allowing determination of the optimal testing and conditioning procedure, given an ideal operational scenario for a proposed ASR system. This OR model was used to examine a number of potential methods for improving testing efficiency.

Application of the model allowed a number of conclusions of practical importance for the potential development of ASR in the UK Chalk aquifer.
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Chapter 1

Introduction and Objectives
1. Introduction and objectives

This Chapter will describe the objectives of this work, then provide a brief overview of the context of the project, and a description of some of the concepts involved. These concepts will be returned to and reviewed in greater detail in Chapter 2.

1.1. Objective

Concerns have been raised by those with an interest in developing Aquifer Storage Recovery (ASR) in Chalk aquifers, that the processes occurring during ASR operations within a double-porosity medium such as the Chalk aquifer have yet to be fully described. Initial investigations (Wright and Barker, 2001) have noted that characterising the nature of the Chalk will require testing of a longer than usual duration in order to successfully predict behaviour. It is also believed that optimal operation is only likely to be reached after a number of years of operational cycling, due to the slow but continuous removal of solutes from the aquifer. This thesis aims to address these concerns, by showing that the removal of solutes is predictable. Furthermore, although this thesis will show that a significant period of preparation is required prior to the operational running of an ASR system (i.e. an ASR system cannot be installed and operated economically in the short term), it will be demonstrated that an operational ASR scheme in the Chalk may be developed on a medium rather than long time-scale (i.e. in under five years).

Results obtained from the Lychett Minster test site will be used to calibrate a semi-analytical double-porosity model, DP-Pulse, in order to both provide insights into the characterisation of a significant Chalk aquifer and assess the conceptual validity of the DP-Pulse model. The DP-Pulse model will then be incorporated into an operational research model, in order to examine the process of testing an aquifer prior to the implementation of ASR in the Chalk aquifer.

1.2. Project Context

It may be of use to the reader to have an understanding of the larger body of work of which this thesis forms just one part.

In the late 1990s, Wessex Water decided to conduct an ASR test in the Chalk aquifer using an existing well at a site in Dorset, on the south coast of the UK. The testing procedure was carried out under contract by CH2M HILL UK. Analysis of the data
was undertaken by a number of parties, including Wessex Water, CH2M HILL UK and the British Geological Survey (BGS). These parties formed a working group to answer site specific questions regarding a number of aspects, including the local geology and hydrogeology (Buckley, 1996, CH2M HILL, 1998, 2000a, 2000c; University of Birmingham, 1997; Wessex Water, 1995), the hydraulic response of an ASR system (CH2M HILL, 1998, 2000a, 2000b, 2000c; Williams et al., 1999), the environmental impact of the system (CH2M HILL, 1998), and geochemical interactions within the aquifer (CH2M HILL, 1998, 2000a, 2000b; Buckley et al., 1998; Williams et al., 1999; BGS 1996, Gaus et al., 2002). The working group additionally examined the potential for ASR within the Chalk aquifer, drawing on the data collected from the ASR test, and applying a series of standard numerical models, notably including SWIFT and PHREEQC (Gaus, 2001; Gaus et al., 2000).

The work described in this thesis was completed as a parallel project, with the objective of trying to understand in more general terms the applicability of ASR to double-porosity systems and the UK Chalk aquifer in particular. It was decided that in order to predict this applicability, it would be necessary to develop a means of determining the required investment at a given site, incorporating the costs and benefits of site specific investigation of ASR at any given location.

1.3. Artificial Recharge and Aquifer Storage Recovery (ASR)

The use of artificial recharge to augment natural water resources has become increasingly important for the management of groundwater reservoirs. This artificial recharge takes many forms, from simple infiltration basins to complex aquifer storage and recovery systems. A design for an artificial recharge system has to take account of a number of factors, including the hydrogeology of the area, availability of recharge water and the financial viability of the scheme. Artificial recharge may be undertaken for a variety of reasons: to provide a groundwater reservoir, to prevent saline intrusion, or simply to replenish depleted aquifers.

As artificial recharge usually requires that surface water pass directly into the aquifer, contamination of the native groundwater can be a major problem. To protect the quality of groundwater, many regions have introduced legislation requiring, for example, that
“Impaired quality waters used to recharge ground water aquifers must receive a sufficiently high degree of pre-treatment (prior to recharge) to minimise the extent of any degradation of ground water quality, as well as to minimise the need for any extensive post-treatment at the point of recovery” (National Research Council, 1994).

Many sources of water are used for artificial recharge. Surplus supply water at times of low demand can be used in a cyclical system where this water is used for recharge, and then can be abstracted at times of high demand. These systems can even operate on a diurnal basis. Stormwater and wastewater may also be used, although these require extensive treatment and monitoring to protect the aquifer from pollution.

One of the more recent forms of artificial recharge is known as Aquifer Storage Recovery (ASR). ASR is described in great detail by Pyne (1995) in his book dedicated to the subject. He states:

“Aquifer Storage Recovery may be defined as the storage of water in a suitable aquifer through a well during times when water is available, and recovery of the water from the same well during times when it is needed” (Pyne, 1995).

The water injected into the aquifer invades a volume of the aquifer around the well from which it can then be extracted as required (Figure 1-1). The same borehole is used for both injection and abstraction, which leads to a number of operational difficulties as well as some benefits. These have been discussed at length, chiefly by Pyne (1995).

One of the most significant benefits of ASR is that as the injected “bubble” displaces poor quality native groundwater, thus an ASR system can potentially make use of otherwise unused aquifers for water storage.
Currently, within the UK, experience of ASR is relatively limited. A number of small schemes are operational in the Nottingham area. An artificial recharge scheme is operational in North London, although injection and abstraction are from different wells and cannot be considered true ASR. Tests in the Sherwood Sandstone in Yorkshire have shown good results, with good operational ASR becoming a practical possibility in the next two years. A number of other sites are currently undergoing testing, with little likelihood of operational running within the short term. These include the Chalk of East Anglia and the Lower Greensand in the Southern region. Testing procedures at other sites, such as the Lychett Minster test site in Dorset, developed by Wessex Water, have identified difficulties in the possible application of ASR.

Further areas are under consideration, and more information can be found in two BGS reports. The potential for Aquifer Storage and Recovery in England and Wales, Jones et al. (1998) provides a good overview of the potential for ASR across the UK, while Williams et al. (2001) describes in more depth some of the issues that have arisen during attempts to develop ASR systems.

The modelling of an ASR system has to take into account many factors, most importantly the interaction of the native groundwater and the injected recharge water. Previous experience within the United States and other countries has involved a
variety of aquifers, including sands and limestones. Most literature describes ASR situations involving a primary porosity, such as sandstone. Fractured rock, cavernous limestones and Chalk all require a more intricate modelling approach due to the double-porosity nature of the rocks.

1.4. The Chalk aquifer

The United Kingdom relies on aquifers, using groundwater resources to provide approximately 27% of all public water supplies, although this increases to 75% if the Southern region alone is considered (data for 2000, supplied by the Department for Environment Food and Rural Affairs; DEFRA, 2003). One of the most important, and distinctive, of these is the Chalk, which provides 55% of the groundwater supply in the UK (Lloyd, 1993). In many areas abstraction is roughly the same as recharge, limiting the potential for future development of the resource. One of the main Chalk-dependent areas is the southeast, where high land costs make surface water storage systems such as reservoirs prohibitively expensive. The nature of the confined Chalk, which in many areas has very low flow velocities and ancient groundwaters, leads to many potential aquifers having brackish or otherwise mineralised waters that are not suitable for potable supply. Were the potential of potable water storage in these non-potable Chalk aquifers to be fully realised, the potential for groundwater to supplement other water resources in these areas would be great.

The most distinctive characteristic of the Chalk is its double-porosity nature. Formed from blocks of very fine matrix material, fractures dominate the flow behaviour. The large volumes of relatively immobile water stored within the matrix blocks can therefore have a different chemistry to that in the fractures. Diffusion of solutes from the matrix, especially if highly mineralised, will have a strong control over the solute concentrations within the fracture waters over long periods of time. This characteristic of the Chalk has been described in the literature as a double-porosity. Although ASR has been developed in double-porosity rocks such as karstic limestone in Florida, within the USA, it has never been fully developed in the highly double-porous Chalk. The results of initial testing, undertaken by Anglian Water, near Colchester, and Wessex Water, in Dorset, have highlighted concerns about the quality of injected water being impacted, prior to abstraction, by solutes diffusing from the relatively immobile matrix pore water. Since diffusion is a slow process, this appears to have the potential to keep ASR efficiency low for long periods. The work described in this thesis addresses this potential.
1.5. **Distribution of work**

In order to clarify the content of the thesis, this section will delineate the responsibility for the various parts of the thesis. Work that was completed by the author alone will be separated from that which is the product of joint work between the author and Prof. John Barker, of University College London, and that which is wholly the work of Prof. Barker.

The thesis itself has been produced entirely by the author guided by editorial comments mainly from Prof. Barker.

Chapters 1 and 2 provide a review of current thinking on a number of relevant topics, including artificial recharge, ASR and the Chalk aquifer. The information within these chapters was compiled by the author.

Chapter 3 describes the DP-Pulse model, used throughout the thesis to simulate a double-porosity system. The DP-Pulse model formulation is the original concept of Prof. Barker, who developed a FORTRAN 77 code of the model to allow basic simulation of an ASR system. The author independently developed the model, recoding to take advantage of the increased functionality of Fortran 90, as well as incorporating some approximations and an automated calibration routine. These adaptations are fully described in the text.

The theories behind the error analysis and the comparison of the relative importance of mechanical dispersion and double-porosity diffusion were developed in discussion between Prof. Barker and the author, with the author completing the body of work supporting the theory. Model verification, through comparison with the DP1D analytical model, was entirely the work of the author.

Chapter 4 describes the work carried out at the Lychett Minster test site, and some of the results obtained. The project design and testing of the ASR well was entirely carried out by CH2M HILL, with advice from the author and Prof. Barker. The author carried out the analysis of the data in this chapter.

Chapter 5 describes the calibration of the DP-Pulse model to data from the Lychett Minster test site, and provides a critical discussion of both the quality of, and the implications of this calibration. This is entirely the work of the author.

Chapter 6 utilises the DP-Pulse model to examine a number of implications of Double-Porosity for the effectiveness of current ASR testing procedures, and for the applicability of ASR in double-porosity aquifers. This is entirely the work of the author.
Chapter 7 describes the concept of OR, and the potential for application of OR techniques to ASR problems. The description of OR was developed from a general review of the literature, while the author applied the techniques to the scenario of an ASR test.

Chapter 8 describes the development and application of an OR model to the problem of optimising an ASR test prior to the development of an ASR system. This is entirely the work of the author. Implementation of this model, described in Chapters 9 and 10, is entirely the work of the author.

1.6. Structure of thesis

The main body of the thesis is divided into a number of chapters as follows:

1) Introduction and objectives – provides a preliminary overview of the topic, and outlines both the objectives of this work, and the structure with which the thesis presents the work. This chapter also provides an outline of the distribution of work, clearly stating which sections are drawn from different sources, and which sections are original research.

2) Background – provides general information about artificial recharge, and specifically ASR. It also contains information about the characteristics of the Chalk aquifer, and some of the methods that are used to simulate double-porosity behaviour.

3) Description of the DP-Pulse model – introducing the DP-Pulse model, which simulates double-porosity diffusion processes. This chapter also provides an error analysis and partial verification of the model.

4) The Lychett Minster Test Site – gives background on the Lychett Minster Test Site, the source of the experimental data used in this thesis. A brief analysis of the geochemical data is completed, as well as analyses of the piezometric data collected during the ASR testing procedures.

5) Calibration of DP-Pulse model to data from the Lychett Minster Test Site – describes the calibration of the DP-Pulse model to the data collected from the Lychett Minster Test Site, and provides a critical analysis of the calibration.

6) Characterising the Chalk aquifer, and the resultant implications for ASR – utilises the DP-Pulse model to examine a number of implications of Double-Porosity for the effectiveness of current ASR testing procedures, and for the applicability of ASR in double-porosity aquifers.
7) Operational Research: Procedures and application – describes the concept of Operational Research (OR), and the potential for application of OR techniques to ASR problems.

8) ‘Risk Reduction’ methodology: A tool to design an ASR test that will guarantee ‘low-risk’ operation of an ASR system – describes the formulation of an OR model to the problem of optimising an ASR test prior to the development of an ASR system. Verbal, mathematical and graphical representations are used to illustrate the formulation of this novel OR model.

9) ‘Risk Reduction’ model use: Initial application of the ‘Risk Reduction’ model – applies the model previously described to a simple scenario, in order to clarify the formulation and the usage of the model.

10) Further developments of the ‘Risk Reduction’ model – makes use of the Risk Reduction model to illustrate potential variations to the design of an ASR test.

11) Summary and discussion – summarises the contents of the thesis.

12) Conclusions and further work – details the author’s conclusions and outlines the author’s suggestions for further work required to develop this concept.

Following the references, a short glossary provides information on a few important terms, and a series of appendices contain data sets from the OR models. There are also appendices which elaborate on statements made within the main body of the thesis. A compact disk, enclosed with this volume, contains water chemistry data sets from the Lychett Minster Test Site and the code for the DP-Pulse model.
Chapter 2

Background
2. Background

Prior to an in-depth investigation of ASR in the UK Chalk aquifer, and the development and application of an original model, it is important to provide both an overview and a review of the work that has previously been completed within the field. This chapter outlines a number of relevant factors. Initially the process of artificial recharge is discussed, and the potential benefits of developing an ASR system are examined. An overview is provided of previous ASR related research, and indication is given of the value and limitations of this previous work for ASR in the UK Chalk aquifer.

Subsequently, the Chalk aquifer itself is described, and the process and importance of the double-porosity diffusion effects that occur within it are discussed. Finally, models that have been developed in order to simulate behaviour of the Chalk aquifer are detailed, and the limitations of those methods are outlined.

2.1. Artificial Recharge

“Artificial Recharge is a means of supplementing the natural infiltration to an aquifer.” (Brandon, 1986).

Artificial Recharge (AR) has been practised for many years as a method for managing groundwater resources. Amongst the many current uses of AR schemes, the most common include the supply of potable water during times of peak demand on annual to diurnal time-scales, banking water against potential times of drought and augmenting river flows. In addition to ground water storage, AR schemes have also been used for waste disposal, secondary oil recovery, land subsidence problems and salt-water intrusion control (Argo and Cline, 1985; Espina, 1980). AR schemes have developed from ancient infiltration basins in Turkmenistan (Pyne, 1995) to the most recent ASR systems in the USA.

Modern research into AR techniques dates back to the 1880's, when water was spread over surfaces to recharge an aquifer in Denver, Colorado (Dvoracek and Peterson, 1971). By 1895 floodwaters were being spread across the alluvial fan at the mouth of the San Antonio Canyon to sustain artesian wells in the Upper Santa Ana Valley in southern California (Toups, 1974). Unfortunately, this practice resulted in limited water availability for residents living downstream of the recharge scheme.
Use of AR in the UK has been relatively limited, but during the 1970's a series of investigative experiments were carried out by the Water Resources Board, in cooperation with several river authorities (Edworthy and Downing, 1979). Combined with experience from around the world, a number of summaries have been produced, detailing different approaches to AR. Bouwer (2002), Bouwer (1996), Edworthy and Downing, (1979) and Brandon (1986) provide good summaries of techniques. As well as summarising the techniques, Huisman and Olsthoorn (1983) deal in depth with the mathematics describing the hydraulics of injection, injection wellfield design, dispersion, water quality and many other facets.

The major forms of artificial recharge are described below.

2.1.1. Infiltration basins

The simplest form of artificial recharge is through the use of infiltration basins. This is where a permeable soil zone exists, or direct access to the aquifer is available, usually in a karstic environment or through swallow holes. Recharge water is let into small artificial lakes or recharge trenches which drain into the aquifer. A typical recharge lagoon is about 3 m deep, with sides sloping at 1:2, giving a maximum recharge head of about 2.5 m. Artificial filters on the base of the lagoon, approximately 0.5 m thick protect the aquifer, and increase the time before the infiltration rate through the base of the lagoon is unacceptably reduced as a result of silt and clay accumulation, as well as microbial growths. The filter may be cleaned, either through removal of the surface layer, or by light ploughing, and experience in the UK suggests this should be completed monthly, taking about 7 days (Brandon, 1986).

Recharge by this process can result from actions deliberately taken to augment water resources within the aquifer, as in Arizona (Quanrud et al., 1996) and Atlantis (Tredoux et al., 1999), both in the USA. Equally, and perhaps more frequently, this may occur as the unintended result of some other operation such as land irrigation, as in Léon, Mexico, which recharges wastewater into the aquifer (Chilton et al., 1998). Lerner et al. (1982) estimated that the alluvial fan under Lima, Peru, received 20% of its recharge from irrigation losses.

Irrigation of this form, through ‘spreading basins’ or ‘playa lakes’ has a number of drawbacks. The main concern with this method is that even ‘unpolluted’ waters may contain suspended solids, which will clog the recharge pathway requiring regular drainage and cleaning of the infiltration basins. In addition, this method can also be
very open to pollution from storm-water runoff or pollutant spills. The importance of infiltration as a source of groundwater pollution was outlined with respect to Chalk and soakaways in Robinson and Barker (1999).

This form of recharge is also very inefficient. Experience in the USA has found that due to the large surface areas, significant quantities of water are lost through evaporation. This large surface area requirement also restricts land available for agricultural uses. Also, in certain areas the large bodies of standing water led to significant mosquito breeding problems (O’Hare et al., 1986).

2.1.2. Well recharge

In areas with low permeability soils or thick soil zones, wells may be used to inject recharge water. If required, this water may then be abstracted through either the same well, or another. There are a number of considerations when designing a recharge well. These include: the diameter being as large as possible, with diameters of 600 to 900 mm being recommended for UK aquifers; in the UK Chalk aquifer, wells should penetrate about 50 m of saturated aquifer (Brandon, 1986). The gravel pack should not be so thick as to prevent easy rehabilitation.

Recharge wells are the only feasible method of AR in areas where a thick impermeable layer overlies the aquifer. This applies to much of the UK. Recharge wells also avoid the issues of evaporation and land usage identified as concerns with infiltration basins.

Injection into a well is not without problems, however. Severe clogging has been found to result if precautionary measures are not taken (Sniegocki and Brown, 1970). Once clogged however, a well can be redeveloped in order to remediate the situation and bring the well back into operation.

The main factor responsible for clogging is suspended solids, either within the recharge water or formed through microbiological activity, which may clog both the well screen and the aquifer. These can be reduced by appropriate treatment of the water, including reduction of: organic carbon, nutrients (including nitrates and phosphorous), and micro-organisms. Chlorination of the water will also help prevent organism growth, and many successful schemes incorporate a permanent trickle feed of chlorine solution into the well. Storage in the aquifer successfully reduces the quantities of chlorine reaction products, commonly known as ‘disinfection by-products’, in the treated water via microbial action (Singer et al., 1993).
Mixing of the recharge water and the native water may result in the precipitation of calcium carbonate, iron oxides and other compounds in the aquifer, again leading to a reduction in the permeability of the rocks. A further clogging process is air binding, a process that occurs when the recharge water is cooler than the aquifer water so that on warming the recharge water exsolves some of the dissolved air, forming air pockets in the aquifer. Prevention of this process requires that injection water should have a low dissolved gas content.

Other recharge issues concern the production of water that is non-potable. As an example, certain recharge waters (e.g. the very low TDS waters that result after reverse osmosis treatment processes) can react with the aquifer rocks, releasing undesirable compounds into the recharge water.

Recharge wells have been developed within the UK: a good example is the North London AR scheme, operated by Thames water in the UK (O'Shea and Sage, 1999; Hawnt et al., 1981; Water Resources Board, 1973; Water Resources Board, 1974; Boniface, 1959), which is used to supplement supply to North London from the Chalk aquifer. This system uses a network of wells to inject water, which then flows as a result of the piezometric gradient within the aquifer. A network of wells is then used to abstract this water. Some of the wells, midway along the flow path, are used to both inject and abstract water, but significantly, they do not abstract the same water that they inject, as the natural flow will remove the injected water from the influence of that well.

Further applications have met with reasonable success, although no similar schemes have become operational in the UK. Investigations have been carried out into AR into the Triassic Sandstones at Edwinstone and Clipstone, Nottinghamshire (IWES, 1986) and Stourbridge (Jones, 1983) as well as the Lower Greensand at Hardham, Sussex (O'Shea, 1984).

Internationally, though mostly within the USA, AR through recharge wells has been used with mixed results. Injection of high quality water has generally been successful (e.g. Brown and Silvey, 1973, 1977). Well design issues reducing irreversible clogging were addressed with wastewater injection in New York (Baffa, 1970). Other recharge wells are used to recharge reclaimed water e.g. Atlantis, South Africa (Tredoux et al., 1999) and to form salinity intrusion barriers, for example in Orange County, California (Pyne, 1995).
2.1.3. Vadose-zone wells

In areas where the ground water level is at depth (100 to 300 m), a cheaper and simpler form of well recharge is to discharge the water into vadose-zone wells. This process is limited by the possibility of clogging of the wells, and the impossibility of redevelopment or remediation of the well via pumping. Because of this the life span of vadose-zone recharge wells is strictly limited.

2.2. Artificial Recharge and Recovery

A development of the use of recharge wells for AR, Aquifer Recharge and Recovery (ARR), uses one or more wells to inject potable water within an aquifer, and additional wells to abstract this water when required. The significant difference between ARR and ASR is that in ARR the same well is not necessarily used for both injection and abstraction. ARR provides an integrated water resource management system, which, when applied within one drainage basin, has a number of potential benefits. Firstly, ARR clearly allows temporary storage of groundwater. The duration of storage is limited by the rate of groundwater flow – water that has moved beyond the region of influence of the abstraction wells cannot be recovered. Secondly, ARR allows the movement of water, along the direction of groundwater flow, without the need for major infrastructure. This can, in certain scenarios, have significant benefits.

The AR scheme in North London, described in Section 2.1.2 is a major ARR scheme in the UK. One conclusion of importance that can be drawn from the success of this scheme for the development of AR in the UK, is that the storage of potable water within a double-porosity system is feasible. Albeit that the overlying sands may play a significant role in the storage of groundwater at this site.

The major drawbacks to ARR are identical to those identified in the section describing recharge wells (Section 2.1.2), most notably the high potential for wells solely used for injection to be become blocked. This issue is somewhat alleviated in those wells midway through the scheme, where both injection and abstraction take place, as the repeated alternating pumping phases have a ‘development’ action on the wells.

A further development of ARR is the aborted hybrid artificial recharge scheme developed by The Severn Trent Water Authority in Norton, near Stourbridge. This scheme, which utilised a semi-confined Triassic sandstone aquifer, had a well
designed for both recharge and abstraction (in the manner of ASR). Additional wells located around the site could also be used for abstraction (as in ARR), (Jones, 1983).

Figure 2-1 Wellhead at the Norton ASR scheme. Four recharge lines allow variable rates of recharge without cavitation in the pipework, limiting unwanted aeration of the water which can lead to clogging of the ASR well.

2.3. **Aquifer Storage and Recovery**

ASR operates on a cyclical basis, with water being injected into the aquifer in times of plenty and being abstracted again during times of shortage; the water injected into the aquifer fills a volume of the aquifer around the well from which it can then be extracted as required. The principle behind any ASR system is very simple. A single well, specifically designed for the purpose (or retrofitted), is used to inject clean water into an aquifer, forming a ‘bubble’ of injected water around the well. After a period of storage, this water is abstracted, chlorinated and then passed into a water supply network. Finally the system is left dormant for a period. This cycle is repeated, occasionally diurnally but more often annually on a seasonal basis (Pyne, 1995). A system may also operate on longer timescales, with long periods of
injection, up to several years in duration, being followed by periods of abstraction during times of drought, for example the Rome Avenue scheme in Tampa (Guillory et al., 1997).

Apart from simply forming a groundwater reservoir, ASR systems may also be used in similar ways to other artificial recharge systems, helping to prevent saline intrusion or replenishing historically depleted groundwater levels.

2.4. Previous research into ASR

There has been surprisingly little research into the processes that occur within an operational ASR system. Most ASR applications have been developed through general experience in the water resource field, and through site specific implementation. As a result, although there are numerous publications outlining ASR case studies (for examples see Brown and Silvey, 1973; Pyne, 1995; Mirecki et al., 1998) and summarising ASR potential (Bouwer, 1996; Jones et al., 1998), there has been little basic research and little interpretation of field observations made during the development and operation of the schemes.

Most ASR systems have been sited so as to use single porosity lithologies, including sandstones and conglomerates. Several systems have been developed in limestone aquifers especially in Florida, USA, but even these show minimal double-porosity effects. As a result, the main thrust of research has been into the effects of mechanical dispersion within the aquifer.

Beginning in the late 1960’s, investigations into the possibility of injecting potable water into a saline aquifer, storing it and then abstracting it were investigated (Bear and Jacobs, 1965). The effects of dispersivity during both the injection and abstraction of water were also investigated. As water with a low solute concentration is injected into an aquifer, this water will interact through dispersive mixing processes, resulting in a potentially significant increase in the solute concentration of the low solute concentration water when it is subsequently abstracted. Analytical solutions building on early site trials were developed to aid in the identification of the significant controls on this dispersive mixing. These solutions were supported experimentally through the construction of miniature artificial aquifers.

This research also investigated the effect of the injection of low solute concentration water into an aquifer saturated with water with a high solute concentration. The ‘saline interface’ within the aquifer becomes tilted due to the density difference, and this results in lower recovery efficiencies for the ASR system. This work is
discussed in Esmail and Kimbler (1967); Kumar and Kimbler (1970); Kimbler (1970), Moulder (1970), Gelhar et al. (1972a,b). Perhaps the best summary can be found in the Bulletin written by Kimbler et al. (1975) who summarises the findings of this research:
• "... the cyclic storage of fresh water in horizontal salaquifers\(^1\) that possess primary permeability and porosity is technically feasible."
• "The economic feasibility of any particular project ... can be determined only after detailed engineering studies have been completed and evaluated with reference to the availability of surface water and treatment plant capacity."
• "The recovery efficiency of the I/S/P\(^2\) cycle can be predicted..."
• "The deleterious effect of pre-existing ground-water movement in the salaquifer upon the cyclic storage of fresh water can be counteracted."

The authors determined that the counteraction in the last conclusion may be effected in two different ways. Firstly through the development of a 'buffer zone' of injected water that remains permanently within the system, and secondly through the use of a wellfield of injection and abstraction wells to create an 'isopotential zone', a flat potentiometric surface across the region affected by the ASR well. The effects of different flow regimes were examined by Streetly (1998).

This important body of work does recognise the limitations of ASR. Kimbler et al. (1975) include a note to the effect that limestones and other aquifers in which there is an important secondary porosity cannot be fully described by the mathematical solutions developed. This is both because of the introduction of double-porosity diffusion effects, and the inhomogeneous nature of dispersion within fractured aquifers.

Recent research has examined the theoretical effect of vertical aquifer heterogeneity (Huntley and Bottcher, 1997), although this had been previously addressed in association with the dispersion and gravitational segregation issues, by Kumar and Kimbler (1970).

Important work examining the issues of clogging, and determining methods of both prevention and rehabilitation has been completed. The causes of biological, chemical and physical clogging have been discussed by a number of authors, both specifically (Sneggocki and Brown, 1970; Pavelic et al., 1998) and in general

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\(^1\) A "salaquifer" is a deep saline aquifer.

\(^2\) I/S/P = Injection / Storage / Pumping
discussions of AR and ASR (Pyne, 1995; O’Hare et al., 1986). The interrelationship between these processes was examined in the laboratory by Rinck-Pfeiffer et al. (2000). Further work has looked at how the quality of the injected water will affect the clogging issues, and Dillon and Pavelic (1995) provide summary guidelines on the quality of stormwater and treated wastewater for injection into aquifers. Other notable works include the modelling of ASR operations within a dual-permeability system (Chen, 1985), and consideration of the implications of chloride disinfection of injected water for disinfection by-product levels (Mirecki et al., 1998).

More recently, preliminary investigations into the role of double-porosity diffusion processes in the applicability of ASR schemes have begun. ASR systems in double-porosity aquifers have been successfully modelled using different double-porosity codes. Gaus et al. (2000) modelled an ASR system using the SWIFT/486 code, incorporating double-porosity effects and calibrating to the Lychett Minster ASR test site. Work within this thesis using the DP-Pulse code (version 1) has been presented, and new approaches in the characterisation of double-porosity aquifers have been developed (Barker et al., 2000), (Wright and Barker, 2001). Initial attempts have also been made to simulate both double-porosity diffusion processes and hydrochemical interactions (Gaus, 2001). Finally, the implications of double-porosity on the time required to fully characterise a double-porosity aquifer has been considered (Wright and Barker, 2001).

2.4.1. Benefits of ASR

The growing interest in ASR as a means of augmenting groundwater management systems is not without due cause. Much has been made of the flexibility of operation and purpose, and this has great appeal for those who plan expenditure on the development of water systems. The low environmental impact of an ASR scheme is also important, as this allows development of schemes in both environmentally sensitive areas and within the urban environment.

ASR schemes have a number of other benefits over other artificial recharge schemes, outlined here and explained more fully below:

- ASR allows the use of aquifers containing non-potable water;
- ASR is a relatively cheap water resource management tool, which allows a staged investment approach;
ASR circumvents the clogging problems that can arise within injection wells, as injection and abstraction through the same well reduce difficulties arising from injection-induced clogging in the well;

ASR is a very flexible system, which can be applied for a wide range of purposes;

Natural processes in the aquifer can improve the quality of injected water.

Firstly, and perhaps of most importance, ASR potentially enables the use of non-potable aquifers for the storage of potable water. Many areas within the UK, and especially in the Chalk regions, have aquifers that either contain extremely old mineralised water, or water that is in direct connection with the sea and therefore saline. The injection of potable water creates a ‘bubble’ of potable water around the ASR well, although in fractured aquifers this ‘bubble’ will actually consist of an extended network of fractures filled with potable water. During the abstraction process this water will be removed and, although some will certainly be affected by mixing processes and the diffusion processes of a double-porosity system (see Section 1.4), potable water can still be removed from the aquifer. This allows the possibility of a guaranteed year-round supply to areas with only seasonably available fresh water, and no potable groundwater supply. This ability to utilise non-potable aquifers as an additional resource is one of the most important aspects of ASR.

Taking into account the usual purpose of an ASR system, that of water storage, the likely alternative would be a surface reservoir. These have extremely high costs, take up large areas of valuable land, and have a recognised ecological and sociological cost. It is estimated that a total of 40-80 million people worldwide have been displaced by reservoir construction (World Commission on Dams, 2000).

The cost of a surface reservoir is dependent on a number of factors, one of the greatest being land value. In many cases displaced people will have to be rehoused and compensated. Large costs also arise in the construction of the structure. This may either consist of a dam, which may also require that the basin to be flooded be lined with impervious clay, or it may take the form of a large tank to contain the water. Either structure can cost large sums of money. The World Commission on Dams (2000) found that:

“Large dams built for municipal and industrial water supply have generally fallen short of intended targets for timing and delivery of bulk water supply and have exhibited poor financial cost recovery and economic performance.”

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While both ASR and surface reservoir systems share many costs, including those of water transportation and pumping, the large construction costs are avoided by an ASR system, which will require little more than a well. The small land requirement often means that a developer need not purchase any land at all, simply building within the grounds of a water treatment plant.

Surface water reservoir systems will, of necessity, take a long time to implement. The time from the first decision, through the application process for permission to the end of construction and filling may take years. By contrast, an ASR installation may be completed within months, and while the development of the aquifer prior to operational use may take anything up to a few years, the overall time for implementation will be equivalent to or, more likely, shorter than that required for a surface water reservoir.

The simplicity and rapidity of construction also allows easy expansion of an ASR system. Increasing the capacity requires little more than the construction of an additional well, allowing for phased investment. This ideally suits those with limited resources, including both smaller public and private bodies.

ASR systems may be used as safeguards against years of drought. Whilst the cost of building a surface water reservoir is immense, and any increase in capacity will need to be thoroughly justified, an ASR system can store water in preparation for years of shortage through the simple process of injecting more water than is abstracted. Year on year, this will provide a surplus within the aquifer which may be drawn upon in dryer periods. On a much smaller time-scale, ASR systems may be used to provide very short term supplements. A system may easily be devised purely for use at time of unusual demand, such as public holidays.

Finally, it is worth noting the potential of ASR to change the solute chemistry of injected waters, with beneficial results. For example, the UK has increasing problems with nitrate contamination of surface waters as the result of excessive fertiliser usage in farming practice. There is evidence (Edmunds and Walton, 1983) that reduction of nitrates will take place in anoxic aquifer conditions, leading to an improvement in the quality of the injected water, although the time-scale of the denitrification processes may be greater than those of any ASR scheme.

### 2.4.2. International experience of ASR

World-wide there have been numerous developments, mostly within the USA where there are currently 50 operational schemes (www.asrforum.com, 2002), with about
100 others under testing. Other schemes are either operational or undergoing testing in Israel (Jerusalem and Hadera), Australia (Adelaide) and Canada. Aquifer types include glacial drifts (e.g. Seattle, Washington) and limestones (e.g. Lake Manatee, Florida, see Figure 2-2). In the USA there is large commercial usage of ASR to provide water supplies for large cities.

Figure 2-2 ASR Wellhead at Lake Manatee, Florida. In the background the water treatment works supplying potable water for ASR injection can be seen.

Artificial recharge has been used in Kuwait to store the output from desalination plants, and also to reduce the depletion of brackish groundwater by reuse of wastewater. Well and basin recharge were used (Viswanathan and Al-Senafy, 1998). Field trials suggested that storage and recovery from the two major aquifers was feasible. Injection at rates of 650 to 1300 m$^3$/d through each of 35 to 40 wells is planned for the Damman Limestone aquifer (Mukhopadhyay et al., 1998).

2.4.3. UK experience of ASR

As has previously been mentioned, within the UK current experience of ASR is relatively limited. A number of small schemes are operational in the Nottingham area, extracting water from low yield Magnesian Limestones and injecting into the Sherwood Sandstone, currently abstracted to capacity. This allows short periods of high abstraction for crop irrigation during the summer months, which could not have otherwise been licensed. An artificial recharge scheme is operational in North
London, although injection and abstraction are from different wells and cannot be considered true ASR (see Section 2.1.2 for further details of this scheme).

A number of other sites are either currently undergoing testing, with little likelihood of operational running within the year, or have been tested and are now awaiting further development. These include the Chalk of East Anglia (Cook and Moncaster, 1998) where pilot scale ASR testing has been carried out to the north of Colchester, with the injection and recovery of 2800 m$^3$ of treated water into a semi-confined aquifer. Extensive testing has been carried out on the Sherwood Sandstone aquifer in Yorkshire (CH2M HILL, 2002; see Figure 2-3), and the deeply confined Lower Greensand aquifer at Stockbury in Kent, a joint project between Southern Water and Mid Kent Water (CH2M HILL, 1999). The Chalk of the Wareham basin, Dorset, was tested by Wessex Water, however there are no current plans to develop the scheme further.

![Figure 2-3 Well drilling at the Yorkshire Water ASR site. Cable percussion techniques are suitable for monitoring wells (foreground), however reverse circulation techniques are best for drilling ASR wells (rear).](image)

Further areas are under consideration, and more information can be found in the BGS report, “The potential for Aquifer Storage and Recovery in England and Wales”, Jones et al. (1998) and also in “ASR - UK: elucidating the hydrogeological issues
associated with aquifer storage and recovery in the UK”, Gale et al. (2002). A recent review of research into ASR in the UK is provided by Jones et al. (1999).

2.4.4. A generic ASR scheme

The typical ASR scheme is designed to provide water to potable supply during times of peak demand, whether these last a few days or for longer periods. In this situation, the injected water can be obtained from a groundwater or surface water source, which is then treated to potable standards before being injected. Under ideal circumstances this water then only requires disinfection before it can be delivered to the distribution network.

Currently in the UK some water authorities surpass their peak capacity for a few days each year. This problem is likely to increase with the growing population density in certain areas. In many of these areas it would not be possible to build reservoirs, as land is prohibitively expensive. It would seem that ASR would be a very effective solution. In England and Wales, ASR would probably be used to smooth out annual variability in water supply, as well as meeting times of peak demand (public holidays and the like).

2.5. Standard ASR practices and definition of terms

2.5.1. Cycle testing

The current standard practice is to test an ASR scheme before operational implementation by performing a number of cycles, of short duration, involving injection and abstraction. These cycles are designed to improve the aquifer over time, while also giving data for the determination of the characteristics of the aquifer. Proprietary methods are used to analyse the collected data in order to identify the possibility of successful ASR operation in the locality.

Initially the cycle tests are of short duration and as confidence grows they become more drawn out, with more water injected as well as periods of storage. Putting the recovered water into supply occurs as soon as possible despite low recovery efficiencies, and with repeated operational cycles recovery efficiencies increase.

This thesis will refer to both cycle testing and ASR tests. Cycle testing will be used as a general term, describing the injection, storage and abstraction undertaken when testing an aquifer prior to implementing an ASR system. The term ‘ASR test’ will be used in a more precise manner. An ASR test is a test carried out in order to
characterise the nature of an aquifer prior to preparations for implementing operational ASR. This thesis will examine the capability of an ASR test to determine specifically the nature of the double-porosity of the aquifer. An ASR test will consist of one or more cycle tests.

As has been discussed earlier, concerns have been raised that characterising the nature of double-porosity aquifers will require testing of a longer than usual duration in order to successfully predict behaviour (Wright and Barker, 2001). It is also believed that optimal operation is only likely to be reached after a number of years of operational cycling, due to the constant but slow removal of solutes from the aquifer (Jones et al., 1998).

2.5.2. Maximum abstracted solute concentration

The maximum abstracted solute concentration is the maximum solute concentration of the water that is abstracted during the operational cycle. This will be of interest to those wishing to use the water as they may have limits on the maximum allowable concentrations to be put into supply. These limits vary from site to site. As an example, it is clear that the legislative controls on drinking water quality provide a basic limit on the quality of water that may be utilised. Water from an ASR well may be diluted with water from another source, however, and so the maximum abstracted solute concentration cannot be determined from a simple examination of legal controls.

2.5.3. Recovery efficiency

The operational efficiency of an ASR system is often characterised by a 'recovery efficiency'. A number of definitions of recovery efficiency exist within the literature. Definitions vary according to the requirements of the site / topic under discussion; for example, the availability of water for supply.

Within this thesis, recovery efficiency is defined as the ratio of the volume of water abstracted while meeting a target water quality criterion to the volume of water injected, expressed as a percentage. The quantity of injected water does not include any of the pre-operationally injected water that may have been added during testing or conditioning.

The control on recovery efficiency is the concentration of the abstracted water. It is necessary to specify a maximum abstracted solute concentration, the maximum that it is viable to put into supply. During abstraction, the solute concentration in the
abstracted water increases until this maximum concentration is reached. From this abstracted quantity we can work out the recovery efficiency of the system (Figure 2-4).

Figure 2-4 Defining recovery efficiency: Abstracted solute concentrations after 100 days injection with a maximum abstracted concentration of 0.5 native concentration demonstrate recovery efficiencies of 25%, 50% and 100%.

2.5.4. Conditioning period

As has been discussed, current methodologies for ASR application implement a series of cycle tests. As well as serving to provide information about the aquifer, these cycle tests act to improve the condition of the aquifer. For application in double-porosity aquifers, a proposed variation on the current ASR testing methodology is the inclusion of an amount of pre-operational preparation, consisting of a period of injection, here termed the conditioning period. The conditioning period would act to improve conditions in the aquifer, accelerating the achievement of standard commercial operations from an ASR well.

The purpose of the conditioning period may be seen as twofold. Firstly, prolonged injection will result in increased diffusion of solutes from the matrix water into the fracture waters, from where they will pass into the aquifer and away from the ASR
well. In this way, the aquifer close to the ASR well will be ‘flushed out’. Secondly, the conditioning period builds up an extensive ‘buffer zone’. This volume of water is between that which is injected and abstracted as the ASR cycle progresses, and that which is native in the aquifer. The buffer zone performs an important function in preventing significant diffusion of solutes from the fracture water back into the matrix at the end of abstraction cycles, when native water from the aquifer is brought closer to the ASR well. The buffer zone ensures that water with a native solute concentration never interacts with the volume of aquifer filled by the water injected during the ASR cycle.

This methodology has been successfully implemented in the USA, in the Florida Miami-Dade ASR wellfield scheme. This scheme was developed in a limestone aquifer, and the first well was tested in the usual manner, with a series of short cycle tests. As the aquifer had been sufficiently characterised during the testing of the initial well, subsequent wells were not tested prior to operation, but rather underwent a period of long-term injection of potable water, of the order of one year (Pyne, 1995).

2.6. Solute transport in double-porosity media

A great deal of work has been conducted on groundwater flow and solute transport in double-porosity media, commonly also described as fractured porous media. This work covers a broad variety of topics. As this thesis is concerned with the UK Chalk aquifer, and specifically with ASR within this aquifer, this review will be limited to relevant topics.

2.6.1. Groundwater flow through fractured aquifers

In a flowing groundwater system, the majority of solute transport takes place as a result of advective flow through the fractures. Flow through fractured aquifers is significantly different to flow through a non-fractured porous system. The principles of fracture flow are relatively simple, and de Marsily (1986) provides a good review.

An important factor is the form of the flow, i.e. whether the flow is laminar or turbulent in nature.

The basic equations for flow through a fracture are derived from the equation for flow through a cylindrical pipe. The transition from laminar to turbulent flow within a cylinder is governed by the Reynolds number:
where $V$ is the mean velocity of the fluid, $d$ is the diameter of the pipe, $\rho$ is the density of the fluid, and $\mu$ the viscosity of the fluid. For a planar fracture, $d$ is replaced by $D_h = 4S/\rho$, the hydraulic diameter of the fracture where $S$ is the cross sectional area of flow and $\rho$ is the outside perimeter of the cross sectional area of flow. For a very long fracture $D_h$ is equal to twice the fracture aperture.

The relative roughness of a fracture also affects the nature of flow within a fracture:

$$R_e = \frac{Vd\rho}{\mu}$$

where $\varepsilon$ is the mean height of the irregularities in the fracture. Louis (1974) applied the Reynolds number and relative roughness to empirically define five regimes of steady state fracture flow:

1. Smooth laminar flow
2. Smooth turbulent flow
3. Rough turbulent flow
4. Rough laminar flow
5. Very rough turbulent flow.

Each of these regimes has a different flow velocity under the same head gradient.

**Figure 2-5 Flow regimes for flow in a fracture (from de Marsily, 1986).**

### 2.6.2. Solute diffusion

One of the most important characteristics of fractured porous media is effect of molecular diffusion within the matrix, and diffusive exchange between the fracture
and matrix waters. The nature of diffusion within a matrix, and the methods for
diffusive exchange are described qualitatively by Freeze and Cherry (1979) as well
as by Grisak and Pickens (1980). The latter authors implemented a numerical model
to simulate the diffusive exchange between fracture and matrix in a double-porosity
system, with advective fracture flow.

The rate at which a solute diffuses in water is proportional to a constant of the
diffusing solute, the tracer diffusion coefficient, \( D_T \). Within a porous media,
however, diffusive movement is impacted by the presence of impermeable material
(i.e. rock matrix). The amount of interconnected porosity and the complexity of
diffusive pathways (tortuosity) act to reduce the rate at which diffusive solute
movement occurs. Diffusion of a solute within a porous medium is therefore
classified by an effective diffusion coefficient \( D_E \), which is proportional to but
less than \( D_T \):

\[
D_E \propto D_T
\]  

(3)

The mass of solute diffusing through a unit cross section of porous material per unit
time is proportional to the concentration gradient, and is described by Fick’s first
law:

\[
J_{\text{diff}} = -D_E \frac{dC}{dz}
\]  

(4)

\( J_{\text{diff}} \) is the diffusive flux, \( C \) is the concentration, \( z \) is the direction of the flux.

Consider mass balance in a rectangular prism of porous material, of area \( A \) and
length \( Az \) in the \( z \) direction (Figure 2-6).

\[ A \Delta z \phi_D \Delta C \]  

(5)

**Figure 2-6 A rectangular prism of porous material, of area \( A \) and length \( Az \) in
the \( z \) direction**
where $\phi_D$ is the porosity accessible to the diffusing solute and we ignore retardation. Through the application of conservation of mass, this must equal the net flux in, which is given by:

$$A\left(J_{z+\Delta z} - J_z\right)\Delta t = AD_E \left( \frac{dC}{dz}_{z+\Delta z} - \frac{dC}{dz}_z \right) \Delta t$$

(6)

Equating the quantities in equations 5 and 6:

$$\Delta z \phi_D \Delta C = D_E \left( \frac{dC}{dz}_{z+\Delta z} - \frac{dC}{dz}_z \right) \Delta t$$

(7)

or

$$\frac{\Delta C}{\Delta t} = \frac{D_E}{\phi_D} \left( \frac{dC}{dz}_{z+\Delta z} - \frac{dC}{dz}_z \right) / \Delta z$$

(8)

Which, taking limits, can be written:

$$\frac{\partial C}{\partial t} = \frac{D_E}{\phi_D} \frac{\partial^2 C}{\partial z^2}$$

(9)

Equation 9 gives the equation for the concentration of a diffusing solute in space and time. This equation, Fick's second law, is normally written:

$$\frac{\partial C}{\partial t} = D_A \frac{\partial^2 C}{\partial z^2}$$

(10)

where

$$D_A = \frac{D_E}{\phi_D}$$

(11)

is called the apparent diffusion coefficient.

Gooddy et al. (1996) provide a method for rapid determination of apparent diffusion coefficients in the Chalk, along with a summary of previously determined diffusion coefficients for a variety of solutes.

2.6.3. Double-porosity concepts and conceptual models

Early solute transport theories made the assumption that groundwater flow occurred through a porous medium, that could be represented by a porous continuum. Work describing the 'smearing' of a solute concentration pulse as flow occurs through the continuum was carried out by Scheidegger (1954), de Josselin de Jong (1958) and Bachmat and Bear (1964). This work described dispersion, which occurred through two processes – mechanical and diffusive. Mechanical dispersion accounts for the effect of variable microscopic flow velocities on the solute pulse amongst other
factors. Diffusion occurs according to Fick's Second Law, for diffusion through a porous material (Section 2.6.2). This resulted in the advection-dispersion equation (ADE).

It was discovered that in certain situations the ADE failed to represent experimental results (Scheidegger, 1961; Biggar and Nielsen, 1962). Solute pulses through certain lithologies were found to produce 'tailing effects', where solutes were retained in the lithology, and released at a slower rate than predicted by the ADE. The reason suggested for this behaviour was that 'dead-end' porosities received solute purely by diffusion, and then released this solute slowly back into the flow, again through diffusion only (Coats and Smith, 1964). Passioura (1971) suggests that, in a soil system, the solute is diffusing into soil aggregates, while Skopp and Warwick (1974) propose that water around solid particles forms an immobile 'halo', and that diffusive exchange occurs between this immobile water and the mobile water.

In the above examples, the volumes of immobile water, and therefore the potential effect on solute concentrations, are small. By comparison, a number of aquifers, including the Chalk and the Lincolnshire Limestone, are characterised by a series of 'blocks' of material separated by fractures. The matrix 'blocks' are generally characterised as having a high porosity and a low hydraulic conductivity, while the fractures are characterised by low porosity and a high hydraulic conductivity. These aquifers are normally considered to behave as two interconnected systems, with the majority of flow occurring through the fracture network, and little flow through the matrix. Solute exchange between the two systems occurs as a result of diffusive movement of solutes from volumes with a high solute concentration to volumes with a low solute concentration. These systems were first described as having a double-porosity by Barenblatt et al. (1960). Because of the high porosity of the matrix blocks, the volume of immobile water is potentially very high, and therefore the potential impact on solute concentrations is also high.

Modelling fracture flow in porous media, i.e. the simulation of a double-porosity system, has been a recognised problem for a number of decades. Significant progress was made when Barenblatt & Zheltov (1960) and Barenblatt et al. (op. cit.) published on the problem of flow in a fractured reservoir. Barenblatt & Zheltov (op. cit.) developed flow equations for both the fracture and matrix volumes, each described as a continuous volume, and a coupling term providing mass transfer between them, using the term dual permeability, as flow is simulated through the
matrix volume. Later Warren & Root (1963) developed an alternative conceptual model, in which the fracture and matrix volumes are again described as two continuous volumes, but the matrix is represented as a periodic array of identical blocks, completely surrounded by fractures, with no 'regional' flow occurring within the matrix.

The further development of double-porosity theory resulted in a number of different conceptual models for flow within, and solute transport through the system. Lichtner (1999), in a paper in the published symposium monograph titled “Dynamics of fluids in fractured rock” (Witherspoon, 1999), provides a general summary of these model types. Table 2-1, adapted from this paper, provides an overview of the different conceptual models.

### Table 2-1 Conceptual models for the development of numerical models of fractured rock systems (adapted from Lichtner, 1999).

<table>
<thead>
<tr>
<th>Definition</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCM</td>
<td>Single Continuum Model</td>
</tr>
<tr>
<td>ECM</td>
<td>Equivalent Continuum Model</td>
</tr>
<tr>
<td>DFM</td>
<td>Discrete Fracture Model</td>
</tr>
<tr>
<td>DCM</td>
<td>Dual Continuum Model</td>
</tr>
<tr>
<td>DCCM</td>
<td>Dual Continuum Connected Matrix</td>
</tr>
<tr>
<td>MDCCM</td>
<td>Multiple Node Dual Continuum Connected Matrix</td>
</tr>
<tr>
<td>DCDM</td>
<td>Dual Continuum Disconnected Matrix</td>
</tr>
</tbody>
</table>

2.6.4. Single Continuum Model, SCM

The SCM simulates flow through a fracture, with no interaction with the surrounding matrix (i.e. the effective porosity $\phi_e$, is equal to the fracture porosity $\phi_f$). Although suitable for fracture systems in igneous rock formations, this type of model will fail to successfully simulate a double-porosity system as there is no account made for
diffusion of water from the (porous) matrix into the fracture volume. SCM are, however, useful tools for determining the first arrivals of solute at a point away from the source, and also for investigating the hydraulics of fracture flow.

### 2.6.5. Equivalent Continuum Model, ECM

On large scales, it is common to model fractured aquifers as ‘equivalent porous media’ (EPM). This methodology simulates the aquifer by creating an analogous aquifer with a single (effective) porosity, and similar hydraulic characteristics (transmissivity and storativity), i.e. a continuum equivalent to the fractured aquifer – an ECM. The effective porosity needs to be chosen according to the problem under consideration: normally this will be either equal to the fracture porosity, or the total (fracture plus matrix) porosity. The UK Environment Agency often applies this approach in an attempt to delineate groundwater protection zones in fractured aquifers (Environment Agency, 1998). For this purpose the specific yield is used as a surrogate for the kinematic porosity, which is similar to the fracture porosity. Whilst capable of successfully modelling large-scale hydraulic regimes, as over a large volume of aquifer piezometric heads will tend to equilibrate over time, it is a very uncertain approach to apply to solute transport modelling. The nature of a fractured aquifer may allow solutes to travel in a different manner compared to an equivalent porous medium, leading to erroneous results (Bradbury and Muldoon, 1993). These errors arise as predicted flow paths determined by the ECM may not coincide with the limited flow paths provided by a fracture network. Also, local variations in fracture properties may result in significantly higher flow velocities within individual fractures than those predicted by the ECM.

### 2.6.6. Discrete Fracture Model, DFM

The term ‘discrete fracture model’ has been used in the literature to describe a model of solute transport within a fracture or fracture network, with no interaction with the surrounding volume of rock. This form of the model has no double-porosity. For the purposes of this discussion, however, an alternative use of the term suitable for double-porosity models will be applied: the ‘discrete fracture model’ describing a single fracture, or a series of fractures, surrounded and separated by volumes of matrix material. The volumes within the fractures and the matrix are connected by a mass transfer equation, which represents diffusive solute transfer between the
fracture and matrix. The DFM is probably the simplest conceptual model of a fractured rock system.

It is possible to formulate this type of model to obtain an analytical solution describing flow in the fracture, diffusion between the fracture and the matrix volume and diffusion within the matrix volume. This form of model is powerful, but limited in its application. One example of a model employing this formulation is DP1D (described in Appendix X). Although it is possible to simulate flow through complex fracture systems with this model, the simplest application allows the simulation of flow through a discrete defined fracture, with parallel walls and infinite width. This model is used in Section 3.9.

2.6.7. Dual Continuum Models, DCM

The DCM describes a system in which there are two continuous volumes, one formed by the matrix 'blocks', and one by the fracture network. These two continua have a separate parameterisation. The DCM can be subdivided into two types. One, the DCCM (Dual Continuum Connected Matrix) describes a fully connected matrix volume, i.e. every matrix ‘block’ is fully connected to those matrix blocks around it (Barenblatt et al., 1960; Barenblatt & Zheltov, 1960). The other, the DCDM (Dual Continuum Disconnected Matrix) describes a system in which each matrix ‘block’ is fully separated from surrounding matrix blocks by the fractures (Warren & Root, 1963).

Dual Continuum Disconnected Matrix Models can be further subdivided according to how the matrix continuum is represented. Three types of matrix continuum may exist:

* Fully mixed – In which the matrix continuum is represented by a fully mixed volume

The simplest form of DCDM model describes the matrix continuum as a fully mixed volume. Solute exchange with the fracture continuum is described by a simple exchange coefficient, generally determined through calibration of the model.

The relative simplicity of implementation (as compared to multiple node models) allows the incorporation of DCDM type models into other complex codes. As an example, PHREEQC is a one-dimensional numerical geochemical model, which has the capability to approximate double-porosity (Parkhurst and Appelo, 1999) through a DCDM type model. As an illustration, this model consists of two parts, a series of cells containing a mobile volume of water (the fracture continuum), and a series of
isolated cells containing a static volume of water (the matrix continuum, Figure 2-7). Each cell of the fracture continuum has attached to it an isolated, fully mixed, static volume. Exchange between the static volume, $V_s$, and the mobile volume, $V_m$, is controlled by an exchange coefficient, $\alpha$. The USGS solute transfer models MT3DMS and MOC3D simulate double-porosity processes with a similar approximation.

\[ \begin{align*}
V_s & \quad \alpha \quad V_s \\
\downarrow \quad \alpha \quad \downarrow & \quad V_m \\
V_m & \quad \alpha \quad V_m \quad \alpha \quad V_m
\end{align*} \]

Figure 2-7 Diagrammatic representation of the 'mixing-cell' approximation to double-porosity in a Dual-Domain Mass Transfer model.

This form of model can be used with reasonable success to simulate a double-porosity aquifer, however great care needs to be taken with its application. The application of these models is further discussed in Appendix V. Simulating a doubly-porous system in this manner takes no account of the diffusion depth into the matrix, instead the exchange coefficient used to describe the mass transfer between the fracture and matrix volumes is not a physically extant parameter, but rather one that is determined through calibration. Although the calibration process may identify a parameter set which allows reasonable simulation of a collected data set, through careful selection of exchange coefficient, there is a high potential for predictive model simulations to fail to correctly simulate the processes that occur. The simulation cannot be very accurate, as the exchange coefficient is insufficient to represent the complex solute diffusion process that occur in a double-porosity system. Additionally, as the exchange coefficient is hard to determine in theory or by experiment with any degree of precision, there is greatly increased uncertainty in the calibration of the model. Because of these reasons, some of which are examined quantitatively in Appendix V, the use of these models to predict system behaviour should be treated with caution.
Recent work (McKenna et al., 2001) has attempted to overcome some of the major failings of the DCDM model through the use of a distribution of exchange coefficients. Although this enables more accurate simulations of data, the potential of the model to predict behaviour, and the uncertainty in the calibration remain.

**Discretised matrix – in which the matrix continuum is represented by two or more discreet fully mixed volumes**

By describing each matrix volume using two or more volumes, through the use of nodes, or multiple concentric ‘shells’ each of which consists of a fully mixed volume, it is possible to develop a DCDM type model that is better able to simulate double porosity processes.

This approach has been used to develop a number of models, including SWIFT II (Reeves et al., 1986), as well as being presented by Dershowitz and Miller (1995), and Bai et al. (1994). A further development used this form of model to simulate the behaviour of multiphase fluids in a double-porosity medium (Lewis and Ghafouri, 1997).

**Continuum matrix – in which the matrix continuum is represented by a continuum**

Using analytical formulations, it is possible to fully describe the matrix continuum, allowing ‘true’ (i.e. non-discretised) representation of solute diffusion in double porosity systems. Implementation of such models allows ‘true’ representation of double porosity processes, in terms of solute movement through the matrix material, however the analytical formulation can lead to difficulties in developing models that are capable of representing real world situations (i.e. 3 dimensional flow systems, heterogeneous formations, geochemical interactions etc.).

Both the DP-Pulse model (described in Chapter 3 and applied throughout this thesis), and DP1D (described in Appendix X) may be considered DCDM type models, in which the matrix continuum is fully described. Through use of analytical solutions the concentration is fully variable throughout the matrix.

### 2.6.8. Experimental double-porosity investigations

Double-porosity systems have been investigated on a laboratory and field scale to some extent in recent years, although much of the investigations have been restricted by the limited ability to successfully simulate double-porosity behaviour.

A significant attempt to apply the theory of double-porosity behaviour to a field scale model was made by Bibby (1981). Bibby used a finite element numerical code (a
DCDM type model) to simulate contaminant transport through the Chalk aquifer from a colliery in the south-east of the UK across a distance of approximately 7 km, and over a timescale of 83 years. Using solutions based on Carslaw and Jaeger (1959) to represent the double-porosity, the model successfully simulated solute concentration changes in a nearby water supply borehole.

A simple DFM model, in which a single fracture diffusively interacted with the matrix, was applied by Maloszewski and Zuber (1993) to simulate a series of tracer tests carried out in fractured gneiss by Raven et al. (1988) amongst others. One series of these tracer tests was carried out using two tracers with significantly different diffusion coefficients. The results of this work indicated the importance of matrix diffusion on solute transport through this media. A team at the Sandia Laboratories, New Mexico, have recently investigated solute transport through fractured dolomite using similar methods of tracers with different diffusion coefficients (Meigs and Beauheim, 2001; Haggerty et al., 2001). The simulation efforts (McKenna et al., 2001) applied a (DCDM) single node (fully mixed) model for the matrix volumes, and used a distribution of mass transfer coefficients to describe diffusive solute exchange between the fracture and matrix volumes. Although the single node assumption limits the application of the findings, the tracer tests conducted involved injection into and abstraction from a single well. These tracer tests may well be of interest for the understanding of the behaviour of ASR systems in similar double-porosity rocks.
2.7. *Double-porosity characterisation of the Chalk aquifer*

The Chalk forms a “Major Aquifer” in England. The Environment Agency (NRA, 1992) defines “Major Aquifers” as:

“…highly permeable formations, usually with a known or probable presence of significant fracturing. They may be highly productive and able to support large abstractions for public supply and other purposes.”

The Chalk aquifer exists along the south and east coast of Britain. Large unconfined areas dip gently towards the south east, where it becomes confined by clays and sands. The London and Hampshire basins as well as the Weald also lead to confinement of the Chalk. The general location of Chalk outcrop across Britain is outlined in Figure 2-8.

![Sketch map showing the approximate location of Chalk outcrop in Britain.](image-url)
Unlike aquifers that have been previously used for ASR across the world, the Chalk is a fractured rock with a double-porosity (Price et al., 1993). It is formed of blocks of a small grained highly porous media ($\phi = 30 - 50\%$) (Fretwell, 1999 and Bloomfield et al., 1996), here referred to as 'matrix', separated by few relatively large fractures (see Figure 2-9) giving a total fracture porosity ($\phi = 0.1 - 1\%$) (Bloomfield, 1996). The Chalk was formed in the Cretaceous from the calcareous skeletal plates of microscopic planktonic algae as well as larger shell fragments. As a result of the small particle size (less than 10 μm), pore throats are of the order of between 0.012 and 100 μm (Price et al., 1976). Pore throats of this size indicate very low hydraulic conductivity values, and this is supported by experimental measurements which indicate an average matrix hydraulic conductivity of $6.3 \times 10^{-4}$ m/day (Allen et al., 1997). As a result of these low conductivities groundwater flow through these pores is negligible.
Figure 2-9 Chalk core from a location near Dunstable, UK. The distinctive fracturing of the Chalk can clearly be seen.

Measured matrix porosities within the Chalk aquifer vary between 17% (Patsoules & Cripps, 1990b) and 50% (Lloyd, 1993) with a credible median value being approximately 40%. Measured fracture spacing in the Chalk vary between 0.106 m (Younger and Elliot, 1995) and 2.9 m (Fretwell, 1999). Bloomfield (1996) and Bloomfield *et al.* (1996) indicated that the lower range of fracture spacings measured (averaging 0.34 m) were joints, while the higher range (averaging 2.80 m) were
flowing fracture systems. A summary of different findings for the Chalk aquifer is presented in Table 2-2.

As indicated by the relatively narrow fracture spacings, the Chalk aquifer is heavily fractured and, as a result of the low hydraulic conductivities within the matrix, all groundwater flow tends to occur within these fractures. Thus field measurements of hydraulic conductivities in the Chalk tend to be much higher than those obtained within the laboratory. Measurements of the hydraulic conductivities of core samples range between $1 \times 10^{-5}$ and $1 \times 10^{-2}$ m/day (Price et al., 1976). Hydraulic conductivities of the Chalk measured in the field range between $1 \times 10^{-2}$ and $1.8 \times 10^{2}$ m/day (Allen & Price 1990; Price et al., 1976; Price et al., 1977; Price et al., 1982; Watson et al., 2000).

The Chalk aquifer therefore behaves as two systems. Flow occurs through the fracture network, which is characterised by low porosities, but high hydraulic conductivities. The matrix is characterised by low hydraulic conductivities and high porosities. Solute exchange between the two systems occurs as diffusion results in movement of solutes from volumes with a high solute concentration to volumes with a low solute concentration.

The double-porosity nature of the Chalk aquifer is important when considering the subject of this thesis, ASR. During the operation of an ASR system, water is injected into the fractures, within which it will come into direct contact with the native water within the matrix blocks and diffusion of solutes between the two porosities will occur (Figure 2-10). This causes the solute concentrations in the abstracted water to behave in a different manner to those in an equivalent single porous medium.
Matrix: High $\phi$ Low $k$

Fracture: Low $\phi$ High $k$

Fluid flow through high permeability fractures
Diffusion from high to low solute concentrations

Figure 2-10 Fluid flow and diffusion in double-porosity media.

Table 2-2 A summary of data on the properties of the Chalk aquifer

<table>
<thead>
<tr>
<th>Reference</th>
<th>Matrix Porosity</th>
<th>Fracture Porosity</th>
<th>Fracture Spacing (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bell, Cripps, Edmonds and Culshaw, 1990</td>
<td>Upper 0.244a</td>
<td>Middle 0.248a</td>
<td>Lower 0.398a</td>
</tr>
<tr>
<td>a-Yorkshire b-Norfolk c-Kent</td>
<td>0.406b</td>
<td>0.351b</td>
<td>0.266b</td>
</tr>
<tr>
<td>Bloomfield, 1996</td>
<td></td>
<td></td>
<td>0.34 for all joints &amp; 2.80 for flowing horizons</td>
</tr>
<tr>
<td>Bloomfield et al., 1996</td>
<td>0.34 – Average of 2045 samples</td>
<td></td>
<td>0.34 for all joints &amp; 2.80 for flowing horizons</td>
</tr>
<tr>
<td>a-Northern b-East Anglia c-Thames d-Southern</td>
<td>Upper 0.354a</td>
<td>M&amp;L 0.189a</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.384b</td>
<td>0.343b</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.314c</td>
<td>0.266c</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.388d</td>
<td>0.284d</td>
<td>0.229d</td>
</tr>
<tr>
<td>Carter &amp; Mallard, 1974</td>
<td>a-Kent, N&amp;S Downs b-Norfolk Converted from void ratios</td>
<td>Upper 0.45a</td>
<td>Middle 0.38a</td>
</tr>
<tr>
<td>Downing et al., 1993</td>
<td>0.3-0.4</td>
<td></td>
<td>&lt;1</td>
</tr>
<tr>
<td>Fretwell, 1999</td>
<td>0.366-0.487</td>
<td></td>
<td>2.90 mean average</td>
</tr>
<tr>
<td>Lloyd, 1993</td>
<td>0.4 – 0.5 Upper and Middle Chalk</td>
<td>0.2 – 0.3 Lower Chalk</td>
<td></td>
</tr>
<tr>
<td>Patsoules and Cripps, 1990a</td>
<td></td>
<td></td>
<td>0.18-0.33 Yorks. Chalk</td>
</tr>
<tr>
<td>Patsoules and Cripps, 1990b</td>
<td>0.17 – 0.28 Yorks. Chalk</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Price et al., 1993</td>
<td>0.3 – 0.4</td>
<td></td>
<td>10^-4</td>
</tr>
<tr>
<td>Younger and Elliot, 1995</td>
<td>BP parallel to bedding</td>
<td>BN normal to bedding a-Thames/Cambridge b-Kent</td>
<td>BP 0.106a</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.400b</td>
</tr>
</tbody>
</table>
Chapter 3
Description of the DP-Pulse model
3. Description of the DP-Pulse model

A novel model, DP-Pulse, has been developed by Professor Barker to examine the behaviour of conservative solute diffusion in double-porosity media (Barker et al., 2000), (Barker, unpublished communications 1997-2001). This model has been used as a tool in a number of different areas of research, including the seasonally unsaturated zone (Fretwell, 1999; Fretwell, 2000). The full mathematical description of the model was given as an Appendix to the thesis of Fretwell (1999) but is not currently published in any major journal, and therefore it is worth providing a detailed description of the conceptual model, the mathematical solution and the functionality of the computer implementation. Also of significant importance are investigations into the errors inherent in the model conceptualisation, and also the errors resulting from assumptions made during the formulation of the model. These potential errors are investigated in Sections 3.7 and 3.8. Furthermore, certain developments of the model by the author have taken place during the completion of this work, and these are outlined in this chapter, most important being the automated calibration routine detailed in Section 3.11, but also the more general model developments detailed in the same section.

The model was verified through comparison with a simple analytical solution to a simple problem of 1-dimensional fracture flow in a double-porosity system (Section 3.9) and finally, a sensitivity analysis was undertaken using the model’s unique parameterisation (Section 3.10).

3.1. Introduction to model

DP-Pulse was conceived in order to examine the behaviour of conservative solute diffusion in double-porosity media, and subsequently adapted to simulate this process under an ASR regime (Barker et al., 2000), (Barker, unpublished communications 1997-2001). The model has an analytical solution but requires computer implementation, and so we shall refer to it as a semi-analytical model. The model consists of a series of cells, each of identical volume. A single cell consists of both fractures and rock matrix. Whilst the mathematics are generalised to many fracture geometries through the use of Block Geometry Functions (BGF) (Barker, 1985a, 1985b), for the purposes of visualising the model we will consider the mathematics of one specific geometry: parallel identical slabs of matrix separated by a uniform fracture (Figure 3-1). A single cell extends from the centre of one
matrix block across the fracture to the centre of a neighbouring block. The fractures have an aperture of $a$ while the blocks have a (total) thickness of $2b$.
As water flows through the fracture system, mass enters and leaves the fracture component of the cell. The novel feature of this model is that this flow velocity is discretised into a series of instantaneous pulses, therefore water flows in a series of pulses from one cell to the next.

![Figure 3-1 A set of model cells. Each cell extends from a fracture to the centres of the two neighbouring matrix blocks. (Slab geometry.)](image)

The matrix component of each cell in the model is disconnected from the neighbouring cells; there is no solute flux from one block to another, only between the fracture and matrix. The matrix is therefore discontinuous. As there is a solute flux with time through the length of the fracture, the fracture component of each cell is continuous. As the model is semi-analytical in nature, it does not represent the matrix material with either one, or a series of nodes. Rather, it fully describes the variation of solutes within the matrix volume over distance and with time. Using the terminology described in Table 2-1 the model is therefore a DCDM (Dual Continuum Disconnected Matrix) type model.

### 3.2. **Model Capabilities**

The functionality of the DP-Pulse model is an improvement on many other double-porosity models in two major respects.
• The formulation of the model allows reversible advective flow of the water in the fractures. This has never been achieved in an analytical model form before.

• The model allows the determination of diffusive exchange of solutes between fracture and the matrix based on Fick's laws. Many so-called 'double-porosity' models approximate the matrix block as a fully mixed cell, from which solutes can diffuse into the fracture by means of an 'exchange coefficient'. While allowing an approximation of double-porosity for calibration purposes, this approach cannot sufficiently simulate true double-porosity in order to allow behavioural predictions. (The limitations of this approach are more fully discussed in Appendix IV).

In addition to these functional capabilities, the formulation of the DP-Pulse model is such that it is significantly different to other available double-porosity models. The model makes use of a unique parameterisation and can be invariant to both flow rate and, more importantly, to the geometry of groundwater flow within the aquifer. Each of these topics are discussed in detail in the following two sections.

The significance of this simple model parameterisation, when compared to the available double-porosity models such as SWIFT (see Section 2.4.4) is large. Most models require the declaration of a large parameter set, including such variables as block size, fracture aperture and matrix porosity. In DP-Pulse these variables are reduced to two 'composite' variables, which allows the model to have, for the purposes of calibration, a unique solution. As a result, under conditions where little is known about the geometrical characteristics of the simulated aquifer, greater confidence can be held in both the results of a model calibration and subsequent simulations.

Additionally, the greater simplicity of the DP-Pulse parameterisation, and the intrinsic geometrical invariances, make the model extremely simple to use, and rapid in application. Other true (Fick's Law based) double-porosity models require the definition of a series of parameters for correct operation including, to use SWIFT as an example, a size describing the cell size within the matrix block, and tolerance levels on solute concentration variations for the iteration regimes. These parameters vary according to the geometry of the system simulated, and inherently affect model stability. The DP-Pulse model has a single variable of this kind, the pulse interval, $\Delta T$. This variable has no impact on model stability, only on the error produced by
the model, and therefore as long as caution is taken when specifying the value of $\Delta T$
to limit the error, automated implementation of the DP-Pulse model is viable.

3.3. Model Assumptions

In order to develop the model, a series of assumptions were required:

1) Steady state flow conditions are established instantaneously.

2) The aquifer is homogenous.

3) The aquifer is fully confined.

4) There is no water movement in the rock matrix.

5) The fracture water remains locally at a uniform but changing concentration.

6) Mechanical dispersion is negligible.

7) Movement of solutes within the matrix is described by Fick’s second law and is
   characterised by an ‘apparent’ diffusion coefficient.

8) Density effects on the flow are ignored.

9) Initially, the solute concentration through the matrix is uniform and at
   equilibrium with the local fracture water.

Through the rest of this section, each of these assumptions will be described in detail,
relevant mathematical boundary conditions will be stated, and the potential
implications for the application of the DP-Pulse model will be discussed.

1. Steady state flow conditions are established instantaneously.

As the compressibility of water is small, the only significant opportunity for transient
flow conditions to arise is when the storativity is significantly large. This is not the
case with most fractured aquifers.

2. The aquifer is homogenous.

This is a standard assumption for most groundwater models, as any groundwater
model must approximate homogeneity on some scale due to the impossibility of
collecting a comprehensive set of data. Despite this, however, the impact of this
assumption should be examined. Stating that an aquifer is homogenous is clearly
hard to justify. All lithologies have variations on both small and large scales. The
Chalk, for example, commonly shows both vertical and lateral variations of fracture
densities.

If an aquifer is inhomogeneous, the solute concentration changes of the fracture
water will vary as the effective characteristic parameters vary. Regional variation of
parameter values within the aquifer will, therefore, impact on measured solute
concentrations, and the assumption of a homogenous aquifer may lead to misleading
results from simulations with the DP-Pulse model. Considering ASR injection and abstraction cycles on different timescales, the injected water will interact with different volumes of rock and so the characteristics of the 'homogenous aquifer' may vary. As a result, different injection and abstraction patterns will result in different calibrated parameter values.

To overcome this potential for error, the DP-Pulse model should be calibrated to data collected from ASR operations on a similar scale to that of the desired predictive simulations.

3. **The aquifer is fully confined.**

The DP-Pulse model described here assumes that the aquifer is fully confined and fully saturated. This will generally be the case for an ASR system as unsaturated aquifers tend to have greater piezometric gradients and hence more rapid natural groundwater flow.

If the aquifer is not fully confined, there is the potential that water table variations will lead to parts of the aquifer being temporarily partially saturated. In this scenario, the model will fail to correctly simulate the solute transport processes.

4. **There is no water movement in the rock matrix.**

If the matrix pore throats are small, the pore throat pressures required to generate significant flow are very great. As a result, movement of water within the matrix will remain small. Thus movement of solutes within the matrix through advective flow will be negligible relative to diffusive flow.

Chalk matrix pore throats vary from 0.012 to 100 μm in size, with a mean of 0.45 μm, and as such result in the chalk matrix having a hydraulic conductivity of between $1 \times 10^{-2}$ and $1 \times 10^{-5}$ m/day (Price et al., 1976). This can be compared with an overall hydraulic conductivity as measured in the field of between $1 \times 10^{-2}$ and $1.8 \times 10^{2}$ m/day (Allen and Price 1990; Price et al., 1976; Price et al., 1977; Price et al., 1982; Watson et al., 2000). As a result of this the majority of flow will be fracture flow.

5. **The fracture water remains locally at a uniform but changing concentration.**

The model assumes that the solute concentration of matrix pore water at the very edge of a matrix block is equal to the solute concentration of the water in the fracture:

$$C_m(x,\pm b, t) = C_f(x, t)$$

(12)
Where $C_m$ is the solute concentration in the matrix, $C_f$ is the solute concentration in the fracture, $x$ is the distance along the fracture and $t$ is the time from the start of the simulation.

This is generally likely to be true. Within each ‘cell’ of the model, the solute concentration in the fracture is assumed to remain at a uniform concentration. This assumption can be discussed in two dimensions, across the width of, and along the length of the fracture.

The model assumes that across the width of the fracture aperture the solute concentration is uniform (for example, in a horizontal fracture there will be little vertical variation in the solute concentration of the fracture water). As long as the fractures are narrow, diffusion and the mixing effect of advective dispersion resulting from flow within the fracture will ensure good mixing across the fracture and this assumption is realistic. In an aquifer with wide fractures, in which diffusion across the fracture will take a significant amount of time, this assumption will only hold if flow within the fracture is sufficiently turbulent to ensure mixing.

The assumption that the solute concentration along the length of the fracture, within a single cell, remains constant, is harder to justify. As the model simulates a changing solute concentration along a fracture (across a series of cells), it is clear that the solute concentration within the fracture along the length of a single cell cannot be uniform. This assumption needs to be examined in terms of the error implied for the model. This is undertaken in Section 3.6, which concludes that the interval between the pulses of flow needs to be selected with care, to ensure that the error arising from this assumption is not too great.

6. **Mechanical dispersion is negligible.**

The model assumes that the effects on solute concentration of mechanical dispersion are negligible. Mechanical dispersion is widely used in groundwater models to describe the dispersive effect of heterogeneous flow velocity within the aquifer, which is affected by many factors including tortuosity, ‘dead-end’ pore spaces and variable fracture apertures. Dispersion coefficients are derived empirically. The assumption that mechanical dispersion is zero clearly cannot be true, however it can be shown that, under certain conditions, the effects of double-porosity diffusion have a more significant effect on solute concentrations than dispersion.
The relative importance of double-porosity diffusion and mechanical dispersion is investigated more fully within Section 3.8, in which the validity of this assumption is tested.

7. **Movement of solutes within the matrix is described by Fick’s second law and is characterised by an ‘apparent’ diffusion coefficient.**

Fick’s first and second laws provide the basis on which the advection diffusion equation is constructed. Diffusion within the matrix is according to Fick’s second law:

\[
\frac{\partial C_m}{\partial t} = D_A \frac{\partial^2 C_m}{\partial z^2}
\]  

(13)

Diffusive exchange at the edge of the matrix block, i.e. diffusive exchange between the matrix and fracture waters is described by Fick’s first law:

\[
J_{\text{diff}} = -D_E \frac{dC}{dz}\bigg|_{z=b}
\]  

(14)

Where \( J_{\text{diff}} \) is the diffusive mass flux (per unit area of water and rock) in the \( z \) direction in saturated rock.

It is widely recognised that Fick’s second law suitably describes the movement of solutes by diffusion. As long as Fick’s second law describes all movement of solutes, i.e. that there is no movement of water in the matrix volume as previously assumed, this assumption is valid.

8. **Density effects on the flow are ignored.**

Flow occurring in an aquifer defined by long narrow fractures with relatively low connectivity is unlikely to be significantly affected by density effects. Previous work, discussed in Section 2.4, describes how, within a single porous medium, gravity can induce rotation of a saline/fresh water interface, leading to reduced recovery efficiencies during ASR operation. The impact of this assumption on the model has not been investigated. It is believed to be dependent on fracture geometry and connectivity, and therefore variable according to the characteristics of the system being simulated.

9. **Initially, the solute concentration through the matrix is uniform and at equilibrium with the local fracture water.**

The solute concentration of matrix waters throughout a matrix block at \( t = 0 \) are equal to a constant:

\[
C_m(x, z, 0) = C_{m0}
\]  

(15)
Where $C_{m0}$ is the concentration in the matrix at $t = 0$.

Taken with equation 12, equation 15 implies that at $t = 0$, the solute concentration of the fracture waters is also identical to the initial solute concentration of the matrix waters.

Although it is highly likely that water within the fracture network would be in equilibrium with the water at the surface of the matrix blocks (equilibrium will be reached in a matter of days in all but the largest fractures), the time required for a large matrix block to come to equilibrium can be of the order of years. If this assumption is not satisfied, the results from the DP-Pulse model will be misleading.

### 3.4. Mathematical description of the DP-Pulse model

The full mathematical development for the DP-Pulse model is described in Appendix IV; a simplified description is presented here. The conceptual model which was developed into the DP-Pulse model is relatively simple, however, due to the invariance with respect to flow geometry (discussed in Section 3.6) it can be difficult to illustrate. To simplify the model description we will examine a specific flow geometry: that of radial flow in a medium formed from slabs of matrix. Figure 3-2 illustrates the piecewise variation of the groundwater flow rates and solute concentrations injected into a well penetrating a confined fractured aquifer.

- $C_{in}$ is the solute concentration of the injected water;
- $Q$ is the flow rate of injection;
- $C_f$ is the solute concentration of the fracture water;
- $C_m$ is the solute concentration of the matrix water;
- $r$ is the radius from the well;
- $r_w$ is the radius of the well;
- $b$ is half the slab thickness;
- $z$ is the distance from the centre of the slab;
- $a$ is the fracture aperture;
- $t$ is the time.
Figure 3-2 Injection of water with varying solute concentrations and rates into a confined fractured aquifer.

Once conceived, the expression of the model is achieved using the standard advection-diffusion mass balance equation for flow through a fractured system. For the radial case this can be expressed:

\[
\frac{\partial C_f}{\partial t} + \frac{Q(t)}{2\pi r N_f} \frac{\partial C_f}{\partial r} = \frac{2D}{a} \frac{\partial C_m}{\partial z}_{z=b} \]

(16)

where \( N_f \) is the number of identical fractures along which flow occurs.

In order to obtain a solution to this equation, however, it is necessary to use a number of mathematical boundary conditions. Two simple boundary conditions describe the solute concentration of water entering the fracture network from the well, and from the distant aquifer. When water is being injected into the well, the solute concentrations of the fracture waters immediately adjacent to the well (i.e. at \( r = 0 \)) are equal to that of the injected water:

\[
C_f(r_0, t) = C_{in} \quad Q > 0
\]

(17)
At a long distance from the well (i.e. such a distance that no water injected into the
well has arrived) the solute concentrations in the fractures are identical to the initial
solute concentration of the matrix waters:
\[
\lim_{r \to \infty} C_f(r,t) = C_m(0)
\]
(18)

3.4.1. Model parameterisation

The model characterises the aquifer with two parameters. The parameters are the
ratio of matrix porosity to fracture porosity, \( \sigma \), and \( t_{cb} \), the ‘characteristic block
diffusion time’.

In terms of the particular model shown in Figure 3-1, the first parameter, \( \sigma \), is
described by equation 19:
\[
\sigma = \frac{2bD_E}{aD_A}
\]
(19)

Where \( D_E \) is the effective diffusion coefficient and \( D_A \) is the apparent diffusion
coefficient. If the retardation coefficient is assumed to be 1, a reasonable assumption
for conservative solutes, \( D_E \) and \( D_A \) are related as in equation 11. For the slab
geometry discussed here, the total matrix porosity volume is proportional to \( 2b\phi_0 \)
and the fracture geometry is proportional to \( a \).

The second parameter, \( t_{cb} \), is described by equation 20:
\[
t_{cb} = \frac{b^2}{D_A}
\]
(20)

\( t_{cb} \) can be regarded as the time taken for a matrix block to approach diffusive
equilibrium. (For blocks with shapes other than a slab, \( b \) is the ratio of block volume
to surface area in contact with the fracture system.)

A third parameter, the ‘characteristic fracture time’ is introduced:
\[
t_{cf} = \frac{t_{cb}}{\sigma^2}
\]
(21)

\( t_{cf} \) describes the time necessary for the fracture water to come to diffusive
equilibrium with an identical volume of matrix water, and can also be described by
equations 22 and 23.
\[
t_{cf} = \frac{a^2D_A}{4D_E^2}
\]
(22)
\[
t_{cf} = \frac{(a/2\phi_0)^2}{D_A}
\]
(23)
A second method of defining the characteristic times $t_{cf}$ and $t_{cb}$ is in terms of ‘half-times’. Figure 3-3-A illustrates the time taken for diffusion of solutes from an infinite matrix into a fracture. The matrix water has an initial solute concentration of $C$, while the fracture water has an initial solute concentration of 0. The time taken for diffusion of solutes to raise the solute concentration of a fracture to $C/2$ is equal to $t_{1/2} = 1.69 \, t_{cf}$. In Figure 3-3-B the diffusion of solutes from an infinite fracture with a fixed solute concentration of 0 into the matrix is described. The time taken to lower the mean solute concentration of the matrix from an initial solute concentration of $C$ to $C/2$ is equal to $t_{1/2} = 5.08 \, t_{cb}$. 
Figure 3-3 Visualising the characteristic times $t_{cb}$ and $t_{cf}$ as proportional to ‘half-times’.

At early times, when diffusion does not penetrate far into the matrix, the model behaviour is characterised by $t_{cf}$ alone, so only this parameter can be deduced from short-term tests. At later times both $t_{cb}$ and $\sigma$ are needed to characterise the system. As $t_{cb}$ and $t_{cf}$ describe diffusion times, they are not intrinsic to the aquifer, but vary according to the solute. $t_{cb}$ and $t_{cf}$ are inversely proportional to the free-water diffusion coefficient and the retardation coefficient of the solute as well as according to the aquifer characteristics. $\sigma$ is intrinsic to the aquifer.
3.4.2. Solution

The solution of equations 16 and 13 subject to the boundary conditions (equations 12, 17 and 18) and the initial conditions specified in equation 15 gives the concentration in the fracture in cell \( n \) at time \( t \):

\[
c^n(t) = c^n(0) + \sum_{i \in \{c \iff c_i \}} \Delta c_i^n G[(t - t_i) / t_{cb}, \sigma] \quad n = 1, \ldots, N
\]

(24)

where \( t_i \) is the time of movement (pulse time) and \( t_{cb} \) is the characteristic 'block' diffusion time (Section 3.6). (Other terms are explained below.) The full derivation of this solution was described by Fretwell (1999) and is repeated in Appendix IV.

Equation 24 shows that the solute concentration of the water in the fractures can be found by taking the solute concentration of the fracture water at \( t = 0 \) and adding the sum of all the changes of the solute concentrations in that fracture water, resulting from both advective flow \( (\Delta c_i^n) \) and diffusion \( (G(\tau, \sigma)) \), up until the time \( t \). The concentration jumps \( (\Delta c_i^n) \) given by equation 25 depend on the direction of flow relative to the well. When the velocity of flow within the fracture \( (v) \) is away from the well \( (v > 0) \), water flows from one cell, \( n-1 \), to the next, \( n \), but the solute concentration of that volume of water immediately either side of the pulse is identical. The change in solute concentration of the water within an individual cell \( (n) \) either side of a pulse interval, therefore, is the difference between the solute concentrations of the water in the previous cell \( (n-1) \) and the water in cell \( n \) immediately prior to the pulse interval. When the direction of the flow of the water within the fracture is reversed, water flows from the cell \( n+1 \) to the cell \( n \).

\[
\Delta c_i^n = \begin{cases} 
\lim_{t \to t_i} [c^{n-1}(t) - c^n(t)] & v > 0 \\
0 & v = 0 \\
\lim_{t \to t_i} [c^{n+1}(t) - c^n(t)] & v < 0
\end{cases}
\]

(25)

The Green's function, \( G(\tau, \sigma) \), describes the solute diffusion within the matrix block that results from the change in solute concentrations given by an instantaneous unit change in concentration in the fracture. The solution is given by an inverse Laplace transform:

\[
G(\tau, \sigma) = \begin{cases} 
L^{-1}\left\{ p^{-1} \left[ \frac{1}{1 + \sigma B(\sqrt{p})} \right] \right\} & \tau \leq 0 \\
L^{-1}\left\{ p^{-1} \left[ \frac{1}{1 + \sigma B(\sqrt{p})} \right] \right\} & \tau > 0
\end{cases}
\]

(26)

\( p \) is the transform variable;
\( \tau \) is equal to \( t / t_{cb} \);
B is the Block Geometry Function (BGF), which describes the block/fracture geometry, and is described in Section 3.5.

3.4.3. Pulsed flow

The formulation of the model requires that the velocity be divided into a series of discrete pulses. Each pulse occurs at the beginning of a pulse interval (\(\Delta T\)). These need not be equally spaced in time, but are assumed to be so in this work. If there is groundwater flow occurring then, at the start of the pulse interval, water will pass instantaneously from one cell to the next, then, during the period of the pulse interval, diffusive exchange between the fracture and matrix waters will occur. This pulsed velocity is, of course, an approximation of the continuous groundwater flow of reality, and it is here that one of the sources of error in the model arises. The potential magnitude of this error will be discussed in Section 3.6.

3.5. Block Geometry Functions

Within the DP-Pulse model, the block/fracture geometry is described by the Block Geometry Function (BGF). This function can characterise the fracture geometry, for example as a series of slabs or a series of spheres (Barker, 1985a, 1985b). The fracture geometry can also be characterised as being a mixture of different proportions of different geometries (Barker, 1985a, Barker et al., 2000).

![Figure 3-4](image)

A - Slab Geometry  B - Sphere Geometry

C - Mixed Sphere Geometry

Figure 3-4 Different block/fracture geometries described by the Block Geometry Function (BGF)
The DP-Pulse model currently allows the selection of a slab geometry (Figure 3-4A, equation 27), a sphere geometry (Figure 3-4B, equation 28) or a mixture of either slabs or spheres of different sizes (Figure 3-4C, equations 29 and 30).

The BGF solutions include:

Slab geometry

\[ B(x) = \left( \frac{\tanh x}{x} \right) \]  

(27)

Sphere geometry

\[ B(x) = \left( \frac{\coth x}{x} - \frac{1}{3x^2} \right) \]  

(28)

Mixed block geometries

\[ B(x) = \sum_{i=1}^{N} \int_{0}^{\infty} p_i(\beta) B_i \left( \frac{xf}{b} \right) d\beta \]  

(29)

\[ \frac{1}{b} = \sum_{i=1}^{N} \int_{0}^{\infty} \frac{p_i(\beta)}{\beta} d\beta \]  

(30)

Where \( p_i(\beta) \) \( d\beta \) is the proportion by volume of the composite block mixture occupied by blocks of shape \( i \) \((i=1,...,N_i)\) in the size (volume to area) range \( \beta \) to \( \beta + d\beta \) and \( b \) is the characteristic length (block volume/surface area). In the slab geometry \( b \) is equal to half the thickness of a slab, while in a sphere geometry \( b \) is equal to one-third of the radius of the sphere.

Further geometries (Barker, 1988, Barker et al., 2000) include:

- An infinite cylinder
  \[ I_1(2x)/xI_0(2x) \]  

(31)

- Sphere of dimension \( n \)
  \[ I_{n/2}(nx)/xI_{n/2-1}(nx) \]  

(32)

\( I_n \) = modified Bessel function

These final two functions are rather more complex to evaluate, and will not be used within this thesis.

### 3.6. Model invariance to flow geometry and flow rate

The model assumes that the effects of dispersion are negligible with respect to those of diffusion. As a result there is no dispersive term in the model formulation. One result of this is that as long as the relative rates of flow are the same, the model is invariant to either flow velocity or flow geometry.
By definition, the cells each have the same mobile fracture volume, i.e. the fracture volume of each cell is the same, and the ratio of mobile to ‘dead end’ fractures is the same. If we consider a number of different flow geometries, it is possible to visualise flow as being 1D linear or radial. In the linear case water flows in a series of pulses from one cell to another (Figure 3-5a). In the radial case flow passes radially out from a central point (Figure 3-5b). In the extreme case, the flow may be anisotropic in 3 dimensions (Figure 3-5c). In each scenario the cells are of identical volume, if not shape.

This invariance to flow geometry is extremely important as it allows the model to be applied to many scenarios with relative simplicity. If the only known solute concentrations in the system are the initial solute concentration in the fracture and matrix, and the solute concentration of water injected and abstracted through the single well, it is not necessary to state the flow geometry of the model. This invariance also means that a lack of knowledge of the actual geometry of the flow system does not prevent satisfactory application of the DP-Pulse model.

![Figure 3-5 DP-Pulse model invariance to flow geometry](image)

Although each cell has an identical fracture volume, the absolute volume is not specified. This volume may be considered to be that required to hold the quantity of water that is injected or abstracted during one pulse interval. Increasing the pumping rate will increase the absolute size of the cells, but within the formulation of the DP-Pulse model the cell size is not specified. As long as the pumping rate, and therefore cell size, is consistent, the model is invariant with respect to that pumping rate.
It should be emphasised that this invariance to flow geometry only applies to concentrations at the injection/pumping well. Away from the well (for example at an observation well) the model is not invariant with respect to flow geometry.

3.7. **Analysis of the error resulting from the pulse interval**

The DP-Pulse model does not simulate a continuous flow velocity, but rather moves the water from one cell to the next with a series of instantaneous pulses of flow, separated by a pulse interval. Errors may arise during the simulation as a result of this discretisation of velocity, which is performed as an essential operation during the model calculations. It is this discretisation that allows the simplification of the code to produce a semi-analytical model, but also raises the potential for error. In order to have confidence in the model, it is necessary to be confident in the size limits on the time step that will maintain reasonable accuracy. The error analysis will be completed for three scenarios. Firstly, the case where $t_{cb}$ is large compared to the simulated duration, will be examined. The second case is a special case of the first scenario, where $t_{cb}$ is infinite. The final scenario is one where $t_{cb}$ is less than the simulated model duration, or as $t_{cb}$ tends to zero.

3.7.1. **Finite matrix case – $t_{cb}$ is large**

We can visualise the error arising in the DP-Pulse through the discretization of the velocity by comparing the two possible limits on the case of a solute concentration pulse with a duration of a single pulse interval. We can put these pulses through a simple 1-dimensional model describing a single fracture through a porous matrix - the simplest double-porosity system. The pulse could either be an instantaneous input of the entire quantity of solute (Case I – the delta input function), or a continuous input of the solute over the period of the pulse interval (Case II – the ‘top hat’ input function). Case II approximately represents the situation described by the DP-Pulse model, in which the pulse interval is analogous to the period over which solute input occurs, $T$. Case I describes the possible scenario that is most different to the DP-Pulse model. If the DP-Pulse model attempted to simulate a delta input function, the resultant input would be similar to Case II. Comparison of the solute curves resulting from each of these models will provide an estimate of the possible error that may occur as a result of the DP-Pulse model formulation. The two solute input cases are illustrated in Figure 3-6 along with the probable breakthrough curve.
Figure 3-6 Two input cases for the DP-Pulse model error analysis, along with their predicted breakthrough curves.

The pulse is passed through a simple double-porosity system (Figure 3-7). We can then compare the two breakthrough curves, find the difference between the two breakthrough curves at the maximum of and relative to the value of Case I, and define this as the error.

Figure 3-7 Model for the finite matrix error analysis

First, we need to define the input functions.

Case I – The delta function

\[ C_0^I(t) = \frac{M}{VA} \delta(t) \quad (33) \]

Case II – The ‘top hat’ function

\[ C_0^{II}(t) = \frac{M}{VA\Delta T} \quad 0 < t < \Delta T \quad (34) \]

Then the equation for solute diffusion across the matrix block, as well as the boundary conditions must be defined. Restating Ficks’ second law:

\[ \frac{\partial C_m}{\partial t} = D_A \frac{\partial^2 C_m}{\partial z^2} \quad (35) \]
Three boundary conditions are applied. The first, analogous to equation 12, ensures that the solute concentration of matrix pore water at the very edge of a matrix block is equal to the solute concentration of the water in the fracture:

\[ C^m(x, b, t) = C_f(x, t) \]  \hspace{1cm} (36)

The initial solute concentration of the matrix is zero:

\[ C^m(x, z, 0) = 0 \]  \hspace{1cm} (37)

Solute concentrations about the centre of the matrix block are symmetrical:

\[ C^m(x, z, t) = C^m(x, -z, t) \]  \hspace{1cm} (38)

We need to define the equation for advective flow through the fracture as well as solute diffusion between the matrix and fracture waters. Restating the advection-diffusion equation described in equation 16.

\[ \frac{\partial C_f}{\partial t} + V \frac{\partial C_f}{\partial x} = \frac{2D}{a} \frac{\partial C_m}{\partial z} \]  \hspace{1cm} (39)

With the boundary conditions ensuring that the solute concentration in the fracture waters adjacent to the source (i.e. at \( r = 0 \)) is equal to the input function (either Case I or Case II):

\[ C_f(0, t) = C_0(t) \]  \hspace{1cm} (40)

The solute concentration in the fracture water at \( t = 0 \) is zero:

\[ C_f(x, 0) = 0 \quad x > 0 \]  \hspace{1cm} (41)

And, where the advective front has not reached, the solute concentration of the fracture water is also zero:

\[ \lim_{z \to -\infty} C_f(x, z) = 0 \]  \hspace{1cm} (42)

Finding a solution through the use of Laplace transformation:

\[ \tilde{f}(p) = \int_0^\infty e^{-pt} f(t) dt \]

Take the Laplace transform of Ficks' second law (equation 35, using 37):

\[ \frac{d^2 \overline{C_m}}{dz^2} = \frac{P}{D_a} \overline{C_m} \]  \hspace{1cm} (43)

Using equations 36 and 38 we obtain:

\[ \overline{C_m} = \frac{C_f \cosh(\lambda z)}{\cosh(\lambda b)} \]  \hspace{1cm} (44)
where

\[ \lambda^2 = \frac{P}{D_A} \]  

(45)

This gives us

\[ \left. \frac{\partial C_x}{\partial Z} \right|_b = C_f \lambda^2 b B(\lambda b) \]  

(46)

Where

\[ B(x) = \frac{\tanh x}{x} \]  

(47)

Take the Laplace transformation of the advection-diffusion equation (equation 39), using 41 and 46:

\[ pC_f + V \frac{dC_f}{dx} = \frac{2D_b}{a} C_f \lambda^2 B(\lambda b) \]  

(48)

\[ \frac{dC_f}{dx} = -\mu C_f \]  

(49)

where:

\[ \mu = \frac{P}{V} \left[ 1 + \sigma B(\sqrt{ptcb}) \right] \]  

(50)

and use has been made of

\[ \lambda^2 b^2 = pt_{cb} \]  

(51)

Solution of 49, using 40 and 38

\[ \overline{C_f} = C_{f0} \exp(-\mu \alpha) \]  

(52)

If we then apply the two input functions (Cases I and II)

Case I

\[ C_{f0}'(t) = \frac{M}{Va} \delta(t) \]  

(33)

\[ \overline{C_{f0}'} = \frac{M}{Va} \]  

(53)

\[ \overline{C_f'} = \frac{M}{Va} \exp[-\mu \alpha] \]  

(54)
Case II

\[ C_{f0}^{II}(t) = \frac{M}{Va\Delta T} \delta(t) \]  
\[ \bar{C}_{f0}^{II} = \frac{M}{Va\Delta T} \frac{1}{p} \]  
\[ \bar{C}_{f}^{II} = \frac{M}{Va\Delta T} \left(1 - e^{-\rho \Delta T}\right) \exp\left(\frac{-\mu x}{p}\right) \]  

We can then compute:

\[ \Delta C_f = \bar{C}_{f}^{II} - \bar{C}_{f}^{I} \]  

For computational purposes it is convenient to define the following Laplace-transform functions:

\[ \overline{G^I}(p,\alpha) = \exp\left[-\alpha p \sqrt{p}\right] \]  
\[ \overline{G^II}(p,\alpha) = \frac{1}{p} \exp\left[-\alpha p \sqrt{p}\right] \]  

where:

\[ \alpha = \frac{\sigma a}{t_{eb}} \]  

in which the advection time, \( t_a \), is given by:

\[ t_a = \frac{x}{V} \]  

Then the required concentrations are found in terms of the inverses of these functions as:

\[ C_{F}^{I}(t) = \frac{M}{Vat_{eb}} \overline{G^I} \left(\frac{t-t_a}{t_{eb}},\alpha\right) \]  

and

\[ C_{F}^{II}(t) = \frac{M}{Vat} \left[ \overline{G^II} \left(\frac{t-t_a}{t_{eb}},\alpha\right) - \overline{G^II} \left(\frac{t-t_a - \Delta T}{t_{eb}},\alpha\right) \right] \]  

3.7.2. Results of the finite matrix error analysis — specifying time, \( T \), and varying travel distance, \( x \).

Initially we will examine the error that occurs in a specific system as a result of the discretisation of the velocity. Using the two analytical solutions describing different pulses, one, Case I, a ‘top hat’ function (equation 62) and the other, Case II, a delta
function (equation 63), will be passed through identical systems. The only variation will be the duration, \( T \), of Case II. \( T \) can be considered as analogous to \( \Delta T \), the pulse interval used in the DP-Pulse model. 

\( \tau_{eb} \) was specified as 1000 days, and \( \sigma \) as 50. A total solute mass of 1 kg was passed through a fracture aperture of 0.005 m in which water with a solute concentration of zero flows at a velocity of 1 m/d for 100 days. Figure 3-8 shows the solute concentration along the fracture after 100 days, after the solute was input using both a delta input function and a ‘top hat’ input function with \( T \) values of 10 and 20 days.

![Figure 3-8 Solute concentration in a fracture, according to two analytical solutions (Equations 62 and 63), 100 days after injection of 1 kg solute into a finite matrix system (\( \tau_{eb} = 1000 \text{ days}, \sigma = 50, \text{fracture aperture} = 0.005 \text{ m}, \text{velocity} = 1 \text{ m/d}).

Clearly the two curves are different, most notably near the maximum solute concentration. In Case I, the maximum solute concentration, 0.53 kg/m\(^3\), occurs 8.9 m from the point of injection. Comparing this with the equivalent solute concentrations obtained with Case II, we can see that increasing \( T \) increases the difference between the different modelled input functions. This difference may be used as a measure of the error resulting from the description of an instantaneous pulse of solute (Case I) with a pulse of specified length (Case II). As the two different input functions were selected to describe the two ‘end member’ possibilities of the DP-Pulse model, we may also surmise that increasing the pulse interval, \( \Delta T \), in the DP-Pulse model, i.e. the period between pulses of flow, will increase the error in
the DP-Pulse model. In this scenario the error, relative to the Case I solution, arising from a $T$ of 10 days is 4.9%, while that resulting from the use of a $T$ of 20 days is 5.7%.

Using this method of analysis, it is possible to determine the maximum acceptable value of $\Delta T$ that may be used in the DP-Pulse model, to maintain the peak solute concentration within a certain level of error. By specifying the maximum allowable error, we can increase the value of $T$ until a suitable difference between the Case I solution and the Case II solution is found.

This may then be repeated for different values of $t_{cb}$ and $\sigma$, and then plotted as a contour plot. (The range used to produce for these contour plots is chosen to approximately correspond with that used in contour plots later within this thesis.)

![Contour plot](image)

**Figure 3-9** Contour plot illustrating the variation in maximum acceptable $T$ required to produce a 1% difference between Case I and Case II solutions after 100 days for different $t_{cb}$ and $\sigma$ values ($v = 1$ m/d, $a = 0.01$ m).

Figure 3-9 illustrates the variation with $t_{cb}$ and $\sigma$ in the $T$ that will produce a difference of 1% between the Case I and Case II solutions with $t = 100$ days, $v = 1$ m/d and $a = 0.01$ m. The maximum acceptable value of $T$ varies between 0.25 days and 0.45 days. The value is almost entirely insensitive to $\sigma$, and only sensitive to $t_{cb}$ within the region $t_{cb} = 100 - 1000$ days.
Figure 3-10 Contour plot illustrating the variation in maximum acceptable $T$ required to produce a 1% difference between Case I and Case II solutions after 50 days for different $t_{cb}$ and $\sigma$ values ($v = 1$ m/d, $a = 0.01$ m).

Figure 3-10 illustrates a similar system, but with a $t$ of only 50 days. The maximum acceptable $T$ values vary between 0.12 and 0.22 days, approximately half that of the system where $t = 100$ days.

Comparison of Figure 3-9 and Figure 3-10 shows that if the simulated duration is longer, the maximum acceptable value of $T$ is larger. This is important as it suggests that DP-Pulse models simulating long time periods may be completed with increased $\Delta T$ values, and hence reduced model size, without unacceptably impairing model accuracy.
Figure 3-11 Contour plot illustrating the variation in maximum acceptable $T$ required to produce a 5% difference between Case I and Case II solutions after 100 days for different $t_{cb}$ and $\sigma$ values ($v = 1$ m/d, $a = 0.01$ m).

Figure 3-11 shows how a system ($v = 1$ m/d, $a = 0.01$ m, $t = 100$ days) with a greater allowable error (5%) can have much larger values of $T$ (between 10 and 25 days). Preliminary investigations in which accuracy may be less important than the identification of trends could therefore be completed with very small, and hence rapidly run, models.
Figure 3-12 Contour plot illustrating the variation in maximum acceptable $T$ required to produce a 1% difference between Case I and Case II solutions after 100 days for different $t_{cb}$ and $\sigma$ values ($\nu = 1$ m/d, $a = 0.005$ m).

Figure 3-12 illustrates the effect of decreasing the fracture aperture to 0.005 m ($\nu = 1$ m/d, $t = 100$ days). There is little difference between this figure and Figure 3-9, indicating that the error is insensitive to the fracture aperture.

Figure 3-13 Contour plot illustrating the variation in maximum acceptable $T$ required to produce a 1% difference between Case I and Case II solutions after 100 days for different $t_{cb}$ and $\sigma$ values ($\nu = 2$ m/d, $a = 0.005$ m).
Figure 3-13 illustrates the effect of increasing the flow velocity to 2 m/d \((a = 0.01 \, \text{m}, \, t = 100 \, \text{days})\). Again, there is little difference between this figure and Figure 3-9, indicating that the error is insensitive to the flow velocity.

In summary:

- The error introduced with changing values of \(T\) is relatively insensitive to \(\sigma\);
- The same error is insensitive to the fracture aperture and the flow velocity;
- Increasing the maximum acceptable error allows large increases in the size of \(T\);
- Increasing the duration simulated by the model enables a larger \(T\) to be selected while maintaining an acceptable error on solute concentrations at times near the end of the simulation.

### 3.7.3. Infinite matrix case – \(t_{cb}\) is infinitely large

A special case of the above error analysis is the infinite matrix case. This would be suitable for application where the total duration of the model is small compared to \(t_{cb}\). The advantage to this case is the fact that the result is analytical.

The model in the infinite matrix case is little different from that in the finite matrix case (Figure 3-14).

**Figure 3-14 Model for the infinite matrix error analysis**

In the infinite matrix case we need to change one of the boundary conditions describing fracture concentrations in the matrix block. Equation 38 is replaced by equation 64, specifying that the solute concentrations of the matrix waters at a distance from the fracture waters such that no diffusive solute exchange has occurred will be 0:

\[
\lim_{z \to \infty} C_m(x, z, t) = 0
\]  

\((64)\)
Solving equation 43 by the method of Laplace transformation, using 36 and 64 gives equation 65:

\[
\overline{C_m} = \overline{C_f} \exp\left(-z\sqrt{\frac{p}{D_A}}\right) \tag{65}
\]

\[
\frac{d\overline{C_m}}{dz} = -\frac{p}{D_A} \overline{C_f} \tag{66}
\]

Take Laplace transformation of 39, using 41 and 66:

\[
-pc_f + V \frac{d\overline{c_f}}{dx} = \frac{2D_E}{a} \left(-\frac{p}{\sqrt{D_A}}\right) \overline{C_f} \tag{67}
\]

\[
\frac{d\overline{C_f}}{dx} = -\mu \overline{C_f} \tag{68}
\]

where

\[
\mu = \frac{1}{V} \left(p - \frac{2D_E}{a\sqrt{D_A}}\sqrt{p}\right) \tag{69}
\]

Solution of 68, using 40 and 42:

\[
\overline{C_f} = \overline{C_o} \exp(-\mu x) \tag{70}
\]

\[
= \overline{C_o} \exp(-pt_a) \exp\left(-\frac{t_a}{\sqrt{t_{cf}}}\sqrt{p}\right) \tag{71}
\]

where

\[
t_a = \frac{x}{V} \tag{72}
\]

and

\[
t_{cf} = \frac{(aD_A/2D_E)^2}{D_A} = \frac{(a\phi/2)^2}{D_A} \tag{73}
\]

Case I

\[
C_o'(t) = \frac{M}{Va} \delta(t) \tag{74}
\]

\[
\overline{C_o'} = \frac{M}{Va} \tag{75}
\]

Using

\[
L^{-1}\left\{e^{-a\sqrt{p}}\right\} = \frac{a}{2\sqrt{\pi^3}} e^{-a^2/4t} \tag{76}
\]

\[
C_f' = \frac{M}{Va} \frac{t_a}{\sqrt{4\pi\phi(t-t_a)^2}} \exp\left[\frac{-t_a^2}{4t_{cf}(t-t_a)}\right] \tag{77}
\]

\[
98
\]
\[
\frac{M}{V a t_{cf}} \frac{t_a/t_{cf}}{\sqrt{4\pi(t/t_{cf} - t_a/t_{cf})}} \exp\left[ \frac{-\left(t_a/t_{cf}\right)^2}{4(t/t_{cf} - t_a/t_{cf})} \right] 
\]

(76)

\[
\frac{M}{V a t_{cf}} \frac{\alpha}{\sqrt{4\pi(\tau - \alpha)^3}} \exp\left[ \frac{-\alpha^2}{4(\tau - \alpha)} \right] 
\]

(77)

where

\[ \tau = \frac{t}{t_{cf}} \]

(78)

\[ \alpha = \frac{t_a}{t_{cf}} \]

(79)

\( C_f \) is at maximum when \( \frac{\partial C_f}{\partial t} = 0 \) giving:

\[ \tau_{\text{max}} = \frac{\alpha(\alpha + 6)}{6} \]

(80)

\[ C_f(\tau_{\text{max}}) = \frac{M}{V a t_{cf}} \frac{3}{\alpha^2} \sqrt{\frac{6}{\pi e^3}} \approx \frac{M}{V a t_{cf}} 0.925 \]

(81)

Case II

We can decompose Case II into two solutions, one indicating a step up in concentration (Case IIA) and the other giving a step down in concentration (Case IIB). When summed, these two cases will give the ‘top hat’ shape of Case II.

Case IIA:

Using

\[ L^{-1}\left\{ \frac{1}{p} e^{-a\sqrt{p}} \right\} = \text{erfc}\left( \frac{a}{2\sqrt{t}} \right) \]

For \( t > t_a \)

\[ C_f^{\text{IIA}} = \frac{M}{V a \Delta T} \text{erfc}\left( \frac{t_a/\sqrt{t_{cf}}}{\sqrt{4(t - t_a)}} \right) \]

(82)

Case IIB

For \( t > t_a + \Delta T \)

\[ C_f^{\text{IIB}} = -\frac{M}{V a \Delta T} \text{erfc}\left( \frac{t_a/\sqrt{t_{cf}}}{\sqrt{4(t - \Delta T - t_a)}} \right) \]

(83)

Combining

For \( \tau > \eta + \alpha \)

\[ C_f^{\eta} = \frac{M}{V a t_{cf}} \frac{1}{\eta} \left[ \text{erfc}\left( \frac{\alpha}{\sqrt{4(\tau - \alpha)}} \right) - \text{erfc}\left( \frac{\alpha}{\sqrt{4(\tau - \eta - \alpha)}} \right) \right] \]

(84)
where
\[ \eta = \Delta T / t_{cf} \]  
\[ \alpha = t_a / t_{cf} \]  

Having determined the maximum point on the breakthrough curve of Case I (equation 81) we can determine the solute concentration at this time and distance for Case II from equation 84 and so find the relative error:

\[ E(\tau, \alpha, \eta) = \frac{C_f^{(\tau, \alpha)} - C_f^{(\tau, \alpha, \eta)}}{C_f^{(\tau, \alpha)}} \]  

where, from 80:
\[ \tau = \tau_{max} = \alpha(\alpha + 6)/6 \]  

If we specify that the error should be 10%, we find that by solving equation 89 we get a solution in terms of the pulse interval, \( T \), the total advection time, \( t_a \), and the characteristic fracture time, \( t_{cf} \) (equation 90). This solution will give us a limit on the size of the pulse interval that will ensure the relative error is never greater than 10%.

\[ E(\tau_{max}, \alpha, \eta) = \frac{1}{10} \]  

\[ \frac{\alpha^2}{\eta} = 12.259 \]  

or

\[ \frac{\alpha}{\eta} = 12.259/\alpha \]  

\[ \frac{\alpha}{\eta} = \frac{t_a}{\Delta T} \]  

Simply put, if \( T \) is the pulse interval (i.e. the residence time in one cell), the total number of cells, \( N \), traversed in time \( t_a \), the advection time, is given by \( N = t_a/T \). To ensure that the relative error in solute concentrations arising from the discretization of time is less than 10%, we need to ensure that:

\[ N > 13t_{cf}/t_a \]  

Similarly, if we want an error of less than 1%, we find that:

\[ E(\tau_{max}, \alpha, \eta) = \frac{1}{100} \]  

gives
\[
\frac{\alpha^2}{\eta} = 32.96 \quad (95)
\]

Therefore, to ensure a relative error of less than 1% error, we need to ensure that
\[N > 33t_{cb}/t_a \quad (96)\]

The minimum pulse interval indicated by the infinite matrix error analysis is significantly larger than that indicated by the finite matrix solution. It is important, therefore, to apply the finite matrix solution if required.

### 3.7.4. Analysis of the error resulting from the pulsing when \( t_{cb} \) is small.

The error analysis carried out in Section 3.7.1 accounts for the potential error arising from the discretisation of the flow velocity when the period simulated by the model is less than \( t_{cb} \). The special case, describing a system with an infinite thickness of matrix block (Section 3.7.3), characterises the error in a system where the simulated duration is significantly less than \( t_{cb} \).

As \( t_{cb} \) becomes smaller (smaller blocks and denser fractures), or the simulated period increases, the characteristic block time will become small relative to the simulated period. In this situation, the main function describing the double-porosity behaviour: \([l + \sigma \cdot B(0)t_c] \) (from equation 26) tends to \((l + \sigma)\) since \(B(0) = 0\) (equation 27).

Therefore, equilibrium between the fracture and matrix water is reached instantaneously, and the solute transport mechanism described is effectively identical to advective flow through a single porosity.

The discretisation of time in the model formulation, however, results in the model behaving in a different manner. Equilibrium will be reached during a single pulse interval, then the fracture water will pulse through the system, coming into contact with matrix water with which it is not in equilibrium.

To illustrate this, we will consider the situation of a finite pulse of solute passing through a system.

In the first case (Figure 3-15a), illustrating the ideal behaviour of a double-porosity model, the solute pulse will travel through the system without change, as the model does not include dispersion and the fracture water is in constant equilibrium with the matrix water.

In the second case (Figure 3-15b), illustrating the behaviour modelled by DP-Pulse, the solute pulse, here illustrated as having the same length as one cell of the model is in equilibrium with the matrix, until the start of the next time step. At this point, the solute pulse in the fracture is displaced by one cell, from cell A to cell B. The matrix
in cell A is therefore not in equilibrium with the fracture, and the fracture is not in equilibrium with cell B. As a result, numerical dispersion can be said to occur when $t_{cb}$ is small.

This dispersion will occur with increasing $\Delta T$ and reducing $t_{cb}$.

\[
\begin{align*}
  & t_a = t_0 & & t_a = t_0 + \Delta T \\
  & \text{Fracture} & & \text{Fracture} \\
  & \text{Matrix} & & \text{Matrix} \\
  & \text{Flow direction} & & \text{Flow direction} \\
  \hline
  & A & B & A & B \\
  & \text{Fracture} & & \text{Fracture} \\
  & \text{Matrix} & & \text{Matrix}
\end{align*}
\]

Figure 3-15 Comparison of true double-porosity behaviour when $t_{cb} = 0$ days, and behaviour simulated by the DP-Pulse model. (a = true double-porosity behaviour; b = behaviour simulated by the DP-Pulse model.)

In order to illustrate both this effect, and to quantify how large $\Delta T$, and how small $t_{cb}$ must be for this numerical dispersion to have a significant control on the solute concentration changes simulated by the model, a scenario was picked, and modelled with varying $t_{cb}$ and $\Delta T$ values. This was repeated for different values of $\sigma$. Figure 3-16 and Figure 3-17 illustrate the solute concentrations close to the well at the end of an ASR cycle, indicating how varying the pulse interval affects simulated solute concentrations. Furthermore, it is apparent from these figures that for $t_{cb} > 10$ days, the simulation is insensitive to $\Delta T$ for $\Delta T < 1$ day.
Figure 3-16 Changes in solute concentration simulated by the DP-Pulse model resulting from varied time step, ΔT, when $t_{cb}$ is small. ($\sigma = 20$; Cycle = 100 days injection, 100 days storage, 100 days abstraction.)

Figure 3-17 Changes in solute concentration simulated by the DP-Pulse model resulting from varied time step, ΔT, when $t_{cb}$ is small. ($\sigma = 50$; Cycle = 100 days injection, 100 days storage, 100 days abstraction.)
3.7.5. Guidelines on the selection of $\Delta T$

The last sections have identified the error that results from the discretisation of velocity, and that is therefore dependent on the pulse interval $\Delta T$. In order to ensure that the error that arises is minimised, careful selection of $\Delta T$ is required. The infinite matrix special case indicated that when

$$N > \frac{33t_e}{t_a} \quad (96)$$

The difference between the two input cases was less than 1%. This, therefore, provides a good start point for the selection of $\Delta T$. This $\Delta T$ will be suitable for initial exploratory simulations, and for simulations where $t_a$ is significantly smaller than $t_{cb}$.

Subsequent $\Delta T$ selection should be made through the process described for the finite matrix case (see sections 3.7.1 and 3.7.2). The application of a similar algorithm can be used to determine the largest acceptable value of $\Delta T$ for use in simulation of a specific system. This value is, however, more complex to obtain.

Finally, the sensitivity of the model to $\Delta T$ should be examined by running simulations with $\Delta T$ set at half, or double, the selected value. If the model output changes significantly, the selected $\Delta T$ is too large.

It should be remembered that while the selection of a small $\Delta T$ reduces possible error (resulting from the discretisation of velocity), a small $\Delta T$ can considerably increase the time taken for a single model run, and therefore a compromise may have to be made.

3.8. Relative importance of double-porosity diffusion and mechanical dispersion

The assumption was made that mechanical dispersion in the fractures is negligible in comparison with the dispersive effects of matrix diffusion. We now investigate the conditions under which that will be valid.

Consider a pulse input with a positive solute concentration to a one-dimensional linear system (i.e. flow along a single fracture) with a solute concentration of zero. We can, for a given distance from the source, compare the maximum concentrations given by the double-porosity and the advection-dispersion models. This gives an 'effective dispersivity' for the double-porosity model. This effective dispersivity is the dispersivity that would be required to reproduce the solute concentration curve in a single porosity system, i.e. entirely through mechanical dispersion. Given that dispersivity is normally only a fraction of the distance travelled (Peaudecerf and
Sauty, 1978) – typically one-tenth of that distance – we can reasonably adopt the
criterion that mechanical dispersion is negligible if the effective dispersivity is
greater than the distance travelled.

We start by considering the situation where the time of travel is small when
compared to the time for diffusion across a matrix block. Under these conditions the
double-porosity model reveals a simple analytical solution for an instantaneous
injection of solute at the origin:

\[
\begin{align*}
c_f^1(x,t) &= \frac{m \tau_a}{vt_{cf} \sqrt{4\pi(\tau - \tau_a)}} \exp \left[ - \frac{\tau_a^2}{4(\tau - \tau_a)} \right] \\
\end{align*}
\]

where

\[
\begin{align*}
\tau &= t / t_{cf} \\
\tau_a &= t_a / t_{cf}
\end{align*}
\]

and \( m \) is the mass injected per unit area of the fracture. This function has a
maximum of

\[
\begin{align*}
c_f^1_{\text{max}} &= \frac{m}{vt_{cf}} \sqrt{\frac{54}{\pi e^3}}
\end{align*}
\]

when

\[
\begin{align*}
\tau &= \frac{\tau_a (\tau_a + 6)}{6}
\end{align*}
\]

We can compare this solution with that representing simple advection dispersion in
the fractures (with no diffusion into the matrix):

\[
\begin{align*}
c_f^2(x,t) &= \frac{m}{\sqrt{4\pi Dt}} \exp \left[ - \frac{(x - vt)^2}{4Dt} \right]
\end{align*}
\]

An adequate approximation, for current estimation purposes, to the maximum over
time of equation 102 is:

\[
\begin{align*}
c_f^2_{\text{max}}(x,t) &= \frac{m}{\sqrt{4\pi Dt}}
\end{align*}
\]

where

\[
\begin{align*}
t &= x / v = t_a
\end{align*}
\]

We now introduce an 'effective' dispersivity, \( \alpha_{\text{eff}} = D / \nu \), which makes the two
maximum concentrations the same:
As previously stated, dispersivity is normally only a fraction of the distance travelled – typically one-tenth of that distance – we can therefore adopt the criterion that mechanical dispersion is negligible if the effective dispersivity is greater than the distance travelled \((\alpha_{\text{eff}}/x > 1)\). This leads to:

\[
t_a > t_{cf} \sqrt{\frac{e^3}{216}} \approx 3t_{cf}
\]

(106)

In summary, dispersion is negligible with respect to diffusion as long as the criteria in equation 107 are fulfilled.

\[
3t_{cf} < t_a < t_{cb}
\]

(107)

Although fulfilment of the criteria in equation 107 will ensure that dispersion is negligible, they may not be necessary. This thesis has not attempted to examine the scenario where \(t_a\) approaches \(t_{cb}\) or is large; in the latter case dispersion cannot be ignored.

From Table 3-1 we see that \(t_{cf}\) will rarely be larger than 5 days while advection times of interest will normally be much larger than 3 times that amount (15 days). As a result, fulfilment of the stated criteria should not be limiting to application of the model.

Table 3-1 Characteristic fracture diffusion time \((t_{cf}, \text{in days})\) as a function of fracture aperture and porosity, \(\phi_D\). (For \(D_x = 3 \times 10^{-10} \text{ m}^2/\text{s}\).)

<table>
<thead>
<tr>
<th>Aperture (mm)</th>
<th>'Diffusion' porosity, (\phi_D)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.1</td>
</tr>
<tr>
<td>0.1</td>
<td>0.01</td>
</tr>
<tr>
<td>0.5</td>
<td>0.24</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>24</td>
</tr>
<tr>
<td>10</td>
<td>96</td>
</tr>
</tbody>
</table>

### 3.9. Model verification

#### 3.9.1. Verification: Selection of models for comparison

In order to determine whether DP-Pulse is capable of correctly simulating a double-porosity system, it is necessary to verify the model, i.e. check that the model is solving the correct transport equations. A common way of doing this is to compare
the model with another model, which is known to be well tested. If the two models
behave in a similar way under identical conditions, this provides good evidence that
both models are simulating the same processes, and that the algorithms forming the
model in question have been correctly coded.

The selection of the model for comparison is important as the model should not only
represent the same system as the DP-Pulse code, but should be similar in the
purposes of the application. The DP-Pulse model is designed to provide a simple
tool that may easily and rapidly represent a double-porosity system through the use
of a novel parameterisation. The DP-Pulse model is not designed to simulate the
hydraulic pressure changes that occur, nor to simulate non-conservative ion transport
within the aquifer.

The DP-Pulse code predictions were compared with those of a similar simpler code:
DP1D (version 3). This code is capable of simulating a number of processes that
DP-Pulse cannot handle (e.g. production and decay) but when those features are
turned off the two codes solve the same problem. The key difference is that DP1D
requires a constant velocity in the fractures. Hence, provided the velocity remains
constant, as the pulse interval used in DP-Pulse tends to zero (which implies that then
the cell size tends to zero) the DP1D and DP-Pulse models become identical.

DP1D is a 1-dimensional analytical code describing advection within fractures with
matrix exchange where the matrix diffusion described by Fick's second law.

Solutions are determined through posing the problems as a set of partial-differential
equations for concentration as a function of time and one spatial dimension (along
the fractures) and solved using the Laplace transform method (Barker, 1982). The
code inverts the Laplace transform solution numerically, to give concentration as a
function of time. A document describing DP1D version 3 is included in Appendix
X.

Comparison of the two models allows us, in particular, to understand the errors that
arise through the discretisation of the flow velocity in DP-Pulse.

3.9.2. Comparing DP-Pulse with DP1D

The input parameters describing rock matrix diffusion in DP1D (Version 3) are:

$\phi_m$ = matrix porosity [-]

$D_E$ = effective diffusion coefficient for solute [ML$^{-2}$T$^{-1}$]

$a$ = fissure aperture [L]

$2b$ = fissure separation [L]
\begin{align*}
\nu &= \text{velocity in fissures } [LT^{-1}] \\
n &= \text{decay constant } [T^{-1}] \text{ (set to } 0.0) \\\nC &= \text{solute concentration } [ML^{-3}] \\
\end{align*}

The input solute concentration and its duration of injection are set, as well as the duration of the model run and the locations at which the concentration is to be determined.

The initial process involves ensuring the two programs could be used to model exactly the same scenario. Both models were used to produce the results from a hypothetical tracer test, whereby a slug of water with a relative solute concentration of 1.0 is followed by a flow of water with a relative solute concentration of 0.0. Values of concentration can then be determined with DP-Pulse at a given travel time before, during and after the passage of the slug, and compared with those determined through DP1D.

For comparison with DP-Pulse, it was necessary to select annuli within DP-Pulse which would be reached by the advective flow front at identical times to the locations chosen in the DP1D model. Concentrations from these locations/annuli over a period of time could then be compared.

The two models were set up to model a wide range of different scenarios, in order to test the bounds within which the two models would produce similar results. The parameters that were input into each model are detailed in Table 3-2. Three parameter sets were chosen: one with \( \sigma \) and \( t_{cb} \) set being well below the normal expected in reality (i.e. with a high fracture porosity, and a small block size); one being within normal range; and one with very high values of \( \sigma \) and \( t_{cb} \) (i.e. with a low fracture porosity, and a large block size). The parameters were chosen to show the possible extremes that could be modelled. The low parameter values are indicative of an aquifer with very small double-porosity effects (relatively high volume of mobile water, and rapid equilibrium across small matrix blocks.). The high parameter values (relatively high immobile water volume, and slow equilibrium across matrix blocks) describe an aquifer with a very strong double-porosity effect.

The parameters selected were then converted to parameters conventionally used to describe fractured rock systems through the use of equations 19 and 20. In order to achieve this, assumptions were made about the block geometry (a slab geometry was assumed), the effective diffusion coefficient, the matrix porosity and the flow velocity. The decay function within DP1D was left inactive. A pulse interval, \( \Delta T \), of
0.1 days was used for the DP-Pulse model, as this is of similar magnitude to the $\Delta T$ that used within this thesis for simulations of similar magnitude to those detailed below.

**Table 3-2 Input parameters for the DP1D and DP-Pulse models used in the comparison of the two.**

<table>
<thead>
<tr>
<th>Low parameter values</th>
<th>Medium parameter values</th>
<th>High parameter values</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>DP1D</strong></td>
<td><strong>DP-Pulse</strong></td>
<td><strong>DP1D</strong></td>
</tr>
<tr>
<td>$D_E$</td>
<td>$1.2 \times 10^{-10}$ m$^2$s$^{-1}$</td>
<td>$1.2 \times 10^{-10}$ m$^2$s$^{-1}$</td>
</tr>
<tr>
<td>$a$</td>
<td>$4.0 \times 10^{-3}$ m</td>
<td>$t_{cb}$ 0.96 days</td>
</tr>
<tr>
<td>$2b$</td>
<td>$1.0 \times 10^{-2}$ m</td>
<td>$\phi_m$ 0.4</td>
</tr>
<tr>
<td>$k$</td>
<td>0 days$^{-1}$</td>
<td>$K$ 0 days$^{-1}$</td>
</tr>
<tr>
<td>$C$</td>
<td>0</td>
<td>$C$ 0</td>
</tr>
<tr>
<td>$\nu$</td>
<td>1 m day$^{-1}$</td>
<td>$\nu$ 1 m day$^{-1}$</td>
</tr>
</tbody>
</table>

The pumping cycle was a simple tracer test, with water with a relative solute concentration of 1 injected for 10 days, followed by 20 days of injection of water with a relative solute concentration of 0. The breakthrough curves of the two models were then compared (Figure 3-18). Solute concentrations were determined at a point 10 metres from the well (i.e. at a point reached 10 days after the initiation of solute injection).
Figure 3-18 Comparison of DP-Pulse model with DPID model - for verification purposes.

The results from DP1D can be replicated using DP-Pulse over a broad range of parameter values. At the peak concentrations, the difference between the two models is significantly less than 10%, and for realistic and low parameter values the difference is 1% or less, therefore the model appears to be verified for use in this particular case.
3.10. **Analysis of DP-Pulse sensitivity to parameter variation**

In order to examine the sensitivity of the model to the different parameters, a series of model runs were completed, all operating a cyclical pumping pattern, consisting of periods of injection, no flow (storage), abstraction, and no flow (dormancy). This “cycle” is selected to be similar in design to the ASR cycling that is commonly applied. The cycle was completed five times during each simulation. Due to the time dependent nature of the models, in which parameterisation can either be undertaken with $t_{cf}$ and $\sigma$, or with $t_{cb}$ and $\sigma$, the cycle examined should be of two different time-scales. It should, however be remembered that on short timescales, diffusion only occurs across the surface of the block, and therefore the model is only sensitive to $t_{cf}$. On longer timescales the model is sensitive to both $t_{cb}$ and $\sigma$.

Therefore, for the examination of $t_{cf}$, the short time-scale cycle is shown in Table 3-3. For the examination of $t_{cb}$ and $\sigma$ the long time-scale cycle is described in Table 3-4. The BGF will be discussed on both time-scales. Sensitivity of the DP-Pulse model to $\Delta T$ was discussed in Section 3.7.4.

### Table 3-3 Short time-scale injection cycle for the sensitivity analysis.

<table>
<thead>
<tr>
<th>Injection period</th>
<th>10 days</th>
</tr>
</thead>
<tbody>
<tr>
<td>Storage Period</td>
<td>10 days</td>
</tr>
<tr>
<td>Abstraction Period</td>
<td>10 days</td>
</tr>
<tr>
<td>Dormant Period</td>
<td>6 days</td>
</tr>
</tbody>
</table>

### Table 3-4 Long time-scale injection cycle for the sensitivity analysis.

<table>
<thead>
<tr>
<th>Injection period</th>
<th>100 days</th>
</tr>
</thead>
<tbody>
<tr>
<td>Storage Period</td>
<td>100 days</td>
</tr>
<tr>
<td>Abstraction Period</td>
<td>100 days</td>
</tr>
<tr>
<td>Dormant Period</td>
<td>60 days</td>
</tr>
</tbody>
</table>

The initial solute concentrations of the matrix and fracture waters were set at 1, while the injected water had a solute concentration of 0.

#### 3.10.1. Sensitivity of DP-Pulse to $t_{cf}$

In order to outline the sensitivity of the model to $t_{cf}$ at early times the model was run on the short time-scale cycle outlined in Table 3-3 for a $t_{cf}$ values of 0.1 days, 1 day and 10 days. The results are shown in Figure 3-19.
Figure 3-19 Comparison of the effect of different $t_{cf}$ values on solute concentrations resulting from an ASR system operating for five short time-scale cycles (Table 3-3). (Block geometry = slab, $\sigma = 50$, $\Delta T = 1$ day.)

Changing the value of $t_{cf}$ has a significant effect on the model output at these early times. As $t_{cf}$ increases the abstracted solute concentrations decrease. This is because the higher $t_{cf}$ results in a longer period being required for the fracture waters to approach diffusive equilibrium with the matrix waters. As a result, in a system with a high $t_{cf}$ value, water that has only been within the fracture for a short period will not have reached equilibrium with the matrix waters, and will have a lower relative solute concentration. The maximum difference in the relative solute concentrations between the abstracted solute concentrations in the different model runs occurs at the start of the fourth abstraction cycle, where the relative difference in solute concentrations between those when $t_{cf} = 0.1$ days and when $t_{cf} = 1$ day is 208%.

To reinterpret these parameters in terms of a recognised physical characterisation of the system (as was discussed in Section 3.6) it is necessary to make some assumptions about diffusion rates and porosity. If we assume the apparent diffusion coefficient (from Fretwell, 1999) and the matrix porosity (see Section 2.7):

$$D_A = 3\times10^{-10} \text{ m}^2\text{s}^{-1}$$

$$\phi_d = \phi_m = 0.4$$
From equation 23 we can obtain the fracture aperture, $a$. It is possible to restate the result for a slab geometry in terms of fracture aperture as follows. The maximum difference in the relative solute concentrations between the abstracted solute concentrations in the different model runs occurs at the start of the fourth abstraction cycle, where the relative difference in solute concentrations between those when $a = 1.29$ mm and when $a = 4.07$ mm is 208%.

In more general terms, as $a$ increases the abstracted solute concentrations decrease. This is because the higher $a$ results in an increase in the time taken for the fracture waters to approach diffusive equilibrium with the matrix waters. As a result, in a system with large fracture apertures, $a$, water that has only been within the fracture for a short period will not have reached equilibrium with the matrix waters, and will have a lower relative solute concentration.

### 3.10.2. Sensitivity of DP-Pulse to $t_{cb}$ and $\sigma$

In order to outline the sensitivity of the model to $t_{cb}$ the model was run on the long time-scale cycle outlined in Table 3-3 for five cycles. $t_{cb}$ values of 1 day, $1 \times 10^3$ days and $1 \times 10^6$ days were chosen, $\sigma$ was set at 50, and the results are shown in Figure 3-20.

![Figure 3-20](image)

**Figure 3-20** Comparison of the effect of different $t_{cb}$ values on solute concentrations resulting from an ASR system operating for five long time-scale cycles (Table 3-3). (Block geometry = slab, $\sigma = 50$, $\Delta T = 10$ days.)
To outline the sensitivity of the model to $\sigma$ the model was run on the long time-scale cycle outlined in Table 3-3 for five cycles. $\sigma$ values of 1, 50 and 100 were chosen, and $t_{cb}$ was set at 1000 days. These results are shown in Figure 3-21.

**Figure 3-21** Comparison of the effect of different $\sigma$ values on solute concentrations resulting from an ASR system operating for five long time-scale cycles (Table 3-3). (Block geometry = slab, $t_{cb} = 1000$ days, $\Delta T$=10 days.)

In Figure 3-20 $\sigma$ was held at 50 while $t_{cb}$ varied. As $t_{cb}$ increased, the abstracted solute concentrations changed both in the absolute values and the range of values produced.

- The greatest difference between abstracted solute concentrations occurred between the $t_{cb}$ values of 1000 days and 1,000,000 days, at the start of abstraction during the fourth cycle. The difference between the solute concentrations was 460%.
- In Figure 3-21 $t_{cb}$ was held at 1000 days while $\sigma$ varied. As $\sigma$ increased the abstracted solute concentrations increased and the range of values produced decreased.
- The greatest difference between abstracted solute concentrations occurred between the $\sigma$ values of 1 and 50, at the start of abstraction during the fifth cycle. The difference between the solute concentrations was 34%.
These variations occur as a result of the changing aquifer types described by the parameters $t_{cb}$ and $\sigma$.

Again interpreting these results for a slab geometry (as was discussed in Section 3.6), with the assumptions as in the previous section:-

$$D_A = 3 \times 10^{-10} \text{ m}^2 \text{s}^{-1}$$

$$\phi_d = \phi_m = 0.4$$

From equation 20 we can obtain the half block size, $b$, and from equation 19 the fracture aperture, $a$, and hence the fracture porosity, $\phi_f$.

Restating the results:

- In Figure 3-20 $\sigma$ was held at 50 while $t_{cb}$ varied, which in terms of a slab geometry, indicates that by definition of $\sigma$ (the ratio of matrix porosity to fracture porosity) the fracture porosity was maintained at 0.008. As $t_{cb}$ increased, the block size, $b$, increased (equation 20) and the abstracted solute concentrations changed both in the absolute values and the range of values produced.

- The greatest difference between abstracted solute concentrations occurred between the block sizes, $b$, of 0.16 m and 5.09 m, at the start of abstraction during the fourth cycle. The difference between the solute concentrations was 460%.

- In Figure 3-21 $t_{cb}$ was held at 1000 days while $\sigma$ varied, which in terms of a slab geometry, the block size was held at 0.16 m, while the fracture porosity varied. As $\sigma$ increased, the fracture porosity decreased, the abstracted solute concentrations increased and the range of values produced decreased.

- The greatest difference between abstracted solute concentrations occurred between the fracture porosity values of 0.008 and 0.4, at the start of abstraction during the fifth cycle. The difference between the solute concentrations was 34%.

### 3.10.3. Sensitivity of DP-Pulse to the Block Geometry Function

To examine the effect of changing the BGF, the standard ASR cycle on both time-scales was repeated five times. The DP-Pulse model was run with this pumping pattern six times, each a different BGF. In these scenarios, size is defined as the ratio of block volume to surface area.

1. Slab geometry
2. Sphere geometry
3. Slab geometry – 50% of the blocks by volume are 10% of the size of the other blocks (Volume ratio = 0.5, Size ratio = 0.1).
4. Sphere geometry – 50% of the blocks by volume are 10% of the size of the other blocks (Volume ratio = 0.5, Size ratio = 0.1).
5. Slab geometry – 50% of the blocks by volume are 50% of the size of the other blocks (Volume ratio = 0.5, Size ratio = 0.5).
6. Sphere geometry – 50% of the blocks by volume are 50% of the size of the other blocks (Volume ratio = 0.5, Size ratio = 0.5).

The results are shown in Figure 3-22, Figure 3-23 and Figure 3-24.

Figure 3-22 Comparison of the effect of different BGF’s on solute concentrations resulting from an ASR system operating for five years. Constant size vs. mixed size – slab and sphere geometries. (\( t_{cb} = 1000 \) days, \( \sigma = 50 \), \( \Delta T = 10 \) days.)
Figure 3-23 Comparison of the effect of different BGF's on solute concentrations resulting from an ASR system operating for five years. Mixed sizes – slab and sphere geometries. \((t_{cb} = 1000 \text{ days}, \sigma = 50, \Delta T = 10 \text{ days})\)

Figure 3-24 Comparison of the effect of different BGF's on solute concentrations resulting from an ASR system operating for five short cycles. Constant size vs. mixed size – slab and sphere geometries. \((t_{cb} = 1000 \text{ days}, \sigma = 50, \Delta T = 1 \text{ day})\)

In general, it can be said that the block geometry can play an important role. The formulation of the BGF is such that as one function is exchanged for another the
surface area to volume ratio remains constant. The change in block shape does, however, result in a change in the distance from the surface to the nominal centre of the block. At longer times this changes the rate at which solutes can diffuse from the matrix block into the fracture water. The scale of the variation resulting from changing the block shape is discussed more fully below.

As can clearly be seen from the Figure 3-22 and Figure 3-23, at longer time-scales the block geometry plays an increasingly significant role in determining the rate of diffusive exchange between the matrix and fracture waters, and hence the solute concentration of the abstracted water. This relative difference in the abstracted solute concentrations can be up to 30%. At the beginning of abstraction during the fifth cycle, the difference between the solute concentrations in the slab geometry model and the mixed sphere geometry model is 29.9%. At the end of an abstraction phase (i.e. the peak solute concentration within the phase) the greatest relative difference, 19.4% during cycle 5, occurs.

Figure 3-23 shows that changing the size ratio of the two different sized matrix blocks in the mixed BGF also has a significant effect on the modelled solute concentrations. This will be because the solute concentrations within the smaller blocks will fall more rapidly as the total solute mass available to diffuse into the fracture water is less.

At short time-scales, the block geometry plays a less significant role. The maximum difference occurs at the same time, the beginning of abstraction during the fifth cycle, but the relative difference in the abstracted solute concentrations is 21%. The maximum relative difference at the end of an abstraction phase is 9.5%, at the end of cycle 5. Figure 3-25 shows how the relative differences between the solute concentrations resulting from different block geometries change over the duration of the model run. In general, the relative difference increases with time. This is due to both a difference in solute concentrations affecting the solute concentration gradient, hence causing a cumulative difference between the models, and the effect of the block geometry becoming more significant as the fracture water diffuses deeper into the matrix block, leading to solute concentrations becoming more dependent on the block shape.
Figure 3-25 Relative differences between the solute concentrations produced by the different models when a different block geometry is selected. The model consisted of a standard short time-scale repeated five times. \( t_{cb} = 1000 \text{ days}, \sigma = 50, \Delta T = 1 \text{ day} \)

The block geometry is clearly significant when characterising the aquifer, especially when modelling long time-scales (i.e. time-scales of the order of \( t_{cb} \)). The selection of the block geometry, however, may not be simple due to limited knowledge of the fracture geometry.

### 3.11. Further developments of the DP-Pulse model

#### 3.11.1. DP-Pulse simulation processor time requirements

One potential problem with the DP-Pulse model is the time taken to complete a model run. The formulation of the double-porosity solution implemented by the model requires that a solution to the Greens function must be found for each individual annulus, for each individual time step in the model run. These solutions are then summed to provide the simulated concentrations. As a result, increases in the simulation size which may occur through increased simulated durations, reduced size of the time step and increased simulated numbers of annuli lead to large increases in the time taken to run a single model.

This is illustrated in Figure 3-26, which shows the time required to complete a simulation of a simple model on a PC equipped with an AMD Athlon 1000 MHz...
processor, the Windows 98 SE operating system, and sufficient memory. The model consisted of a varying period of injection, while the chosen time step, $\Delta T$, remained constant at 1 day. As a result, increasing the injection period increases the number of annuli, and the number of time steps that need to be modelled. It is clear from this figure that the required processor time increases with model size according to an approximate power ratio.

![Graph showing computational time required for single model run (seconds) vs. duration simulated (days)].

Figure 3-26 Processor time required to complete DP-Pulse model simulations of varying size.

In order to reduce the processor time required by the model, a number of approximations and other changes to the model were made.

3.11.1.1. **Green’s function approximation**

It can be shown that as time increases the value of the Green’s function (see equation 26) tends to a limit (equation 108):

$$\lim_{r \to \infty} G(r, \sigma) = \frac{1}{1 + \sigma}$$  \hspace{1cm} (108)

The new code takes advantage of this fact by calculating and storing only those Green functions required to satisfy this tendency to a specified error margin (nominally 1%). Beyond this number, the limit value is used. This allows a large reduction in both the required memory capacity and the CPU time.

3.11.1.2. **Model size**

When dynamically determining the model size it is necessary to ensure there are sufficient annuli. The safest approach to the problem is to determine the furthest
reach of the injection water, were there no abstraction, i.e. the sum of the durations of all the injection periods;

\[ N = \frac{1}{\Delta T} \sum_{i} t_i^n \]  

(109)

Where \( N \) is the number of annuli, \( n \) is the number of each of the cycles simulated, \( \Delta T \) is the pulse interval and \( t_i \) is the duration of the injection phase of each single cycle. This approach will guarantee that the model is sufficiently large.

3.11.2. Expansion of block geometry function code

Code allowing a generalised mixture of block sizes in the BGF has also been incorporated. See Section 3.5 for details.

3.11.3. Code development

3.11.3.1. Rewriting the code with Fortran 90

The original DP-Pulse code was developed by John Barker in FORTRAN 77. The Fortran environment is ideal for experimental mathematical modelling as it is simple, coherent and fast to use. The original model successfully described the behaviour of double-porosity rocks in an ASR environment. There were, however, a number of limitations to this code, and it became obvious that reprogramming in Fortran 90 could improve the code performance in a number of ways.

FORTRAN 77 requires specific declaration of all arrays. As a result the model had to be created with a standard size. To obtain the most efficient usage of a computer it would be necessary to specify the model size (as a function of model duration, pumping regime and pulse interval) within the code. This would lead to a need to recompile the code for each specific model run. Any compromise would limit either the maximum model size, or greatly increase the memory requirements of an average model run. Fortran 90 allows arrays to be declared dynamically, and they can therefore be created to a size suited to the problem, as determined from within the code.

3.11.3.2. Optimisation for vector processor

Further developments to the code were applied in order to make best use of the Fujitsu VPP300 vector processing computer with 8 processors, each rated 2.2 Gflops peak and each with 2 Gbytes memory, run by the Computer Services for Academic Research (CSAR) at the University of Manchester.
Standard FORTRAN 77 and Fortran 90 operations on matrices require either an explicit `DO .. LOOP` construct (Fortran 77), or an explicit matrix operation function that performs an implicit `DO .. LOOP` type operation. Thus completing an operation on an array requires a processor time in proportion to the size of the array. A vector-processing computer allows operations to be performed simultaneously on multiple elements of a matrix. Any operation acting on an array or part of an array (the total number of elements that may undergo the same simultaneous operation is hardware restricted) can be executed in one step. As a result, vector processing computers can perform certain mathematical operations more rapidly than older versions.

In order to increase code performance on the Fujitsu VPP 300, a vector-processing computer, 'strip-mining' of the code was performed. This mainly involved reducing individual `DO .. LOOP` constructs to below a certain size, in order to maximise processor performance.

### 3.11.4. Automatic calibration

In order to calibrate the model efficiently, it became necessary to incorporate the DP-Pulse model into a fitting routine. A few groundwater models are either self-calibrating, or are used in conjunction with a general-purpose model fitting routine, such as PEST. One concern with the automated calibration of groundwater models in this manner is the possibility of non-uniqueness in the result. As the DP-Pulse model shows, for example, solute concentrations in double-porosity rocks are dependent on the ratio of matrix to fracture water volumes ($\sigma$). This parameter is itself dependent on the fracture aperture and separation, the matrix block size and the diffusion porosity of the matrix (equation 19). The interdependence of these may result in identical calibrations for a number of different combinations of parameter values.

If $t$ is of the order of $t_{cb}$, the solution of the DP-Pulse model is unique. In other words, if the simulation occurs over a sufficient period of time that the entire volume of the matrix block is active in controlling the solute concentration of the fractures, then the solution provided by the model is characteristic of the selected parameter values and no others. Figure 3-27 is a contour plot showing the sum of the squares of the difference between the data collected from test cycles 1 to 9 at the Lychett Minster test site, and the data produced by the DP-Pulse model for a range of parameter values. (The Lychett Minster test site is described in Chapter 4, and the calibration of the DP-Pulse model to the data from the site is undertaken in Chapter...
5. The data is used here for purely illustrative purposes.) There are a number of significant points to this graph.

Most importantly, it is clear that the surface described is very simple. There is only one valley in the surface, and therefore the solution is unique. Secondly, the valley containing the solution, although narrow, is very long. The solution is not well constrained along this line (described by $\sigma^2 = t_{cb}$, i.e. $t_{cf}$ is constant). This indicates that while the calibration is well constrained with regards to $t_{cf}$, the calibration of $t_{cb}$ and $\sigma$ is more uncertain. We may, however, plot a curve along the line of $t_{cf}$, marked in Figure 3-27 as Line A – B, and picture how the solution is constrained (Figure 3-28).

Figure 3-27 Contour plot showing the sum of the squares of the difference between the data collected from test cycles 1 to 9 at the Lychett Minster test site, and the data produced by the DP-Pulse model for a range of parameter values, assuming a slab geometry.
Figure 3-28 Sum of the squares of the difference between the data collected from test cycles 1 to 9 at the Lychett Minster test site, and the data produced by the DP-Pulse model for a range of parameter values along Line A - B in Figure 3-27.

Through examination of these two plots, and the indication of a unique solution for a single BGF, it is possible to determine that a relatively simple approach to calibration may be applied in order to determine $t_{cb}$ and $\sigma$. In addition to the calibration of these two parameters, however, correct selection of the BGF will be necessary. In the simplest case this is an integer problem (either slab geometry, or sphere geometry), however the introduction of mixed geometries introduces a number of different continuous variables (a number which also varies according to the complexity of the block mixture), making the problem significantly more complicated.

Two methods were considered by which the calibration routine could incorporate different block shapes and sizes. The first method is through the use of the mixed BGF (29), which will allow a number of different block sizes and shapes to be set. The calibration routine varies the proportions by volume of each of the different block types specified.

The second method would make use of the BGF describing $n$-dimensional spheres (32). As has previously been stated, this BGF is not trivial to evaluate, so this is a less useful method.

Initial attempts by the author to incorporate the first (mixed block geometry) solution into the calibration routine met with limited success. This is likely to be the result of either complexities in the solutions to the BGFs, or the fact that the calibration data
set was of limited length, and that the block geometries do not, therefore, have sufficient control over the solute concentrations in the abstracted water. The calibration routine developed was unstable, and therefore within this thesis, selection will be made on an empirical basis. Calibration to both geometries will be necessary, and a comparison of the 'goodness of fit' will determine the most likely geometry form. This does, however, limit the calibration to either slabs of one size, or spheres of one size, which represent extremes in either sense (see Section 3.5 and Figure 3-4).

### 3.11.4.1. A simple but robust approach

The first attempt to develop a fitting routine was very simple, effectively the initial calibration was only made to the value of $t_{cf}$. In practice, the model would fit to one parameter, $t_{cb}$, $\sigma$ being specified with each calibration run. The $t_{cb}$ error space thus determined took the form of a transect, with equal $\sigma$, of the error surface in Figure 3-27, and the minimum identified would be the value of $t_{cf}$ that resulted in the least difference between actual and simulated data.

To find the minimum along the transect the model completed a bisectional search of the line, always centring on the lowest point. As the model is insensitive to $\sigma$ and $t_{cb}$ at early times, by combining the specified value of $\sigma$ and the calibrated value of $t_{cb}$ we can obtain a calibrated value of $t_{cf}$. Using a different value of $\sigma$ would result in a different calibrated value of $t_{cb}$, but the same value of $t_{cf}$. As the model is only sensitive to $t_{cf}$ at early times, this is sufficient for the calibration of the DP-Pulse model to a tracer test of relatively short duration.

An extension of this program could, having calibrated to $t_{cf}$, search along another transect described by that $t_{cf}$ value, in a similar way to that shown as Line A-B in Figure 3-27. This would allow calibration to both $t_{cb}$ and $\sigma$, but the low gradient of the transect at high $t_{cb}$ and $\sigma$ values, as shown in Figure 3-28, would lead to difficulties in determining a unique solution.

There are a number of limitations to this method:

- This method, while being robust, requires a large number of iterations. This can lead to extremely long program runs.
- Although reduction of the program to a single parameter is not a major limitation to the fitting of the model at early times, it would constrain the maximum information that could be obtained from a data set collected over a long period of time. To resolve this a similar algorithm could be used to
enable the model to be fitted to both parameters, but this would double the necessary computation time.

- The fitting procedure provides no information as to the quality, and therefore reliability, of the fit.
- When the iteration step length becomes very small, numerical dispersion has a tendency to falsely produce local maxima, which can confuse the program output by indicating a complex error space.

3.11.4.2. Levenberg-Marquardt routine

Due to the failings of the initial fitting program, a more complex fitting technique was required: a standard fitting algorithm developed by Marquardt (1963) was implemented. This algorithm performs least-squares estimation of non-linear parameters through a combination of the Taylor series method, allowing rapid approach to the solution, and the method of steepest descent, allowing rapid convergence. The output of this algorithm includes not only the best-fit parameters, but also the covariance matrix, from which the standard deviation and student t-test confidence values can be obtained. Thus we not only obtain a suitable fit, but a measure of how well constrained the fit can be. The basic Marquardt-Levenberg algorithm was drawn from a standard code (Press et al., 1992).

The program determines the ‘goodness of fit’ of the model by summing the square of the difference between each experimental data point and a value from the DP-Pulse model (equation 110), i.e. the Mean Square Error (MSE). Although in theory the DP-Pulse model can simulate the concentration at any time (i.e. it is not constrained by $\Delta T$), the code available at the time of writing was only capable of producing the concentration at a time defined by an integer multiple of $\Delta T$. Therefore, for the determination of the MSE, when the time at which the experimental data was collected does not coincide with the output from the DP-Pulse model a value is determined by linear extrapolation of the model output.

$$E = \frac{\sum_{i=1}^{n} (y_d^i - y_m^i)^2}{n}$$  \hspace{1cm} (110)

$E = \text{MSE}$

$y_d^i = \text{experimental data}$

$y_m^i = \text{DP-Pulse model prediction}$

$n = \text{total number of data points.}$
The algorithm requires not only the MSE, but also the gradients of the local error surface. To describe the error surface, five repetitions of the model run are performed for each iteration. As well as the initial run, these iterations involve $t_{cb} \pm \delta t_{cb}$ and $\sigma \pm \delta \sigma$. Although it would be possible to cut the computation time by two fifths by only recalculating for $t_{cb} + \delta t_{cb}$ and $\sigma + \delta \sigma$, the error in calculating the gradient is greatly reduced by calculating over two points, equidistant either side of the actual value. This does not significantly affect the fit obtained, but does increase the confidence in the calibration.

The fitting program itself appears fairly robust, but depends on the input parameters. If they are not within the range of reasonable behaviour (i.e. if they are too close to zero or too high), changing the input parameters by a small amount will not create a numerically significant difference in the model output relative to rounding errors implicit in the model code, and hence the model will not be able to approach the correct solution.

Application of the calibration model is very simple. Inputs include preliminary estimates of $t_{cb}$ and $\sigma$ (or, if desired, $t_{cj}$), the pumping cycle (durations of periods of injection, storage, abstraction and dormancy), and the collected conservative solute data. The calibration routine then automatically determines the optimal values of $t_{cb}$ and $\sigma$, and calculates the confidence intervals around these parameters.

In order to test the calibration algorithm, a DP-Pulse simulation was run with known parameter values, and then the calibration routine was used in an attempt to obtain these parameter values. In every scenario the calibration routine was correct to 7 significant figures.

### 3.11.4.3. Weighting the data for optimal calibration

A further development of the automated fitting routine involved weighting the data. Field data are rarely collected according to the precise demands of a numerical routine. As a result, the automated calibration routine may be biased towards periods during which more data were collected. It is possible to weight the data in order to remove this bias. This weighting may be accomplished by applying a numerical weight to each data point which may then be used to scale its influence on the 'goodness of fit' estimation. A simpler method of weighting was chosen for the calibration routine - repeating selected data. Although several methods of selecting the number and location of the data to be repeated were identified (Table 3-5), the simplest approach was chosen for the initial application of the model.
application of the DP-Pulse model is cyclical in nature, selected data from the start of each cycle were repeated to ensure equal numbers of data points were available for each cycle.

**Table 3-5 Methods of selecting data to repeat when weighting a data set prior to automated calibration.**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Ensure equal numbers of data points are available for each cycle. Repeat data from the start of each cycle.</td>
</tr>
<tr>
<td>2</td>
<td>Ensure equal numbers of data points are available for each cycle. Repeat selected data from throughout the duration of each cycle.</td>
</tr>
<tr>
<td>3</td>
<td>Ensure data are consistently dense with respect to time. Repeat selected data to increase density when data collection is sparse.</td>
</tr>
</tbody>
</table>

**3.11.4.4. Confidence intervals**

Due to both the nature of the calibration algorithm and the limited parameterisation of the DP-Pulse model, it is possible to complete a more coherent sensitivity analysis. This would indicate the potential range in model outputs that may be simulated within the confidence bounds of the calibration, showing both the effect of limited parameter calibration resulting from limited and imperfect data sets, as well as allowing visualisation of the confidence in the model calibration.

The calibration algorithm produces a covariance matrix for the parameter field in the region local to the calibrated solution. This may be used to determine confidence intervals for the calibration through the use of a student t-test.

Assuming the error surface local to the calibrated parameter values to be quadratic in form, the covariance matrix, in conjunction with the student t-test, can be used to predict the parameter region defined by a confidence interval.

A confidence interval defines a region about the calibrated parameter within which the true parameter value is likely to be situated. A 50% confidence interval, for example, bounds the parameter range within which it is possible to be approximately 50% sure that the true parameter is situated.
Chapter 4

The Lychett Minster Test Site
4. The Lychett Minster Test Site

One of the first proposed ASR developments in the UK, and the first to complete large scale testing within the UK Chalk aquifer, was the Lychett Minster Test Site, within the Wareham Basin in Dorset (Figure 4-1). The scheme itself eventually proved unfeasible, as the cost of developing the system to a point where it could significantly supplement the water resources of the region proved to be too great. The trial methodology does, however, provide a background against which theoretical developments of ASR practices may be compared and contrasted, and as such proved to be an extremely valuable exercise. In addition, the solute chemistry analyses carried out during the trial provide a data set that may be used to further understanding of the processes occurring during ASR operations in a double-porosity system.

Before discussion of the operations undertaken at the Lychett Minster test site, it is useful to provide an overview of the geology and hydrogeology of the Wareham Basin. The Wareham Basin is located to the west of Poole, Dorset and occupies approximately 300 km² of gently undulating low-lying land from Dorchester to the west and Poole Harbour to the east. The elevation of the Basin ranges from 0 to 50 metres above Ordnance Datum (mAOD) and is flanked by prominent ridges of chalk hills to the north and to the south.

The northern chalk ridge trends in a SW to NE direction and gradually rises to an elevation 220 to 240 m AOD. Several steeply incised valleys carry streams which flow into the Wareham Basin, coalescing into two main rivers: the Rivers Frome and Trent (or Puddle).

The southern chalk ridge trends in a West-East direction and rises steeply to an elevation of 100 to 150 m AOD. A number of tributaries from this chalk ridge flow into the River Frome except the Corfe River which flows directly into Poole Harbour.

The River Stour receives flow from the north-east and flows in a southerly direction into the sea, 10 km east of the Wareham Basin.
4.1. **Geology and Hydrogeology of the Wareham Basin, Dorset**

4.1.1. **Regional Stratigraphy and Geology**

The topography, hydrology and ecology of the Wareham Basin and its immediate environs are strongly influenced by its underlying geology and structure. A lithological summary of the principal geological units is given in Table 4-1, while the geology is summarised in Figure 4-1.

The following geological summary is based on published maps and records from the BGS, Bristow *et al.* (1997), and from a report on a regional hydrogeological model of the area (CH2M HILL, 2000c) which was supplemented by recent confidential records from oil exploration boreholes and Wessex Water’s groundwater investigation.

Further detailed information on the differentiation of the various stratigraphic units and minor fault lineaments can be found in the BGS map of the area (Arkell and Smart, 1981), Bristow *et al.* (1997), and the memoir describing the region (Melville and Freshney, 1982).

![Figure 4-1 Surface Geology of the Wareham Basin](image)
<table>
<thead>
<tr>
<th>Geological Period</th>
<th>Stratigraphic Unit</th>
<th>Description</th>
<th>Thickness (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Palaeogene (Tertiary)</td>
<td>Poole Formation</td>
<td>Alternating sequences of fine to coarse sands, and silty clays.</td>
<td>7 to 80 m</td>
</tr>
<tr>
<td>London Clay Formation divided into: London Clay West Park Farm Member</td>
<td>London Clay</td>
<td>Laminated clays with sandy lenses.</td>
<td>20 to 35</td>
</tr>
<tr>
<td></td>
<td>West Park Farm Member</td>
<td>Variable sequence of clays, sandy clays, sand and gravel units</td>
<td>10 to 25</td>
</tr>
<tr>
<td>Cretaceous</td>
<td>Upper Chalk Formation divided into: Portsdown Chalk Spetisbury Chalk Tarrant Chalk Newhaven Chalk Seaford Chalk Lewes Nodular Chalk Chalk Rock</td>
<td>Smooth, white, massively bedded chalk with flints Hard nodular glauconitised chalk bed</td>
<td>300 to 400</td>
</tr>
<tr>
<td>Middle Chalk Formation divided into: NewPit Chalk Holywell Chalk</td>
<td>White homogenous massively bedded chalk with occasional marl partings and scattered flints.</td>
<td>30 to 40</td>
<td></td>
</tr>
<tr>
<td>Lower Chalk Formation divided into: Plenus Marl Zig Zag Chalk Glaucnitic Marl</td>
<td>Marls and marly limestones Blocky chalk Green grey glauconitic marl at the base of the Lower Chalk</td>
<td>30 to 50</td>
<td></td>
</tr>
<tr>
<td>Upper Greensand</td>
<td>Glaucnitic sands and silts</td>
<td>40 to 50</td>
<td></td>
</tr>
</tbody>
</table>

**4.1.1.1. Poole Formation**

The Poole Formation is the youngest Palaeogene (Tertiary) sediments in the Basin and typically forms the surface strata of the low-lying areas. These sediments comprises a variable sequence of lignitic, fine to coarse-grained sands with interbeds of clay and silt that were deposited in an estuarine environment. The Formation ranges in thickness, but around the Lytchett Minster Test Site it is 7 m thick. It supports an unconfined aquifer whose water table lies just below the ground surface.

**4.1.1.2. London Clay Formation**

The London Clay Formation lies beneath the Tertiary sediments, and immediately above the chalk strata. It is divided into two units, the London Clay and the West Park Farm Member.

Underlying the Tertiary sediments is the London Clay. This unit comprises laminated clays although lenses of sandy and shelly material within the clays have been encountered in a number of boreholes across the Basin. The London Clay is laterally extensive, disappearing only at the northern and southerly edges of the Basin near to the chalk hills. Owing to its widespread occurrence and very low
overall permeability, these sediments form an effective aquiclude hydraulically separating the unconfined aquifer in the Poole Formation sediments and the deeper confined aquifer in the Chalk strata.
The West Park Farm Member comprise a variable sequence of multi-coloured clays, sandy clays, sands and gravely material which collectively form the basal sediments of the London Clay Formation. Although the thickness and the composition of these sediments vary across the Wareham Basin, these sediments are laterally extensive and were encountered in virtually all boreholes drilled across the area.

The sediments of the West Park Farm Member were deposited in a marine estuarine environment on the eroded surface of the Upper Chalk. Being an erosional surface, the interface between Upper Chalk and the West Park Farm Member is likely to be uneven with the uppermost chalk sediments being highly weathered with some solution enhanced fissures. Where sands and gravels overlie the chalk, the West Park Farm Member tends to be in direct hydraulic continuity with the underlying confined Chalk aquifer. For example, at the Lytchett Minster Test Site, an 8 to 11 m thick bed of flinty gravel rests directly on the chalk surface.

4.1.1.3. Chalk

Work conducted by the BGS has enabled differentiation of the three broad chalk formations, Upper, Middle and Lower Chalk, as indicated in Table 2.1. Within the Wareham Basin, the confined chalk is reported to have a thickness of 300 to 500 m.

**Upper Chalk:** comprises approximately 350 to 450 m of fissured fine-grained microporous limestone. The youngest member of the Upper Chalk is the *Portsdown Chalk*, which comprises predominantly of soft chalk with many mm-thick marl seams. To the east of the basin the thickness of this member exceeds 130 metres, but this rapidly thins westwards due to erosion during the onlap of the Palaeogene (Tertiary) and is absent in Dorchester.

Immediately underlying this member is the *Spetisbury Chalk*, which is a white flinty much harder chalk more suited to solution-enhanced water bearing fissures and fractures.

There is some doubt as to which of the *Portsdown* and *Spetisbury* is intersected by higher yielding confined chalk boreholes. For example, the chalk intersected at the Lytchett Minster test site is much harder and yielded significant groundwater compared to a borehole located 5.6 km to the north west (Corfe Hills), which intersected soft chalk with no water bearing fissures. To date initial investigations by
the BGS have designated all of the uppermost chalk beneath the Palaeogene (Tertiary) sediments as belonging to the Portsdown.

The basal unit of the Upper Chalk comprises the hard, nodular glauconitised Chalk Rock, which forms a prominent marker bed that has been identified on the down-hole sonic logs of all oil exploration boreholes in the Wareham Basin.

Middle Chalk: comprises approximately 30 to 40 m of fissured fine-grained microporous limestone with occasional marl partings and scattered flints.

Lower Chalk: is typically a clay rich chalk that lies directly above the older Upper Greensand strata. It is approximately 30 to 50 m thick and is separated from the overlying Middle Chalk by the Plenus Marls.

4.1.2. Structural Geology

The sediments of the Wareham Basin are folded into a major asymmetrical syncline whose axis trends west to east through the centre of the Basin and into Poole Harbour (Figure 4-1). This structural feature is reflected in the topography of the region where the higher land to the north and south forms the outcropping chalk limbs of the syncline. In addition, faults in the Cretaceous and overlying Palaeogene (Tertiary) sediments are known to be present and these play key role in the direction and pattern of groundwater flow in the confined Chalk aquifer.

Recent mapping by the BGS indicates that the Wareham Basin geology is complicated by a series of normal faults, located roughly parallel to the axis of the syncline. A noticeable feature is the abundance of fault lineaments, which correspond with the dry valleys, with moderate offsets on them. These faults are considered to form important hydrogeological boundaries, influencing the pattern of groundwater flow across the Basin and controlling natural recharge into the Basin as more permeable chalk blocks are offset against less permeable chalk blocks.
4.2. **Hydrogeology**

4.2.1. Chalk

The Chalk aquifer in the Wareham Basin is well confined with groundwater levels above ground surface. Artesian yields from the boreholes drilled by Wessex Water across the Basin vary from 1 to 4 Ml/d, with flow substantially arising from sub-horizontal fractures in the upper 50 to 100 m of the Upper Chalk strata. A pumping test was carried out by Wessex Water at the Lychett Minster site in 1994, as part of the original groundwater investigation (Wessex Water, 1995). This pumping test demonstrated that the London Clay acts as an effective aquiclude to groundwater flow between the unconfined aquifer in the Poole Formation and the confined aquifer in the Chalk strata (Wessex Water, 1995).

The strongest artesian heads occur in the eastern part of the Basin around Lychett Minster, while the groundwater is not artesian in the northwestern parts of the basin (Institute of Geological Sciences & Wessex Water Authority, 1979). Figure 4-2 indicates the regional variation of groundwater level in the chalk aquifer across the Wareham Basin. This figure indicates that the principal direction of groundwater flow is southeasterly, towards Poole Harbour.

The matrix porosity of the chalk is typically high, ranging from 15 to 45% in sediments across southern England. However, the pore throats tend to be very small giving rise to very low matrix hydraulic conductivities \(10^{-5} - 10^{-2}\) m/day. The matrix water is therefore generally regarded to be immobile and contributes little to the yield from chalk boreholes. The fissures and fractures provide a secondary component of porosity and the main component of hydraulic conductivity in the Chalk. No core was available from the Chalk in the Wareham Basin.

Records of studies conducted in southern England indicate that fissuring in the confined chalk aquifer is typically greatest in the top 50 to 100 m of the Chalk and where the strata lies close to the axis of valleys. It is here that the weathered zone is deepest and the greatest aquifer yields are usually encountered. In the Wareham Basin, the hydraulic conductivity of the Upper Chalk was reported to range from 0.3 to 2 m/day based on data derived from the 1994 pump test. The greatest hydraulic conductivities were recorded in Lytchett Minster (2 m/day) whilst a nearby production borehole recorded the lowest hydraulic conductivity at 0.35 m/day. A series of geological faults are thought to offset chalk of different ages against one
another. Softer chalk offset against harder more fractured chalk may also help to explain apparent differences in the recorded lithologies, transmissivity and borehole yields across the Basin.

![Hydrogeology of the Wareham Basin](image)

**Figure 4-2 Hydrogeology of the Wareham Basin (Excerpt from Institute of Geological Sciences & Wessex Water Authority, 1979)**

The observed effects of the 1994 pumping test, reported by Wessex Water (op. cit.) and the University of Birmingham (1997) indicate that cones of depressions within the chalk strata were localised and that drawdowns around the well were high. This would suggest that the boreholes were responding inefficiently. Throughout the 1994 pump test, no apparent connection between the flow zones in the confined chalk and the unconfined chalk were observed, either at the Lychett Minster Test Site, or at boreholes located 4 to 5 km from the pumping wells. This finding indicates that natural recharge is limited and that even seasonal abstraction is unlikely to be sustainable without some form of artificial recharge. No impacts on surface water features monitored within the Wareham Basin were recorded.
Analysis of pump test data from both the Lytchett Minster site and other boreholes within the Wareham Basin, indicate that the transmissivity of the Chalk typically ranges from 125 to 500 m²/day. The University of Birmingham's numerical model of the observed data indicates that the regional average is typically 300 m²/day and that storage coefficients are low, typically in the order of $1\times10^{-6}$ (University of Birmingham, 1997).

4.2.2. West Park Farm Member

Lytchett Minster and another installation at Bulbury, approximately 5km from Lytchett Minster, are the only sites where piezometers monitor groundwater levels in the basal beds of the London Clay Formation, i.e. the West Park Farm Member. At Lytchett Minster, the results of the 1994 pump test indicated that the Chalk aquifer and the West Park Farm member are hydraulically connected. Similar behaviour was also observed at Bulbury during the 1994 pump test. The degree of flow across the boundary is dependent on the hydraulic gradient across the boundary, the permeability of the sediments and storage conditions. Although this aquifer is not used for public groundwater supply a number of licensed abstractors use the unconfined parts of this aquifer for irrigation water supply. These boreholes are typically located on the northern and western regions of the Basin.

4.2.3. Poole Formation

The aquifer in the Poole Formation is typically unconfined or partially confined beneath alluvial sediments. No observed impacts to pumping from the Upper Chalk were observed in this aquifer which is understood to be isolated from the groundwater in the underlying chalk aquifer by the London Clay. A number of private licensed abstractors also use this aquifer for irrigation water supply.

4.3. Hydrochemistry of the Confined Chalk Aquifer

The groundwater of the confined Upper Chalk aquifer is a calcium bicarbonate water type. Although relatively fresh in origin, with a conductivity of around 600 µS/cm, geochemical indicators suggest that considerable water-rock interaction has taken place. The groundwater exhibits slight mineralisation with fluoride and iron being the main parameters to exceed the drinking water standards. Anaerobic conditions prevail, as indicated by the elevated concentrations of iron (0.2 to 0.5 mg/l), low concentrations of aqueous nitrogen and low Eh. Indicators of residence times
provided from parameters such as strontium estimate the groundwater to be around 8,000 years old with no history of abstraction to disturb the aquifer (British Geological Survey, 1996; Edmunds, 1996; CH2M HILL, 2000a, 2000b).

The groundwater in confined chalk strata beneath the Wareham Basin appears to be hydraulically unconnected with the groundwater in the unconfined chalk regions. It is suggested that geological faults are present in the chalk that form barriers to horizontal groundwater flow.

4.4. Hydrology

Records of average annual rainfall indicate that the Wareham Basin receives 800 to 900 mm per year. To the north and west of the Basin, in the area of the headwaters of the Rivers Frome and Trent, the average annual rainfall is more typically around 1000 to 1100 mm. Hydrographs of boreholes in these headwater regions indicate that groundwater recharge primarily occurs from November to February.

The low-lying land around Wareham comprises the Catchment basin for three rivers: the Rivers Frome, Trent and Stour. The Rivers Trent and Frome rise from the chalk ridge to the north and west of Wareham, and flow into Poole Harbour just east of Wareham. The headwaters of the River Stour lie north of these Downs and river flows along the northern boundary of the Basin and into Christchurch Bay.

All three rivers show similar characteristics with peak flows occurring in January and February. Thereafter baseflow recessions occur until the end of September with low flow periods typically occurring from July to September. The rivers show a net increase in flows between the upstream and downstream gauging stations confirming that these are gaining rivers, i.e. they receive groundwater discharge throughout the year and runoff during precipitation events (CH2M HILL, 2000c).

4.4.1. Aquifer Interaction with Surface Waters

The upper reaches of the Rivers Frome and Trent are primarily spring fed streams. Flow rates are highly dependant on the relative position of the water table in the unconfined chalk aquifer: receiving flow when the water table is high and losing flow when the water table is below the base of the stream bed. Any groundwater abstraction in the confined chalk aquifer therefore has the potential to impact the groundwater levels in the unconfined chalk and, as a consequence, stream flows. Stream flows increase significantly as soon as they flow into the Basin and onto the clay and sand sediments of the Palaeogene (Tertiary) strata. High water tables in the
Poole Formation, which vary little in elevation between seasons, contribute to the river flows, as does precipitation runoff. Interaction of river water with the deeper confined chalk aquifer is negligible owing to the presence of London Clay between the overlying Poole Formation and the underlying chalk strata. Extensive monitoring of groundwater levels, water quality and stream flow across the Basin during the 1994 pump test confirmed that the low permeability sediments of the London Clay formed an effective aquiclude, hydraulically separating the overlying Poole sediments from the underlying chalk strata.

The unconfined chalk to the north, west and south of the Basin receives groundwater recharge from seasonal precipitation. The elevation of the water table will vary in response to these precipitation events, being typically high in the winter months and low in the summer months. Streams and rivers flows in the unconfined regions are highly sensitive to the elevation of the water table, gaining and losing flows in response to changing groundwater conditions.

4.5. Overview of the Lychett Minster Test Site

The borehole used in the ASR trial was one of five wells drilled in 1993 as part of an investigation of the groundwater resource potential of the Chalk aquifer of the Wareham Basin. In September 1997, Wessex Water retrofitted one of the boreholes, at Lychett Minster, to act in a trial ASR system. A series of cyclical fresh-water injection and groundwater abstraction tests were planned and executed, based on knowledge gained through previous US experience (Pyne, 1995).

4.5.1. Location

The Lychett Minster ASR test site is located over the confined Chalk, as shown in Figure 4-3.
4.5.2. Site description

The Lychett Minster test site, illustrated in Figure 4-4, consists of four wells. Well constructions are shown in Figure 4-9. A main well, called ABH, or the ASR well, was used for injection and abstraction of the water. Piezometric levels were measured in the Chalk aquifer by a main observation well and in the confining sediments by two piezometers. The Lychett Minster Test Site is approximately 6 m above sea level.
Figure 4-4 Sketch map of the Lychett Minster Test Site (No scale available; approximate site size = 30 x 50 m.). See Figure 4-9 for a geological cross section of the site.

4.5.3. The ASR well

The main well (ABH) is 110 m deep, penetrating 51 m into the Upper Chalk. It is cased to a depth of 67 mbgl, and open with a diameter of 600 mm from there to the bottom (see Figure 4-5). From the surface to 53.95 mbgl the casing diameter is 600 mm, between 53.95 mbgl and the bottom of the casing at 67 mbgl a dropset reduces the diameter to 500 mm.

Considering the hardness of the chalk encountered during drilling, and the presence of solution fissures, which provide an important proportion of the water to the well, it is likely that the open section of the borehole largely intersects the Spetisbury Chalk.
4.5.4. The observation wells

The main observation well (OBH) is situated 19 m from the ASR well. It is 141 m deep, penetrating 82 m into the Chalk. The well is cased between 0 and 67 m, with a diameter of 150 mm, and open from there to the bottom with a diameter of 100 to 150 mm. The well is fitted with a pressure transducer.

Two more piezometer wells are drilled 19 m from the ASR well. One records groundwater pressure in the Basal Sand of the London Clay, the West Park Farm Member (P2), while the other measures the pressure in the unconfined Poole formation (P1).

The borehole construction and local geology encountered during the construction of the wells is outlined in Figure 4-9.

Table 4-2 Flange and pressure transducer levels in the Lychett Minster boreholes (maOD).

<table>
<thead>
<tr>
<th></th>
<th>ABH</th>
<th>OBH</th>
<th>P1</th>
<th>P2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transducer level</td>
<td>-50.05</td>
<td>-34.36</td>
<td>-9.88</td>
<td>-26.72</td>
</tr>
<tr>
<td>Flange level</td>
<td>2.95</td>
<td>3.04</td>
<td>3.12</td>
<td>3.28</td>
</tr>
</tbody>
</table>

4.5.5. Analysis of piezometric data

Prior to the ASR testing, a series of pumping tests, both constant and stepped rate, were carried out on the ASR well at the Lychett Minster Test Site. The tests are summarised in Table 4-3 (see Figure 4-6).
Figure 4-6 Measuring the flow during a step discharge test at the Loftsome Bridge Test Site. Inline flowmeters were also used.

Table 4-3 Summary of pumping tests completed at the Lychett Minster Test Site ASR borehole prior to the ASR testing.

<table>
<thead>
<tr>
<th>Action</th>
<th>Date</th>
<th>Time</th>
<th>Rate (m³/d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant rate pump test</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Start</td>
<td>01/06/1994</td>
<td>14:10</td>
<td>5400</td>
</tr>
<tr>
<td>Stop</td>
<td>02/06/1994</td>
<td>00:00</td>
<td></td>
</tr>
<tr>
<td>Step Discharge test</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Start</td>
<td>29/11/1997</td>
<td>11:25</td>
<td></td>
</tr>
<tr>
<td>Stop</td>
<td>29/11/1997</td>
<td>15:25</td>
<td></td>
</tr>
<tr>
<td>Pressure gauges recalibrated</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Step Discharge test</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Start</td>
<td>05/12/1997</td>
<td>21:00</td>
<td>997.92</td>
</tr>
<tr>
<td>Increase rate</td>
<td>05/12/1997</td>
<td>22:00</td>
<td>1994.11</td>
</tr>
<tr>
<td>Increase rate</td>
<td>05/12/1997</td>
<td>23:00</td>
<td>2998.08</td>
</tr>
<tr>
<td>Increase rate</td>
<td>06/12/1997</td>
<td>00:00</td>
<td>3030.05</td>
</tr>
<tr>
<td>Stop</td>
<td>06/12/1997</td>
<td>01:00</td>
<td></td>
</tr>
<tr>
<td>Step Injection Test</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Start</td>
<td>09/12/1997</td>
<td>10:17</td>
<td>698.13</td>
</tr>
<tr>
<td>Increase rate</td>
<td>09/12/1997</td>
<td>11:17</td>
<td>1201.43</td>
</tr>
<tr>
<td>Increase rate</td>
<td>09/12/1997</td>
<td>12:17</td>
<td>1599.87</td>
</tr>
<tr>
<td>Increase rate</td>
<td>09/12/1997</td>
<td>13:17</td>
<td>2000.16</td>
</tr>
<tr>
<td>Increase rate</td>
<td>09/12/1997</td>
<td>14:17</td>
<td>2127.80</td>
</tr>
<tr>
<td>Stop</td>
<td>09/12/1997</td>
<td>15:17</td>
<td></td>
</tr>
</tbody>
</table>
The data collected during the 1994 pumping test at the Lychett Minster Test Site (Wessex Water, 1995) has been analysed a number of times. Results from these analyses, are given below in Table 4-4.

**Table 4-4 Transmissivity and storativity data determined at the Lychett Minster Test Site using data from the 1994 constant rate pumping test.**

<table>
<thead>
<tr>
<th>Analysis</th>
<th>Transmissivity (m²/d)</th>
<th>Storativity</th>
</tr>
</thead>
<tbody>
<tr>
<td>University of Birmingham, (1997)</td>
<td>500</td>
<td>1x10⁻⁶</td>
</tr>
<tr>
<td>CH2M HILL (1998) Analysis of early time data</td>
<td>170</td>
<td>3x10⁻⁴</td>
</tr>
<tr>
<td>CH2M HILL (1998) Analysis of late time data</td>
<td>550</td>
<td>1x10⁻²</td>
</tr>
<tr>
<td>Analysis of data (See Figure 4-7)</td>
<td>172</td>
<td>2.5x10⁻²</td>
</tr>
</tbody>
</table>

Further examination of this data has been carried out for this thesis (Figure 4-7 and Figure 4-8). The analyses in this figure are based on the Hantush and Jacob solution for a leaky confined aquifer (Hantush and Jacob, 1955). The relatively low r/B value (0.1) indicates that leakage is relatively small.
Both the work above and that completed by CH2M HILL identified a lower transmissivity and a higher storage coefficient at early times than that determined in both the analysis of the data from later times and the analysis by the University of Birmingham. The difference between the determined results could be explained by leakage from the upper sediments, a nearby source of recharge or inhomogeneities in the aquifer locally. It is more likely, considering the relatively short duration of the data used for the early time analysis, that the early time data is influenced by well storage, fluctuating pump rates, etc. The higher value, however, is more reasonable for the general characteristics of the Upper Chalk aquifer in this region.

The step discharge test data may be used to determine the efficiency of the well through the use of standard methodologies (Figure 4-8). Concerns about the accuracy of the pressure transducers used during the first test resulted in a repeat of the step discharge test. Data from the second step discharge test (dated 5/12/97) will be analysed.

![Graph](image)

**Figure 4-8 Analysis of well performance at the Lychett Minster Test Site using data from the 1997 step rate pumping tests.**

The analysis indicated a well loss coefficient of between 0.0019 d/m² and 0.0023 d/m², and an aquifer loss coefficient of between $8\times10^{-7}$ d²/m⁵ and $9\times10^{-7}$ d²/m⁵ depending on whether injection or abstraction is taking place.
4.5.6. Local geology and hydrogeology of the Lychett Minster site

The geological profile encountered during the drilling activities at the Lychett Minster test site is summarised in Table 4-5, and in Figure 4-9. There is restricted hydraulic connection between the Chalk and the tertiary sand layers as a result of the low hydraulic conductivity of the basal London Clays. 2D modelling completed by CH2M-HILL indicated no significant flow between the Chalk and the confining sediments (CH2M-HILL, 2000a, CH2M-HILL, 2000b). The Poole formation is unconfined.

The aquifer is naturally artesian with a head of roughly 20 m above ground level. As a result, changes to the well head construction were difficult, and could only be completed with some, unmeasured, abstraction of water. Manual measurements of the piezometric level were not possible. Geophysical logging completed by the BGS identified a number of important fissures (Buckley, 1996; Buckley et al., 1998) at depths of 70.5 m, 76-78 m, 86.5 m, 94 m and 100 m. These fissures contributions to the overall volume of flow is identified in Table 4-6.

Table 4-5 Summary of geology at Lychett Minster.

<table>
<thead>
<tr>
<th>Geological Period</th>
<th>Lithostratigraphic unit</th>
<th>Thickness (m)</th>
<th>Depth to base of unit (mbgl)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tertiary</td>
<td>Poole formation</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>Tertiary</td>
<td>London Clay</td>
<td>37</td>
<td>44</td>
</tr>
<tr>
<td>Tertiary</td>
<td>London Clay – West Park Farm Member</td>
<td>15</td>
<td>59</td>
</tr>
<tr>
<td>Cretaceous</td>
<td>Undifferentiated Upper Chalk</td>
<td>51</td>
<td>110 (base of borehole)</td>
</tr>
</tbody>
</table>
Based on an original drawing by CH2M-HILL

Figure 4-9 Geology and borehole construction at the Lychett Minster Test Site.

Table 4-6 Summary of flow characteristics from the ASR well prior to cycle testing. Data from BGS Geophysical logging (Sept. 1997 and July 1998)

<table>
<thead>
<tr>
<th>Depth of fissure (m below ground level)</th>
<th>Fissure flow (%)</th>
<th>Cumulative flow (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>71</td>
<td>25</td>
<td>100</td>
</tr>
<tr>
<td>78</td>
<td>20</td>
<td>75</td>
</tr>
<tr>
<td>86</td>
<td>10</td>
<td>55</td>
</tr>
<tr>
<td>94</td>
<td>25</td>
<td>45</td>
</tr>
<tr>
<td>100</td>
<td>15</td>
<td>20</td>
</tr>
<tr>
<td>Below 100</td>
<td>5</td>
<td>5</td>
</tr>
</tbody>
</table>

There is a small south-easterly piezometric gradient of 0.004 across the Wareham Basin, and in the region of the Lychett Minster Test Site (Figure 4-3) which, assuming a hydraulic conductivity of 3 m/d (determined in Section 4.5.5) and a flowing porosity of 2%, indicates groundwater flowing at approximately 0.6 m/d to the south east at Lychett Minster. The implications of this relatively small hydraulic gradient for an ASR system are obvious. As water flows through the aquifer, the injected freshwater is carried away from the well. During the abstraction phase, this will mean that native groundwater water will be abstracted through the well at an earlier stage, resulting in a lower recovery efficiency of the system (see Section 2.5.2 for a discussion of this term).
When considering the implication of this factor for an ASR system, it should be realised that the flow velocity is very sensitive to a number of parameters, including the hydraulic gradient, the flowing porosity and the hydraulic conductivity. The latter two parameters are hard to define for a fractured aquifer such as the Chalk, and therefore a detailed examination will not be carried out for this location, for which there is limited knowledge of these parameters. Also, work carried out to characterise the geochemistry of the aquifer at the Lychett Minster Test Site (British Geological Survey, 1996) determined that the groundwater was 8,000 years old. This clearly does not support the calculated flow velocities, and further indicates that there may be errors in the estimated flowing porosity and hydraulic conductivity. Furthermore, ASR projects that operate in the USA have found that the impact of a small hydraulic gradient across the site is minimal, however this is a factor that should be examined prior to the implementation of ASR at any location.

4.5.7. Data collection

The test-pumping regime is outlined in Table 4-7.

Table 4-7 Cyclic pumping regime for the Lychett Minster Test Site.

<table>
<thead>
<tr>
<th>Cycle no</th>
<th>Action</th>
<th>Start time</th>
<th>Stop time</th>
<th>Duration (Days)</th>
<th>Time from start of testing (Days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Injection</td>
<td>10/12/97 10:32</td>
<td>14/12/97 21:42</td>
<td>4.47</td>
<td>4.47</td>
</tr>
<tr>
<td>1</td>
<td>Abstraction</td>
<td>15/12/97 08:46</td>
<td>22/12/97 10:17</td>
<td>7.06</td>
<td>11.53</td>
</tr>
<tr>
<td>2</td>
<td>Injection</td>
<td>29/12/97 09:00</td>
<td>08/01/98 17:30</td>
<td>10.35</td>
<td>21.88</td>
</tr>
<tr>
<td>2</td>
<td>Abstraction</td>
<td>09/01/98 09:00</td>
<td>10/01/98 11:17</td>
<td>1.10</td>
<td>22.98</td>
</tr>
<tr>
<td>3</td>
<td>Injection</td>
<td>11/01/98 08:00</td>
<td>21/01/98 12:05</td>
<td>10.17</td>
<td>33.15</td>
</tr>
<tr>
<td>3</td>
<td>Abstraction</td>
<td>22/01/98 09:00</td>
<td>26/01/98 11:08</td>
<td>4.09</td>
<td>37.24</td>
</tr>
<tr>
<td>4</td>
<td>Injection</td>
<td>27/01/98 17:30</td>
<td>07/02/98 17:34</td>
<td>11.00</td>
<td>48.24</td>
</tr>
<tr>
<td>4</td>
<td>Abstraction</td>
<td>09/02/98 09:00</td>
<td>14/02/98 20:01</td>
<td>5.46</td>
<td>53.70</td>
</tr>
<tr>
<td>4a</td>
<td>Injection</td>
<td>15/02/98 10:00</td>
<td>05/05/98 17:30</td>
<td>79.31</td>
<td>133.01</td>
</tr>
<tr>
<td>4a</td>
<td>Abstraction</td>
<td>19/05/98 10:00</td>
<td>19/05/98 17:30</td>
<td>0.31</td>
<td>133.32</td>
</tr>
<tr>
<td>5</td>
<td>Injection</td>
<td>20/05/98 12:00</td>
<td>01/06/98 20:00</td>
<td>12.33</td>
<td>145.66</td>
</tr>
<tr>
<td>5</td>
<td>Abstraction</td>
<td>02/06/98 09:00</td>
<td>11/06/98 21:30</td>
<td>9.52</td>
<td>155.18</td>
</tr>
<tr>
<td>6</td>
<td>Injection</td>
<td>16/06/98 10:15</td>
<td>29/06/98 16:00</td>
<td>13.24</td>
<td>168.42</td>
</tr>
<tr>
<td>6</td>
<td>Abstraction</td>
<td>30/06/98 12:30</td>
<td>10/07/98 09:00</td>
<td>9.83</td>
<td>178.27</td>
</tr>
<tr>
<td>7</td>
<td>Injection</td>
<td>11/07/98 10:00</td>
<td>24/07/98 10:00</td>
<td>13.00</td>
<td>191.27</td>
</tr>
<tr>
<td>7</td>
<td>Abstraction</td>
<td>24/08/98 12:30</td>
<td>02/09/98 18:00</td>
<td>9.23</td>
<td>200.50</td>
</tr>
<tr>
<td>8</td>
<td>Injection</td>
<td>03/09/98 10:00</td>
<td>07/12/98 10:00</td>
<td>95.00</td>
<td>295.50</td>
</tr>
<tr>
<td>8</td>
<td>Abstraction</td>
<td>07/01/99 12:00</td>
<td>19/01/99 18:00</td>
<td>12.25</td>
<td>307.75</td>
</tr>
<tr>
<td>9</td>
<td>Injection</td>
<td>21/01/99 09:00</td>
<td>26/05/99 08:50</td>
<td>124.99</td>
<td>432.74</td>
</tr>
<tr>
<td>9</td>
<td>Abstraction</td>
<td>01/07/99 15:00</td>
<td>03/09/99 08:45</td>
<td>63.74</td>
<td>496.48</td>
</tr>
</tbody>
</table>

During the abstraction phases, the solute concentrations in the abstracted water were measured. During the cycle tests, groundwater pressure was measured in all of the wells by piezometric pressure transducers and automatically recorded. The pressure transducers were occasionally recalibrated.
4.6. **Water chemistry**

Water samples were collected from the ASR well during the preliminary abstraction tests, prior to the injection of any water, in order to characterise the native groundwater.

Throughout the testing procedure solute concentration data were collected from the ASR well during injection and abstraction by automatic samplers, and recorded by a data-logger. The automatic samplers were supported by less frequent manual sampling at the wellhead, and analysis of these samples was completed by the Wessex Water laboratory according to Wessex Water’s standard procedures. Water samples were not collected from the observation well.

Between ASR test cycles 6 and 7, six multilevel tubes were inserted into the ASR well to allow collection of samples from different levels within the Chalk aquifer. The levels of these tubes are outlined in Table 4-8. The chemistry discussed within this thesis will be limited to the solute concentrations from the abstracted water.

**Table 4-8 Details of the multilevel sample tubes in the ASR borehole at the Lychett Minster Test Site.**

<table>
<thead>
<tr>
<th>Tube Number</th>
<th>Depth to base of tube (mbgl)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>107</td>
</tr>
<tr>
<td>2</td>
<td>99</td>
</tr>
<tr>
<td>3</td>
<td>92</td>
</tr>
<tr>
<td>4</td>
<td>85</td>
</tr>
<tr>
<td>5</td>
<td>75</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
</tr>
</tbody>
</table>

The native Chalk groundwater has a calcium bicarbonate chemistry. The pH of the groundwater ranges from 7.2 to 7.6 and the temperature is typically between 11 and 13°C. The conductivity ranges from 591 to 711 μS/cm.

The major inorganic constituents of the Upper Chalk groundwater are calcium, chloride, sodium, magnesium and silica. The alkalinity typically ranges from 227 to 246 mg/l, primarily in the form of bicarbonate ions. The chloride concentration ranges from 52 to 60 mg/l, with a mean in the measured concentrations of 56 mg/l. The minor inorganic constituents include fluoride, potassium, iron and ammonia. The fluoride concentration is variable, ranging from 2.5 to 4.1 mg/l, and in all instances exceeds the drinking water quality limit of 1.5 mg/l.
The complete solute chemistry of one of the samples taken from the Lychett Minster ASR well, prior to the injection of any water, are given as part of Appendix X, the compact disk enclosed with this thesis.

4.6.1. Data trends

The general trend of a selection of solute concentrations during the abstraction phase of Cycle 1 are illustrated in Figure 4-10. These solute concentrations are then plotted relative to the maximum measured solute concentration in Figure 4-11.

Chloride and fluoride showed a typical diffusion dominated solute concentration curve. Initially solute concentrations close to the injected values were detected, indicating that the injected water had only spent a short time interacting with the matrix water. With time, solute concentrations approached the native water as the injected water had more time to undergo diffusive exchange with the matrix water.

Nitrate concentrations followed a similar pattern, with abstracted solute concentrations showing a value close to injected concentrations and then falling to low native concentrations. This profile is the result of both diffusion of solutes from the fracture water into the matrix water and denitrification.

Sulphate concentrations remained consistently high in the abstracted water, possibly indicating oxidation of pyrite within the matrix material.

Figure 4-10 Selection of solute concentrations in the abstracted water from the first test cycle at the Lychett Minster Test Site.
4.6.2. A brief examination of the chemistry data

It is necessary to identify a suitable tracer from the data collected at Lychett Minster that may be used to calibrate the DP-Pulse model. Because of the simplicity of the DP-Pulse model, which currently has no ability to model radioactive production and decay or chemical reactions, it was necessary to choose a conservative tracer. Initially it was thought that the fluoride solutes behaved in a conservative manner, and that the primary control over fluoride concentrations was the double-porosity effect. As a result, it was proposed that fluoride be used as the conservative tracer, as it has a similarly low reactivity to chloride, yet was main the solute of concern in the Lychett Minster ASR test.

Early cycles (Cycles 1 to 3, Figure 4-12; Cycle 1, Figure 4-13) showed a high correlation between the fluoride and the chloride solute concentrations. However, cycles 4, 5, 6 and 7 showed a marked difference between the chloride and fluoride data (Cycles 4 to 7, Figure 4-12; Cycle 4, Figure 4-13), highlighting that as the two were not behaving in a similar manner, at least one cannot have been conservative. Geochemical modelling of the groundwater/injected water interactions highlighted over-saturation of the native groundwater with respect to fluorite (CaF$_2$), and under-
saturation of the injected and abstracted waters (Williams et al., 1999; CH2M-HILL, 2000a; Gaus et al., 2002). This would indicate the existence of precipitated fluorite within the aquifer, which could be dissolved by the injected water, thus providing a source of fluoride. As a result of this, all modelling of double-porosity processes examined the behaviour of chloride, as in all but the rarest circumstances chloride behaves in a conservative manner.

Figure 4-12 Relative fluoride and chloride concentrations in abstracted water from 8 test cycles at the Lychett Minster ASR test site.
It is also important to describe the solute concentrations being injected into the well. The solute concentrations the injected water were analysed at frequent intervals, and the results for the Chloride analyses for Cycles 1 to 8 are presented in Figure 4-14. From this it can be seen that the injected water had a relatively stable chloride concentration, ranging between 25 and 30 mg/l, but generally falling between 28 and 30 mg/l.

Figure 4-14 Chloride concentrations in the water injected into the aquifer, Cycles 1 to 8.

4.6.3. Noise within the data set
As can clearly be seen from Figure 4-12, the data set obtained from the ASR test is affected by noise. Errors can arise from a number of sources, including lack of
instrument sensitivity, drift of the instrument calibration and mistakes made when
sampling the water. Aquifer heterogeneities will also be significant, as one major
model assumption is that the aquifer is homogenous.
For the purposes of this thesis it is important to be able to characterise the noise, as
this will be simulated in Chapters 8 and onwards.
In order to determine the standard deviation of the data, and to characterise the noise,
it is necessary to establish the trend to subtract to reveal the noise. As the data is
non-linear in nature, it is unsatisfactory to simply complete a linear regression
analysis. Instead, the trend must form a similar shape to the data. There are a
number of means of doing this, each with their drawbacks.
The DP-Pulse model could be applied to simulate the data, and hence provide a
baseline for comparison. This method should reasonably reproduce the shape of the
curve of an individual cycle. Unfortunately, limitations in the DP-Pulse model limit
its capability to reproduce all of the data, including data collected at the start of the
recovery cycle. Certain individual cycles, notably Cycle 4 are also poorly
represented by the model. This would result in a higher value for the measure of
noise than is reasonable.
A suitable method for the determination of noise is to compare a standard equation to
the solute concentration data. A number of different non-linear equations could be
used, the simplest being a quadratic equation. Increasing the complexity of the
equation used to produce the baseline potentially allows the curve to follow the
course of the data more accurately. There is, however, a trade-off between the
complexity of the curve used and the information obtained.
It would potentially be possible to analyse the error in a detailed quantitative manner,
indicating the sources of error, and the relationship between the error and the
sampling plan. This body of work, however, does not attempt this, rather producing
a rough quantitative analysis of the error that will allow the overall pattern of error to
be reproduced. In order to determine the minimum complexity of baseline equation
required to perform this function, both a quadratic and a cubic equation were fitted to
the solute concentration data from each abstraction cycle, by means of a least squares
fitting process. The deviation of the data residual from this baseline was then
visually examined to determine whether the calculated errors in the data change with
time in a systematic manner, an indication that the baseline equation is not
sufficiently complex to reproduce the data set. Further complexity was not
introduced into the baseline equation as the required accuracy of the noise characterisation process was not considered sufficient to demand greater complexity. It is important to note that there may also be a systematic change in the error if there is significant drift in the instrument calibration, if there is significant groundwater flow due to a natural piezometric gradient, if the aquifer is inhomogeneous, or if the solute is unevenly distributed through the aquifer. (These last two possibilities occur as water that is abstracted later in the testing procedure will have passed through a greater volume of aquifer. As water that has flowed through a greater volume of the aquifer will be affected by that greater volume of aquifer, the cumulative effect on the water will be to average across the inhomogeneities, and hence the solute concentration will be close to an averaged value. Water that has passed through a lesser aquifer volume will be more affected by local variations in the aquifer and therefore differ more from the average value.)

Figure 4-15, Figure 4-16 and Figure 4-17 show how the error changes with time for three of the cycles. The solute chemistry data has been normalised so that the injected water chemistry has a solute concentration of 0.0, and the native water chemistry has a solute concentration of 1.0. This normalisation has been carried out as data used by the DP-Pulse model, and the data produced by the model are all normalised in this manner.

Visual inspection indicates that there is no apparent trend in the variation of the absolute error values. There appear to be indications of a recurring variation, with a wavelength of about 1 day in Cycle 3, and a wavelength of about 60 days in Cycles 6 and 9. This variation, however, is a result of the limited precision of the solute concentration analyses. As the solute concentrations are reported to two significant figures, a slowly increasing solute concentration will produce a series of identical results, with an occasional step increase, a pattern not reproduced by the cubic or quadratic equations. Although this may result in small discrepancies in the measure of the error, the amplitude of the variation is small compared to the maximum measured values and therefore there is unlikely to be a significant effect on the measured noise. Additionally, it is worth noting that the divergence of the data from the baseline in this manner will serve to increase the measured level of noise. As there is no significant difference between the results obtained for a quadratic and a cubic equation, the simpler quadratic form will be used for further analyses.
Figure 4-15 Difference between the measured solute chemistry data and a fitted quadratic curve for Cycle 3 of the Lychett Minster ASR test.

Figure 4-16 Difference between the measured solute chemistry data and a fitted quadratic curve for Cycle 6 of the Lychett Minster ASR test.
Figure 4-17 Difference between the measured solute chemistry data and a fitted quadratic curve for Cycle 9 of the Lychett Minster ASR test.

Application of this method found that both quadratic and cubic equations could reproduce the curve shape and therefore provide a suitable baseline for the determination of the noise. This method is not without drawbacks. Although both equations appear to reasonably reproduce the curve shape, there may be subtleties that are missed. As a result, the measured noise may be slightly different to the ‘true’ value. This will be discussed after the application of the method.

The standard deviation was then calculated according to the deviation of the experimental data from the quadratic baseline. There are two possible means by which the error can be measured. One is simply the difference between the measured value and the curve approximation, referred to below as the ‘absolute error’, the other is that difference as a percentage of the total value, below discussed as the ‘relative error’. By plotting histograms of the each measure of error we can look at the distributions (Figure 4-20 and Figure 4-18) of the errors. Probability plots indicate how close to normal the distributions are (Figure 4-19 and Figure 4-21). A normal distribution will plot as a straight line (Shapiro and Gross, 1981). In both cases the errors appear to be close to normally distributed, although the relative error less so.
Figure 4-18 Histogram of the differences between experimental data set and quadratic approximation for nine cycles of the Lychett Minster ASR Test.

Figure 4-19 Probability plot of the differences between experimental data set and quadratic approximation for nine cycles of the Lychett Minster ASR Test.
Figure 4-20 Histogram of the normalised differences between experimental data set and quadratic approximation for nine cycles of the Lychett Minster ASR Test.

Figure 4-21 Probability plot of the normalised differences between experimental data set and quadratic approximation for nine cycles of the Lychett Minster ASR Test.
We can examine the data quantitatively by applying the two-tailed Kolmogorov-Smirnov One-Sample Test (Stevens and D’agostino, 1986). This may be used to test the hypothesis that a sample comes from a particular distribution (including uniform, normal, or Poisson). In this scenario the test was applied to the hypothesis that the data is normally distributed.

For the true error, an asymptotic significance of 0.155 is obtained. This indicates that the distribution may be treated as normal. For the normalised error, an asymptotic significance of 0.000 is obtained. This indicates that the null hypothesis is true, and that the normalised error is not normally distributed.

We can therefore describe the noise as being absolute values (independent of solute concentrations), normally distributed with a specified standard deviation.

\[
\sigma^2 = \frac{\sum_{n=1}^{N} (x_{\text{data}}^n - x_{\text{curve}}^n)^2}{N-1}
\]  

(111)

\[\sigma^2\] = variance in experimental data

\[x_{\text{data}}\] = experimental data value

\[x_{\text{curve}}\] = value from quadratic curve fitted to experimental data

\[N\] = total number of data points

As has been discussed, the use of an equation to produce a trend for comparison has a potential drawback as the curve may not be completely similar to the abstraction curve. The slight change in gradient at the highest percentiles on both probability plots may indicate a slight skew in the data set, alternatively it may be indicative of the fact that the baseline is not ideal.

In summary, for the purposes simulating the noise, it is justifiable to apply normally distributed random noise. This noise should be applied irrespective to the simulated solute concentration at that point in time. Suitable values for the standard deviation of the normal distribution have been calculated using equation 111 and are given in Table 4-9.
Table 4-9 Table of the standard deviation in the absolute error in the data collected at the Lychett Minster Test Site for each of nine cycles, and for the nine cycles as a whole.

<table>
<thead>
<tr>
<th>Cycle No.</th>
<th>Absolute error</th>
<th>Standard deviation</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0009</td>
<td>0.0307</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.0001</td>
<td>0.0088</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.0016</td>
<td>0.0404</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.0004</td>
<td>0.0195</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.0015</td>
<td>0.0386</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.0017</td>
<td>0.0410</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.0007</td>
<td>0.0261</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0.0004</td>
<td>0.0197</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>0.0011</td>
<td>0.0329</td>
<td></td>
</tr>
<tr>
<td>Average</td>
<td>0.0009</td>
<td>0.0301</td>
<td></td>
</tr>
</tbody>
</table>

The difference between the chloride concentration of the native groundwater (52 - 60 mg/l) and the chloride concentration of the injected water (25 – 30 mg/l) is quite small. Caution should be applied when normalising the data, as a change in solute concentration of 1 mg/l will change the relative solute concentration by approximately 2%. The standard deviation of the noise in the data determined above is slightly larger, at 3%. For the purposes of this investigative work, this degree of uncertainty in the data is considered acceptable. Caution should be applied when using this methodology to direct operations when testing and operating an ASR system.
Chapter 5

Calibration of DP-Pulse model to data from the
Lychett Minster Test Site
5. Calibration of DP-Pulse model to data from the Lychett Minster Test Site

The primary use in this thesis for the solute chemistry data collected during the ASR trials at the Lychett Minster Test Site was calibration of the DP-Pulse model. As well as allowing the characterisation of an aquifer with the novel parameterisation of \( t_{cb} \) and \( \sigma \) (see Section 3.4.1), a good calibration of the model would indicate that the model was suitable for use in simulating ASR in a double-porosity system, the function for which it was designed. In short, to successfully calibrate the model, and produce a good simulation of real processes occurring would go a long way towards validating the model for further use.

5.1. Model calibration to the data from the Lychett Minster Test Site.

The model was automatically calibrated to the chloride data collected from the Lychett Minster test site using the Levenberg-Marquardt routine detailed in Section 3.11.4.2. The data input to the calibration model can be seen below (Table 5-1). The initial parameter estimates were \( t_{cb} = 1000 \) days, \( \sigma = 50 \). A pulse interval of 1 day was used.

Table 5-1 Pumping-cycle times input for the semi-analytical model (days).

<table>
<thead>
<tr>
<th>Step</th>
<th>Injection</th>
<th>Storage</th>
<th>Abstraction</th>
<th>Dormancy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.47</td>
<td>0.46</td>
<td>7.06</td>
<td>6.95</td>
</tr>
<tr>
<td>2</td>
<td>10.35</td>
<td>0.65</td>
<td>1.1</td>
<td>0.86</td>
</tr>
<tr>
<td>3</td>
<td>10.17</td>
<td>0.87</td>
<td>4.09</td>
<td>1.27</td>
</tr>
<tr>
<td>4</td>
<td>11.00</td>
<td>1.64</td>
<td>5.46</td>
<td>0.58</td>
</tr>
<tr>
<td>4a</td>
<td>79.31</td>
<td>13.69</td>
<td>0.31</td>
<td>0.77</td>
</tr>
<tr>
<td>5</td>
<td>12.33</td>
<td>0.54</td>
<td>9.52</td>
<td>4.53</td>
</tr>
<tr>
<td>6</td>
<td>13.24</td>
<td>0.85</td>
<td>9.85</td>
<td>1.04</td>
</tr>
<tr>
<td>7</td>
<td>13.00</td>
<td>31.10</td>
<td>9.23</td>
<td>0.67</td>
</tr>
<tr>
<td>8</td>
<td>95</td>
<td>31.08</td>
<td>12.25</td>
<td>1.63</td>
</tr>
<tr>
<td>9</td>
<td>124.99</td>
<td>36.26</td>
<td>63.74</td>
<td>0.00</td>
</tr>
</tbody>
</table>

It was decided that the addition of the capacity to simulate mixtures of different sized blocks, or mixtures of slabs and spheres would significantly increase the complexity of the calibration routine. It was further decided that the application of the data weighting routines would introduce extra complexity, which could not be justified without a rigorous investigation of the implications of weighting the data. As a
result, the calibration used only compares the results from calibrating an unweighted data set to the experimental data with either a slab or a sphere block geometry.

A reasonably successful fit to the solute data was made (Figure 5-1). The calibration routine was run twice for each block geometry. The first run allowed calibration to two parameters, $t_{cb}$ and $\sigma$. The second run calibrated to the two parameters $t_{cf}$ and $\sigma$. Analysis of the quality of the fit was completed by the definition of confidence intervals for each of the parameters. The 95% confidence bound, for example, gives a parameter region within which it is possible to be 95% sure that the actual parameters are situated. The calibrated parameter values, as well as the confidence bounds on the calibration are produced in Table 5-2.

**Table 5-2 Parameters from the calibration of the DP-Pulse model to the Lychett Minster Test Site data. Data set unweighted.**

<table>
<thead>
<tr>
<th>Block geometry</th>
<th>Calibrated Parameters</th>
<th>Parameter</th>
<th>Calibrated value</th>
<th>50% confidence minimum</th>
<th>50% confidence maximum</th>
<th>95% confidence minimum</th>
<th>95% confidence maximum</th>
<th>Calculated $t_f$ value (Days)</th>
<th>'Sum of squares'</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slab</td>
<td>$t_{cb}$ / $\sigma$</td>
<td>$t_{cb}$ (Days)</td>
<td>1086</td>
<td>1024</td>
<td>1149</td>
<td>904</td>
<td>1269</td>
<td>0.44</td>
<td>293</td>
</tr>
<tr>
<td></td>
<td>$\sigma$</td>
<td>( - )</td>
<td>49.5</td>
<td>47.9</td>
<td>51.0</td>
<td>45.0</td>
<td>53.9</td>
<td>0.44</td>
<td>293</td>
</tr>
<tr>
<td>Sphere</td>
<td>$t_{cf}$ / $\sigma$</td>
<td>$t_{cf}$ (Days)</td>
<td>0.44</td>
<td>0.43</td>
<td>0.46</td>
<td>0.39</td>
<td>0.49</td>
<td>0.44</td>
<td>293</td>
</tr>
<tr>
<td></td>
<td>$\sigma$</td>
<td>( - )</td>
<td>49.4</td>
<td>47.9</td>
<td>51.0</td>
<td>45.0</td>
<td>53.9</td>
<td>0.44</td>
<td>293</td>
</tr>
<tr>
<td></td>
<td>$t_{cb}$ / $\sigma$</td>
<td>$t_{cb}$ (Days)</td>
<td>10153</td>
<td>6530</td>
<td>13775</td>
<td>411</td>
<td>20717</td>
<td>0.40</td>
<td>308</td>
</tr>
<tr>
<td></td>
<td>$\sigma$</td>
<td>( - )</td>
<td>158.4</td>
<td>132.2</td>
<td>184.6</td>
<td>82.0</td>
<td>234.7</td>
<td>0.40</td>
<td>308</td>
</tr>
<tr>
<td>Sphere</td>
<td>$t_{cf}$ / $\sigma$</td>
<td>$t_{cf}$ (Days)</td>
<td>0.40</td>
<td>0.39</td>
<td>0.42</td>
<td>0.35</td>
<td>0.46</td>
<td>0.40</td>
<td>308</td>
</tr>
<tr>
<td></td>
<td>$\sigma$</td>
<td>( - )</td>
<td>158.3</td>
<td>132.2</td>
<td>184.4</td>
<td>82.2</td>
<td>234.5</td>
<td>0.40</td>
<td>308</td>
</tr>
</tbody>
</table>
Figure 5-1 Calibration of DP-Pulse model to conservative tracer (Chloride solute) data from the Lychett Minster Test Site (block geometry = uniform slab, \( t_{cb} = 1086 \) days, \( \sigma = 49.5 \), \( \Delta T = 0.5 \) days; block geometry = uniform sphere, \( t_{cb} = 10153 \) days, \( \sigma = 158.4 \), \( \Delta T = 1 \) day).
It is immediately apparent that the calibrated values of \(t_{cb}\) and \(\sigma\) are much larger for the sphere geometry than for the slab geometry, while the calibrated values of \(t_{cf}\) are similar. This discrepancy is interesting as it illustrates the impact that the block geometry has on the data during long simulations. It is difficult to determine which is the correct geometry. Both slab and sphere simulations provide a similar visual match to the experimental data set (Figure 5-1), and the calculated error is too close to enable a selection to be made.

The sizes of the confidence intervals in the fit to a spherical geometry are very large. For the slab geometry, the difference of the 95% confidence interval maxima and minima to the calibrated value is less than 6%. For the sphere geometry, this difference is almost 36%. This indicates poor resolution of the calibration with the sphere geometry.

### 5.1.1. Physical meaning of calibrated parameters

The parameters outlined in Table 5-2, determined through the calibration process, can be converted to a more conventional parameter set. In order to do this it is necessary to estimate the values of two parameters. By assuming the apparent diffusion coefficient (from Fretwell, 1999) and the matrix porosity (see Section 2.7) it is possible to construct Table 5-3.

**Table 5-3 Physical characteristics of the aquifer at the Lychett Minster Test Site, interpreted from calibrated parameters.**

<table>
<thead>
<tr>
<th>Slab Geometry</th>
<th>Sphere Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Calibrated parameters</strong></td>
<td><strong>Calculated aquifer characteristics</strong></td>
</tr>
<tr>
<td>(\sigma = 49.5)</td>
<td>(b = 16.8) cm</td>
</tr>
<tr>
<td>(t_{cb} = 1086) days</td>
<td>(a = 2.7) mm</td>
</tr>
<tr>
<td>(\phi_f = 0.008)</td>
<td>(\phi_f = 0.008)</td>
</tr>
<tr>
<td><strong>Assumed Parameters</strong></td>
<td><strong>Calibrated parameters</strong></td>
</tr>
<tr>
<td>(D_A = 3 \times 10^{-10}) m²s⁻¹</td>
<td>(\sigma = 158.4)</td>
</tr>
<tr>
<td>(\phi_m = 0.4)</td>
<td>(t_{cb} = 10153) days</td>
</tr>
<tr>
<td>Where (2b) is the fracture spacing and (a) is the fracture aperture (Figure 3-1)</td>
<td><strong>Calculated aquifer characteristics</strong></td>
</tr>
<tr>
<td>Assumed Parameters</td>
<td><strong>Calculated aquifer characteristics</strong></td>
</tr>
<tr>
<td>(D_A = 3 \times 10^{-10}) m²s⁻¹</td>
<td>(r = 154) cm</td>
</tr>
<tr>
<td>(\phi_m = 0.4)</td>
<td>(a = 2.6) mm</td>
</tr>
<tr>
<td>Where (r) is the sphere radius and (a) is the ratio of the volume to the surface area</td>
<td></td>
</tr>
</tbody>
</table>

These values indicate blocks between 30 and 154 cm in size, with a wide fracture aperture of at least 2.6 mm. With the exception of the block size when the sphere geometry is selected, these values fall within the parameter range delineated for the Chalk in Table 6-1.

Through application of the cubic law (equation 112) it is possible to reinterpret these physical characteristics as hydraulic conductivities. It should, however, be noted that
the cubic law is unable to capture the complexity of the real system, and therefore these results should be treated with caution. The cubic law indicates a hydraulic conductivity of 3.5 m/d assuming a slab geometry. This value is of the same order of magnitude as those determined from piezometric data collected during the pumping tests carried out at the site (Section 4.5.5).

The correspondence of the calibrated parameters to measured characteristics is a good indication that the DP-Pulse model is capable of correctly simulating the processes occurring, and can therefore be seen as a partial validation of the model for this scenario. There are, however, limitations to the extent to which the model is capable of representing the system. An important uncertainty is the lack of determination of the correct block geometry, discussed below. Further limitations, arising from the failure of the assumptions to correctly describe the system are discussed in the next section.

The block sizes calculated from the two calibrations are very different. The poor resolution of the spherical geometry discussed in the previous section results from the larger block size. For a spherical geometry, the cycle tests undertaken are of insufficient duration to sufficiently characterise the aquifer, as the larger blocks mean that the time required for the fracture water to diffusively interact with the centre of the matrix blocks is significantly larger. This is reflected in the large increase in $t_{cb}$.

Determining the correct block geometry is not possible with this data set. In order to decide if the system is best represented by a sphere or slab (or another) geometry further work would have to be conducted. Ideally, the rock strata would be examined intensively through excavation, but this would be difficult considering the artesian nature of the aquifer. Alternatively, conducting a series of extended tests, of a duration consistent with the identified $t_{cb}$ for a spherical geometry, on the aquifer would then allow recalibration of the model. It would then be possible to determine which model best fitted both early and late time data (divergence of the two models can already be seen by Cycle 9). As the identified $t_{cb}$ for the spherical geometry is so large, the aquifer tests would have to be approximately 10 times longer than those conducted to date. Using the current data set, the only indication of the correct block geometry is found in the difference between the calculated hydraulic conductivities. The hydraulic conductivity determined for the spherical geometry is smaller than those measured by an order of magnitude, possibly indicating that the slab geometry better represents the fracture network.
In Chapter 4 the geophysical logging of the ASR borehole at the Lychett Minster site completed by the BGS was briefly discussed. Fissures were identified at intervals of approximately 7 m, indicating a value for $b$ of around 350 cm. The discrepancy between the measured values, and those determined through calibration of the data set indicates that although a significant proportion of flow is occurring along the large identified fissures, a proportion of the flow is also flowing along smaller fissures. This would imply that standard techniques of fissure detection, including flow logging, are insufficient for the purposes of characterising the double-porosity nature of this aquifer.

The calculated fissure aperture indicates that it is likely that the fissuring through which water is flowing has undergone some dissolution. The fracture porosity identified is low in both cases, being of the same order of magnitude as the lowest fracture porosities identified in the literature. The assumed matrix porosity, used to determine the fracture porosity, is the maximum identified in the literature. This result highlights the extreme doubly-porous nature of the Chalk, with the volume of water within the matrix being significantly larger than the volume of water in the fractures.

5.1.2. The capability of the DP-Pulse model to successfully simulate operations at the Lychett Minster ASR Test Site

It is important to discuss the capability of the DP-Pulse model to successfully simulate operations at the Lychett Minster ASR Test Site. If the DP-Pulse model is not suitable for the purpose, the calibration of the model, and subsequent interpretation, must be treated with caution. As well as a number of assumptions used in the model that may affect the capability of the DP-Pulse, accuracy of the calibration, the formulation of the model results in a number of limitations to the possible accuracy of the calibration.

The first limitation is a result of varying the rate of injection. The DP-Pulse model has been formulated in a manner which results in it being completely rate-invariant, i.e. solute concentrations measured at the ASR well are invariant with respect to rate. This is only true if all flow rates (in and out of the well) are the same. The nine cycles all involved injection or abstraction at either 2 or 3.2 Ml/d. The model assumes that all pumping was at the same rate. This difference between the simulated activities and the actual operations will result in discrepancies between the measured solute concentrations and the simulated concentrations, and hence
inaccuracies in the calibration. Furthermore, continuing variations in the flow rate are likely to lead to a cumulative error. Clearly, for the purposes of this type of calibration, introducing the capability for DP-Pulse to deal with variable flow rates will be important.

Between cycles 5 and 6 and cycles 6 and 7 an uncertain amount of leakage occurred due to works on the well head. During these times an unknown quantity of water came out of the well for an unknown duration under artesian conditions. The resulting flow brought water that had been in the aquifer for a longer period of time, and thus water with a solute concentration closer to equilibrium with the native water, closer to the well. The solute concentration of the water abstracted from the well would be higher than model predictions as a result. As the simulated timescale is much greater than the duration over which this leakage occurred, however, this discrepancy is likely to be of minor significance.

The DP-Pulse model discretises the pumping rate into a series of instantaneous pulses of flow separated by a time, $\Delta T$. In the version of the code used all time periods must be integer multiples of $\Delta T$. This code was selected to simplify the automated calibration routine, other forms of the DP-Pulse model are capable of simulating solute concentrations at any time. With the selected code it is not possible, therefore, to produce a perfect simulation of the pumping sequence. The time-scale of this discrepancy is again small relative to the simulated model duration and hence the significance is likely to be small.

In addition to the limitations already described, a number of assumptions are made that may affect the capability of the model to correctly simulate the processes occurring. These assumptions were discussed in Section 3.4. Each of these assumptions will now be explored, with regard to the implication for the quality of the calibration.

1. **Steady state flow conditions are established instantaneously.**

As has been previously stated, storativities in fractured aquifers are generally small, and steady state flow conditions are rapidly approached. In order to determine how rapidly this occurs, it is possible to examine the drawdown curves measured in the aquifer during testing carried out on the Lychett Minster ASR well. Looking back at Section 4.5.5, and specifically at the drawdown data from the 1994 constant rate pumping test, it can be seen that steady state flow can be seen (i.e. the drawdown in
the well approaches equilibrium) after approximately 30 minutes. As the shortest duration of any of the cycle test phases was a little over 4 days, the duration of the non-steady state flow is less than 1% of the overall phase duration.

This transient flow must result from elastic storage in both the fractures and the matrix. During injection, the increased pressures will lead to extra volumes of water being transiently stored in the fractures, where it will then interact diffusively with the matrix. This will not significantly impact on the capability of the model to simulate the system, as the volume of extra water within a single cell stored under elastic conditions will be too small to have a significant impact on the solute concentration of that cell. There will also, however, be some exchange of water between the matrix and fracture volumes, resulting from elastic storage within the matrix. As the water within the matrix may have a significantly different composition to that in the fractures, there may be some significant impact on the concentration of the water within the fracture. The potential impact of this period during which storage plays a role can be determined by calculating the volume of water that is potentially forced into the matrix.

The argument presented here is limited in that it examines the very worst case scenario – release of water from storage close to the well. The volume of water released in this way is proportional to the decreasing piezometric level. Close to the well, changes in the piezometric level are relatively high in magnitude, and at distances of greater than 50 m the change in piezometric level is likely to be small. The volume of water determined below is, therefore, only representative of a small region of the aquifer in which ASR is taking place. Additionally, the calculation does not allow for the impact of injection on the aquifer, during which increasing piezometric levels will force water back into the matrix.

In Section 4.5.5 the storativity of the aquifer at Lychett Minster was determined to be 2.54×10⁻⁴, indicating a specific storage of 5.8×10⁻⁶ m⁻¹. As the fracture porosity of the Chalk is relatively small, the major contribution to the storativity of the aquifer will be from the matrix volume. Reducing the piezometric head within the aquifer will therefore lead to release of water from the matrix volume, and this water will flow into the fracture network. Using these parameters, the fracture porosity determined through the calibration of the DP-Pulse model in Section 5.1.1, and the piezometric head changes measured during the ASR cycle testing procedure, it is possible to quantify the volume of this water that is exchanged during ASR cycling.
For each metre change in the piezometric head within the aquifer, \(5.8 \times 10^6\) m\(^3\), or 0.006 litres of water per m\(^3\) will be released into the fracture network. The maximum drawdown measured in the well was during the 1994 pumping test, at the end of which the change in the piezometric head close within the well was 19.8 m. In total, therefore, 0.12 litres/m\(^3\) of water would have been released from the matrix through the relaxation of the elastic storage that results from the reduction of the piezometric head. Assuming a matrix porosity of 0.4, and using a \(\sigma\) value of 50, the same cubic metre of aquifer would by definition of \(\sigma\) have a fracture volume of 0.8\%, or 8 litres. As a result, the total addition of water from the matrix to the volume of water fracture resulting from the change in the piezometric head would be 1.5\%.

Assuming a solute concentration for the water in the fracture of 1, and a solute concentration of the water in the matrix of 0, the change in solute concentration within the fracture, resulting from the release of water from the matrix, would therefore be 0.0125. This volume of exchange is therefore unlikely to be significant in controlling the solute concentration in the fractures, and hence in the abstracted water.

This change in the solute concentration is very small, and well within the level of error determined through statistical analysis in Section 4.6.3. It should also be noted that the change in piezometric head decreases rapidly with distance from the well, and the head gradient will rapidly equilibrate with time. Therefore, this exchange will decrease with distance from the well, and with time as equilibrium is reached.

2. The aquifer is homogenous.

The Chalk aquifer at the Lychett Minster site is clearly not homogenous. Although little is known about the aquifer, as limited investigative drilling work has been undertaken, it is almost certain that lateral variation will occur. It is possible to look at the implications of the failure of this assumption through detailed examination of the calibration of the model.

Figure 5-2 shows the results of a sequence of calibrations of the DP-Pulse model to the data from successive cycle tests at the Lychett Minster test site (assuming slab geometry). The calibration to each cycle incorporates the data collected during all previous cycles. There is clear variation in the calibrated parameters with each cycle.
Figure 5-2 DP-Pulse calibration of $t_{cb}$ and $\sigma$ to successive Lychett Minster Cycle tests.

The variations in the calibration can be seen in both the early and the late cycle tests. The early cycle tests are of relatively short duration, and even the cumulative duration of these tests is shorter than the time required for diffusive exchange to occur between the fracture water and the centre of the matrix block. This may account for the variation at early times, as the system is not fully tested. The longer duration cycle tests are of sufficient duration that diffusive exchange between the fracture water and the centre of the matrix block is likely to have taken place. The system is fully 'sampled', however the calibrations of subsequent cycles are not identical. It is probable that variations in the calibration on this timescale result from heterogeneities in the Chalk aquifer, which result in cycle tests of different durations (and hence different scales) interacting with different aquifer volumes. Heterogeneities in the aquifer therefore affect the quality of the calibration to a certain extent in scenarios where the volume of aquifer affected by ASR operations varies, and the potential impact of this should be considered before implementation of the DP-Pulse model.

3. The aquifer is fully confined.

The aquifer at the Lychett Minster test site has a piezometric level of approximately 20 m above ground level. It is therefore correct to say that the aquifer is very well confined.
4. **There is no water movement in the rock matrix.**

There are insufficient data collected from the Lychett Minster test site to confirm the physical characteristics of the Chalk aquifer at this location. Although a nearby borehole was cored, the core was of such poor quality that it was not possible to determine fracture apertures or spacings. Also, there were no attempts to measure the porosity or pore throat size of the cored samples. In order to examine this assumption it is necessary to use previous research completed on the Chalk in different locations. Section 2.7 details measurements taken of the hydraulic conductivities of the Chalk matrix, giving values between $1 \times 10^{-5}$ and $1 \times 10^{-2}$ m/day. Measured hydraulic conductivities of the aquifer at this site range between $3.44 \times 10^0$ and $1.29 \times 10^1$ m/day (Table 4-4). Using the highest measured hydraulic conductivity of the matrix, and the lowest measured hydraulic conductivity of the aquifer (assuming all flow is fracture flow), and assuming a matrix porosity of 0.4 and a fracture porosity of 0.008, a simple calculation of flow under normal conditions (i.e. a piezometric gradient of 0.004) can be completed. This indicates a flow velocity in the matrix of 0.1 mm/day, with an overall flow velocity in the aquifer of 1.72 m/day.

Repeating this calculation for the maximum gradient created between the ASR well and the observation well during the cycle testing (a piezometric gradient of 2.07) indicates a flow velocity in the matrix of 5.17 cm/day, with an overall flow velocity in the aquifer of 889 m/day.

Clearly, although there is significantly more flow within the fracture system than the matrix, in close proximity to the well the piezometric gradient created during injection and abstraction is sufficiently large to induce small amounts of flow through the matrix. As a result, the assumption that there is no movement of water within the matrix is difficult to support close to the well.

At a distance from the well the piezometric gradient will be significantly smaller, as will the flow velocity in the matrix. At a distance from the well this assumption may be reasonable.

5. **The fracture water remains locally at a uniform but changing concentration.**

The potential error resulting from this assumption was discussed in Section 3.6. The specific scenario where $t_{cb}$ is large, but not infinite as is the case with the system
currently being examined, is discussed in Section 3.7.1. For this calibration, the pulse interval used was 1 day. Using the methodology indicated in Section 3.7.1 it was determined that the error in the solute concentrations arising for a pulse interval of 1 day, after 690 days of flow, was less than 0.05%. After 10 days of flow, the error in the solute concentrations was less than 1%.

6. **Mechanical dispersion is negligible.**
The assumption that mechanical dispersion is negligible was discussed in Section 3.8. This section concluded that as long as the criteria stated in equation 107 \( t_{cf} < t_a << t_{cb} \) were fulfilled, the assumption would hold. For both block geometries, \( t_{cf} \) (less than 0.5 days) is significantly smaller than \( t_a \) (690 days), and \( t_{cb} \) (1086 days for the slab geometry, 10153 days for the spherical geometry) is greater than \( t_a \).

7. **Movement of solutes within the matrix is described by Fick’s second law and is characterised by an ‘apparent’ diffusion coefficient.**
As has been discussed, it is widely recognised that Fick’s second law suitably describes the movement of solutes by diffusion. As long as Fick’s second law describes all movement of solutes, i.e. that there is no movement of water in the matrix volume as previously assumed, this assumption is valid. The examination of previous assumptions has, however, highlighted that there is a small, but significant amount of groundwater flow through the matrix volume close to the ASR well. This has the potential to render the assumption invalid close to the ASR well.

8. **Density effects on the flow are ignored.**
The mass of total dissolved solids (calculated from the conductivity) within the injected water (between 390 and 410 mg/l) is not significantly less than in the native groundwater (between 430 and 470 mg/l). As a result, the assumption that density effects on the flow can be ignored is valid.

9. **Initially, the solute concentration through the matrix is uniform and at equilibrium with the local fracture water.**
Work carried out to characterise the geochemistry of the aquifer at the Lychett Minster Test Site (British Geological Survey, 1996) determined that the groundwater
was 8,000 years old. This is sufficient time for equilibrium to be reached between the matrix and fracture waters, and for the matrix waters to be of uniform concentration. This equilibrium could be disturbed by the injection of water, however as the ASR testing operations carried out at this site were the first known periods of injection, this assumption is likely to hold.

5.1.3. Potential implications of the failure of the assumption that there is no flow in the matrix

A number of the assumptions discussed in the previous section rely on the assumption that there is no movement of water within the matrix material. As well as the assumption stating this, the assumption that steady state flow is reached instantaneously, and that the movement of solutes within the matrix is controlled by Fick’s second law implicitly rely on this fact. As has been discussed, although in general water movement within the matrix is so small as to be insignificant, during periods of injection and abstraction high piezometric gradients develop close to the well, and as a result there is a small, but substantial amount of flow within the matrix block. This flow was calculated to be up to a maximum of 5.17 cm/day, with potential to significantly impact the capability of the DP-Pulse model to simulate such a system.

This problem is not as simple as presented, however. Fracture networks are complex and there is a high potential that the piezometric gradient is not applied across a single matrix block. For example, considering the hypothetical situation of a series of horizontal planar fractures of infinite extent. The hydraulic gradient acting across the matrix, on the horizontal plane, would be limited as it would take time for the change in pressure to permeate through the matrix block inducing a piezometric gradient across the matrix block.

Additionally, the porosity of the matrix may not be fully interconnected across a matrix block, which can be on the scale of metres in the Chalk. The failure of this assumption close to the well, however, raises some concerns for the capability of the DP-Pulse model to simulate a system under significant stress, as is the case with an ASR system during injection or abstraction. In addition, this assumption is applied in a large number of models simulating double-porosity behaviour, including both SWIFT and PHREEQC. It is therefore important to look at it in more detail. Using the parameter values obtained from the review of current literature, a standard drawdown curve has been calculated using the Theis formula.
(Theis, 1935), and this has been used to calculate the potential flow velocity within the Chalk aquifer (Figure 5-3).

Figure 5-3 Calculated theoretical flow velocities in the chalk matrix

It can be seen that at a distance of 10 m or more from the well, the flow rate is less than 10 mm/day, and can be considered insignificant.

5.2. **Sensitivity and uncertainty analysis**

It is important to assess the sensitivity of the model to parameter variation in order to quantify both the quality of the calibration and the reliability of any predictions. The standard methodologies for this process are sensitivity analysis and uncertainty analysis. Sensitivity analysis involves changing a particular parameter, and determining the effects of this change. It is then possible to determine the parameters that show most influence over the behaviour of the system being investigated. Uncertainty analysis concerns uncertainties in the choice of conceptual model (i.e. whether the model is capable of simulating all significant processes), as well as the effects of known uncertainty in the values of parameters chosen for use in the model (i.e. the variation in measured values of hydraulic conductivity for the same aquifer). Uncertainty analysis is a process concerned with solution uniqueness and calibration qualities.

While much has been written about the importance of sensitivity and uncertainty analysis in the use of a groundwater model (NRA, 1994), little has been said about
the actual processes involved. The simplest form of sensitivity analysis consists of varying each parameter in turn by a specified amount within a reasonable range of values, and assessing the influence of this parameter change on the model output (Anderson and Woessner, 1994). This was undertaken in Section 3.10 and will not be repeated here.

The application of these analyses can be used in a number of ways. Firstly, they are a good means by which to qualitatively assess the usefulness of a model. If calibration of the model is poor, it may indicate that the model is unsuitable for the chosen use. If a model is highly sensitive to a parameter, it is essential that data collected in order to evaluate that parameter must be obtained as accurately as possible. Another use of sensitivity analyses is to improve the collected data set in order to improve the model reliability. By revealing the more important parameter uncertainties it is possible to develop experimental procedures to gain an optimal data set. This methodology has been developed and described by Freeze et al. (1992).

5.2.1. Uncertainty analysis

The concept of the DP-Pulse model has been discussed previously (Chapter 2.4.4). A visual comparison of the calibrated model output and the experimental data set shows a good correspondence (Figure 5-1). Thus it seems safe to assume that the DP-Pulse model is a suitable model, capable of simulating the important processes involved in the Lychett Minster ASR test.

The major source of uncertainty is in the selection of the block geometry. As has been discussed in the previous section, it is not possible to use the collected data set to determine the BGF that most accurately represents the true physical geometry of the fracture network. As the calibration of the data set to the slab geometry is more constrained, it was decided to proceed on the assumption that this geometry represents the physical characteristic of the Lychett Minster Test Site. Although a slab model is likely to be representative of the nature of fracturing in the Chalk, fracturing has not been observed at the Lychett Minster Test Site, as there is no Chalk outcrop. This decision, therefore, is not made on a factual basis, rather to allow investigation of this site to progress with the limited data available.

Assuming the slab geometry, it is possible to test the uncertainty of the model across the parameter range outlined by the calibration of the DP-Pulse model to the data collected from the Lychett Minster Test Site data (illustrated in Figure 5-1). Rather
than vary each parameter by a specified amount, a group of parameter sets were chosen to describe each confidence interval, and the DP-Pulse model was run with each of these sets of parameter values in order to illustrate the sensitivity of the model. The advantage of this procedure over the standard sensitivity analysis methodology is that it provides quantitative information on both the robustness of the calibration as well as highlighting the relative importance of the parameters.

The parameter sets selected to outline each confidence interval are illustrated in Figure 5-4, and then listed in Table 5-4. To improve the clarity of the presented information, all values of t<sub>cb</sub> and σ in the sensitivity analysis have been rounded to the nearest integer value. As a result the calibration bounds used are not exactly symmetrical about the calibrated parameter value. It was felt that, due to the insensitivity to t<sub>cb</sub> and σ on this scale, greater accuracy was not required for this analysis.

![Figure 5-4 Confidence intervals for the calibration of the DP-Pulse model to the Lychett Minster Test Site data, showing the selected parameter groups for the uncertainty analysis (Slab Geometry).](image)

The DP-Pulse model was then run, with the slab BGF, for each set of parameter values. These model runs are illustrated in Figure I-1, Figure I-2, Figure I-3, Figure I-4, Figure I-5, Figure I-6, Figure I-7 and Figure I-8, which are located in Appendix I.
In order to show the sensitivity of the model to parameter variation the abstracted solute concentration at the end of the operational cycles detailed in Table 5-1 were determined for each of the parameter sets detailed in Table 5-4 below. These results were contoured, to show the variation in the final abstracted solute concentration within the parameter region defined in Figure 5-4. The contour plot is shown below in Figure 5-5. From this figure it can be seen that $t_{cb}$ has a stronger controlling effect on the abstracted solute concentrations than $\sigma$, but that overall the model is not highly sensitive to either $t_{cb}$ or $\sigma$ for the simulated cycles (a 53% increase in $t_{cb}$ leads to a 7% increase in the relative solute concentration).

Figure 5-5 Contour plot of the simulated relative solute concentration of the abstracted water at the end of the cycle testing of the Lychett Minster test site, for the parameter region outlined in Figure 5-4.
Table 5-4 Parameter groups selected to outline the 50% and 95% confidence intervals for the calibration of the DP-Pulse model to the Lychett Minster Test Site data.

<table>
<thead>
<tr>
<th>Calibrated parameter values</th>
<th>Parameter values</th>
<th>50% confidence interval</th>
<th>95% confidence interval</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_{cb}$ = 1086 days</td>
<td>$t_{cb}$ = 1086 days</td>
<td>$t_{cb}$ = 1086 days</td>
<td>$t_{cb}$ = 1086 days</td>
</tr>
<tr>
<td>$\sigma$ = 49.5</td>
<td>$\sigma$ = 49.5</td>
<td>$\sigma$ = 49.5</td>
<td>$\sigma$ = 49.5</td>
</tr>
<tr>
<td>$t_{ef}$ = 0.44 days</td>
<td>$t_{ef}$ = 0.44 days</td>
<td>$t_{ef}$ = 0.44 days</td>
<td>$t_{ef}$ = 0.44 days</td>
</tr>
</tbody>
</table>

A  
$t_{cb}$ = 1149 days  
$\sigma$ = 51  
$t_{ef}$ = 0.44 days  
$\sigma$ = 53.9

B  
$t_{cb}$ = 1024 days  
$\sigma$ = 47.9  
$t_{ef}$ = 0.45 days  
$\sigma$ = 45

C  
$t_{cb}$ = 1149 days  
$\sigma$ = 47.9  
$t_{ef}$ = 0.50 days  
$\sigma$ = 45

D  
$t_{cb}$ = 1024 days  
$\sigma$ = 51  
$t_{ef}$ = 0.39 days  
$\sigma$ = 53.9

E  
$t_{cb}$ = 1149 days  
$\sigma$ = 49.5  
$t_{ef}$ = 0.47 days  
$\sigma$ = 49.5

F  
$t_{cb}$ = 1024 days  
$\sigma$ = 49.5  
$t_{ef}$ = 0.42 days  
$\sigma$ = 49.5

G  
$t_{cb}$ = 1086 days  
$\sigma$ = 51  
$t_{ef}$ = 0.42 days  
$\sigma$ = 53.9

H  
$t_{cb}$ = 1086 days  
$\sigma$ = 47.9  
$t_{ef}$ = 0.47 days  
$\sigma$ = 45

It is apparent from all the listed figures that the model is not greatly sensitive to either $t_{cb}$ or $\sigma$. The greatest difference between abstracted relative solute concentrations occurred at the commencement of the first abstraction cycle. Within the 95% confidence interval the greatest difference was between the solute concentrations arising from models run using parameter sets C95 and D95. Parameter sets D50 and C50 produced the greatest difference within the 50% confidence interval. The relative solute concentration at the start of abstraction during cycle 1 from C50 was 9% less than that from D50. The relative solute concentration at the same time from C95 was 24% less than that from D95.

There are a number of conclusions that can be made from these plots. It is significant that the greatest difference in solute concentrations produced arose from model runs C95 and D95, as these parameter groups had the greatest variation.
in $t_{cf}$. At early times the solute concentrations within the fracture are controlled by $t_{cf}$, and C95 has a $t_{cf}$ value of 0.63 days, more than twice as large as D95 at 0.31 days. This is the largest $t_{cf}$ difference between any two parameter groups.

The increasing influence of $t_{cb}$ and $\sigma$ on abstracted solute concentrations can be seen in all the plots, but is most apparent in Figure I-1. At early times the model is slightly sensitive to the variation in $t_{cb}$ and $\sigma$, but there is only a small change in the solute concentrations. This is because although there is a large difference between the $t_{cb}$ and $\sigma$ values of A95 and B95, the difference between the $t_{cf}$ values is quite small. A95 has a $t_{cf}$ value of 0.44 days and B95 has a $t_{cf}$ value of 0.45 days.

In an ASR system it is often the peak abstracted solute concentration that is of most importance. In the 50% confidence interval, the greatest relative difference between peak concentrations, 3.4%, was again between C50 and D50. In the 95% confidence interval the greatest relative difference was 10.4% between C95 and D95. Both maxima occurred at the end of the second abstraction cycle.

In summary, we can see that within the parameter range outlined by the 95% confidence interval, the model is most sensitive to variations in $t_{cf}$. The maximum error arising from parameter uncertainty on this time-scale is approximately 24% at the start of an injection cycle, and 10.4% at the end.

Significant differences in solute concentrations at early times can be seen between C50 and D50 in Figure I-6, G50 and H50 in Figure I-7, C95 and D95 in Figure I-2, E95 and F95 in Figure I-3 and G95 and H95 in Figure I-4.

Significant differences at later times can be seen between A95 and B95 in Figure I-1 and E95 and F95 in Figure I-3. The figures illustrating these findings are located in Appendix I.

### 5.3. Conclusions drawn from the calibration process

A number of important conclusions can be drawn from this exercise in calibrating a DP-Pulse simulation to solute concentration data from the Lychett Minster ASR Test Site. Perhaps most importantly, the model was able to successfully simulate the data produced, despite the simplicity of the model, and the use of only two parameters, $t_{cb}$ and $\sigma$, and the block geometry function. The parameters indicated by this calibration can be reinterpreted as physical characteristics of the aquifer, and these characteristics fall within the reasonable range as identified earlier in this thesis.
This provides a partial validation of the use of the DP-Pulse model to simulate ASR within a double-porosity aquifer such as the Chalk. During the calibration process it was found that determining the correct geometry to describe the fracture network, and hence choosing the correct BGF is not a simple task. The cycle testing undertaken at the site was of insufficient duration to determine whether a slab or sphere geometry best represented the system. As a result, an important conclusion to draw is that if at all possible, the geometry of the fracture network should be examined, probably at a nearby outcrop. This activity is not possible within the Wareham Basin due to the deeply confined and artesian nature of the Chalk aquifer. Alternatively, further work could be conducted examining all Chalk data to attempt to discern if, in general, Chalk conforms better to one geometry or the other. In addition to the limitation on the understanding of the geometry, there are a number of other factors that impact on the quality of the calibration arising from the assumptions made in the formulation of the DP-Pulse model. Although some of these raise significant concerns about the applicability of the DP-Pulse model to this system, the fact that the model successfully simulated solute concentration variations in some part validates this model.
Chapter 6

Characterising the Chalk aquifer, and the resultant implications for ASR
6. Characterising the Chalk aquifer, and the resultant implications for ASR

It is necessary at this point to characterise the Chalk aquifer. This chapter attempts to characterise the Chalk aquifer with a range of parameter values, expressed as $t_{cb}$ and $\sigma$. The implications of this parameter range for the behaviour and success of an ASR scheme are discussed.

6.1. Outlining the range of plausible parameter values for the Chalk and other significant UK aquifers.

Although site specific measurements using tracer tests are the ideal way to characterise an aquifer, it is possible to outline a range of feasible values for $\sigma$ and $t_{cb}$ through examination of the general characteristics of certain aquifers. Frequently, work has been undertaken to characterise fractured aquifers through the measurement of a number of physical parameters, including the fracture aperture and separation as well as matrix and fracture porosities. Using equations 19 and 20, these parameters can be expressed in terms of $t_{cb}$ and $\sigma$. As the novel characterisation in DP-Pulse requires only these two parameters, it is possible to represent these ranges as zones on a simple 2-dimensional plot of $t_{cb}$ and $\sigma$. For simplicity we use a series of boxes, each of which defines the range of potential aquifer characteristics for an aquifer type. Table 6-1 gives a range of plausible characteristics for a number of important UK aquifers, and the resultant ranges of $t_{cb}$ and $\sigma$, assuming a slab geometry.

Table 6-1 General ranges of aquifer characteristics. (From Allen et al., 1997)

<table>
<thead>
<tr>
<th>Aquifer</th>
<th>Hydraulic Conductivity (m/d)</th>
<th>Porosity (%)</th>
<th>Fracture spacing (m)</th>
<th>Calculated Fracture Aperture (m)</th>
<th>$t_{cb}$ (days)</th>
<th>$\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lincolnshire Limestone</td>
<td>$1 \times 10^{-3}$</td>
<td>10-100</td>
<td>1-10</td>
<td>0.5-5</td>
<td>1-10</td>
<td>$2.5 \times 10^{-3} - 2.5 \times 10^{-1}$</td>
</tr>
<tr>
<td>Chalk</td>
<td>$1 \times 10^{-3}$</td>
<td>1-100</td>
<td>20-40</td>
<td>0.1-2</td>
<td>0.1-10</td>
<td>$5 \times 10^{-3} - 0.1$</td>
</tr>
<tr>
<td>Sherwood Sandstone</td>
<td>1-50</td>
<td>10-500</td>
<td>10-25</td>
<td>1</td>
<td>10-100</td>
<td>0.05 - 0.5</td>
</tr>
<tr>
<td>Lower Greensand</td>
<td>1-100</td>
<td>-</td>
<td>10-35</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

It is possible to refine this range of feasible values for $\sigma$ and $t_{cb}$ through a statistical analysis of the studies of characteristic physical parameters completed by various
authors. This exercise will be carried out for the Chalk aquifer. The general characteristics of the Chalk, as reported within the literature, were reproduced in Table 2-2, Section 2.7.

Assuming that the range of reported values follow a log-normal distribution, we can determine a mean value and standard deviation of these parameters. By adding a single standard deviation to the mean we obtain a reasonable range of parameter values for the Chalk, described in Table 6-2. This range has been plotted as the box labelled “Chalk (Statistically determined parameters)” on Figure 6-1. This box represents the range of parameters which is more likely to represent a Chalk aquifer than those detailed in Table 6-1, as the potential extreme values have been reduced.

**Table 6-2 Parameters characterising the Chalk aquifer providing the bounds on typical Chalk parameters from literature review.**

<table>
<thead>
<tr>
<th></th>
<th>( t_{cb} ) (Days)</th>
<th>( \sigma )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chalk (Statistically determined parameters from literature review, using a slab geometry)</td>
<td>A 62 25</td>
<td>B 62 480</td>
</tr>
</tbody>
</table>

There is a significant reduction in the parameter range for the Chalk aquifer detailed in Table 6-1 when compared to Table 6-2. This is because Table 6-1 is an attempt to comprehensively incorporate all feasible variation in the Chalk aquifer while Table 6-2 is a statistical interpretation of reported values, which will show the more probable variation in Chalk aquifer parameters. It should be noted that the parameters detailed in Table 6-2 tend to show lower values of \( t_{cb} \), and higher values of \( \sigma \). Although this may be a true representation of the actual parameter variation, it could also be an artefact of the difficulty in identifying fractures in aquifers from borehole logs. It is frequently the case that exposed and hence weathered Chalk, from which fracture characteristics are mostly derived, have more frequent fracturing than buried Chalk (see section 4.2.1).

6.1.1. **Using hydraulic conductivities for the Chalk aquifer to restrict possible parameter ranges**

The cubic law for flow through a fracture (equation 112) describes a relationship between fracture aperture and block size:

\[
K = a^3 \frac{gD}{24 \mu b} \tag{112}
\]
\[ K \] = hydraulic conductivity (m·s⁻¹); \[ g \] = gravity (m·s⁻²); \[ \rho \] = water density (kg·m⁻³)

\[ \mu \] = water viscosity (kg·m⁻¹·s⁻¹); \[ a \] = fracture aperture (m); \[ b \] = fracture separation (m)

Using equations 20 and 23 in equation 112, it is possible to describe a relationship between \( t_{cb} \) and \( \sigma \), that varies with \( K, \phi \) and \( D_a \):

\[
\frac{t_{cb}}{\sigma^3} \approx 4 \cdot 22 \times 10^{-9} \frac{K}{\phi^3 D_a} \text{ days}
\]

(113)

\[ \phi \] = matrix porosity = 0.2 - 0.4 (Allen et al., 1997)

\( D_a \) = apparent diffusion coefficient = \( 3.0 \times 10^{-10} \) m²·s⁻¹ (Fretwell, 1999)

Using limit values of fracture separation and hydraulic conductivity for the Chalk with this equation, it is possible to define boundaries for \( t_{cb} \) and \( \sigma \), further refining the parameter range obtained in the previous section.

Looking to the literature for a range of possible hydraulic conductivities (Allen and Price 1990; Price et al., 1976; Price et al., 1977; Price et al., 1982; Watson et al., 2000) a range of between \( 1 \times 10^{-2} \) and \( 1.8 \times 10^{2} \) m day⁻¹ is indicated. Combining these values with the parameter ranges previously identified for the porosity and the apparent diffusion coefficient, two boundary lines can be plotted on a chart of \( t_{cb} \) vs. \( \sigma \) indicating a region within which equation 113 is valid.

Figure 6-1 indicates the set of feasible parameter values for the Chalk determined through statistical analysis (the box titled “Chalk (Statistically determined parameters)”

In addition, two lines (A and B) indicate the bounds on the region within which equation 113 is valid.
Figure 6-1 Bounds on typical Chalk parameters from literature review and aperture analysis (Slab geometry).

It should be noted that the parameter ranges outlined within Figure 6-1 are not to be considered definitive. Firstly, the ranges defined in Table 6-1 and Table 6-2 are broad, but may well not be comprehensive. Also, the interpretation provided does not account for possible correlation between parameter values. For example, it is plausible that there is some association between the fracture separation and the fracture aperture that is currently not clearly understood. Should this be the case, the zones could be further refined.

6.2. Parameters and their implications for ASR

As has previously been discussed (Section 3.6), a double-porosity aquifer can be described by (essentially) two parameters: the ratio of matrix porosity to fracture porosity, $\sigma$, and the ‘characteristic block diffusion time’, $t_{cb}$. These two parameters play an important role in describing the solute concentrations in the abstracted water from an ASR system – and hence the success of that system. In order to overview
the role these parameters play we will need to outline the implications of different parameter values.

When $\sigma$ is greater than 1, more of the total water within the system is contained within the matrix blocks than within the fractures: either the blocks are relatively large and of high $\phi$, or the fracture apertures are small. As all water flows within the fractures, there is a large reservoir of water at native solute concentrations with which diffusive exchange can occur. When $\sigma$ is less than 1, large fracture apertures or small matrix blocks result in more water being contained within the apertures than in the matrix blocks. In order to look at the effect of $\sigma$ on the operation of an ASR system in the Chalk aquifer, we will refer to the previous section, and consider $\sigma$ values of between 25 and 480. It will be assumed that this range will cover the extremes of 'normal' double-porosity rocks.

When $t_{cb}$ is low, of the order of a few days, generally because of small matrix block sizes, the time taken for diffusive exchange with the fracture to occur at the centre of the matrix block is small. As a result the average solute concentration of the matrix block will rapidly approach that of the injected waters. When $t_{cb}$ is high, of the order of years, the average solute concentration of the matrix block will only slowly approach that of the injected water in relation to ASR operations.

We shall examine the effects of four parameter groups chosen according to the parameter delineation undertaken in Section 6.1. These parameter groups are indicated in Table 6-3.

### Table 6-3 Parameter range for qualitative assessment of ASR potential

<table>
<thead>
<tr>
<th></th>
<th>$t_{cb}$</th>
<th>$\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Low $t_{cb}$, high $\sigma$</td>
<td>62</td>
</tr>
<tr>
<td>B</td>
<td>Low $t_{cb}$, low $\sigma$</td>
<td>62</td>
</tr>
<tr>
<td>C</td>
<td>High $t_{cb}$, high $\sigma$</td>
<td>1362</td>
</tr>
<tr>
<td>D</td>
<td>Low $t_{cb}$, high $\sigma$</td>
<td>1362</td>
</tr>
</tbody>
</table>

The selected parameters can be converted to a more conventional parameter set. If we assume the apparent diffusion coefficient and the matrix porosity:

- $D_a = 3\times10^{-10}$ m$^2$/s
- $\phi_m = 0.4$

From equation 20 we can obtain the half block size, $b$, and from equation 19 the fracture aperture, $a$, and hence the fracture porosity, $\phi_f$. This interpretation, however,
is dependent on the value of $D_a$ and $\phi_m$ selected, and should only be considered illustrative.

6.2.1. A - ASR behaviour when $t_{cb} = 62$ days, $\sigma = 134$

<table>
<thead>
<tr>
<th>$\sigma = 134$</th>
<th>$\sigma = 62$ days</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_{cb} = 62$ days</td>
<td>$t_f = 0.003$ days</td>
</tr>
</tbody>
</table>

$D_a = 3 \times 10^{-10}$ m$^2$s$^{-1}$

$\phi_m = 0.4$

$b = 4$ cm

$a = 0.24$ mm

$\phi = 0.003$

These parameters describe a system with small matrix blocks and narrow, but frequent, fractures. This would be characteristic of a densely fractured chalk in which dissolution has not significantly widened fracture apertures. Although there is a large volume of native water able to diffusively interact with the fracture water, this process occurs rapidly. As a result an ASR system would initially produce abstracted solute concentrations that were close to the native water solute concentrations. After a short period of operation these solute concentrations would fall, as the native water became diluted through diffusion with the injected water. Figure 6-7 indicated that with a low maximum abstracted solute concentration, and after a 360 day conditioning period, high recovery efficiencies could be expected, in aquifers with non-potable water.
6.2.2. B - ASR behaviour when $t_{ob} = 62$ days, $\sigma = 25$

<table>
<thead>
<tr>
<th>$\sigma = 25$</th>
<th>$D_a = 3 \times 10^{-10}$ m$^2$s$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_{ob} = 62$ days</td>
<td>$\phi_n = 0.4$</td>
</tr>
<tr>
<td>$t_{cf} = 0.1$ days</td>
<td>$b = 4$ cm</td>
</tr>
<tr>
<td></td>
<td>$a = 1.3$ mm</td>
</tr>
<tr>
<td></td>
<td>$\phi = 0.016$</td>
</tr>
</tbody>
</table>

This aquifer is characterised by wide frequent fractures. It is close in behaviour to a single-porosity medium, although the presence of the small blocks of matrix will still introduce an element of double-porosity behaviour.

The issues surrounding ASR in a single-porosity medium have been widely discussed. ASR has been found to be effective in these areas, but major controls on the ASR system in this situation include dispersive effects and density effects.

Figure 6-7 shows that this combination of parameters would result in a highly effective ASR system, with good recovery efficiencies, even in aquifers in which the water is, for example, extremely saline.

6.2.3. C - ASR behaviour when $t_{ob} = 1362$ days, $\sigma = 377$

<table>
<thead>
<tr>
<th>$\sigma = 377$</th>
<th>$D_a = 3 \times 10^{-10}$ m$^2$s$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_{ob} = 1362$ days</td>
<td>$\phi_n = 0.4$</td>
</tr>
<tr>
<td>$t_{cf} = 0.01$ days</td>
<td>$b = 19$ cm</td>
</tr>
<tr>
<td></td>
<td>$a = 0.4$ mm</td>
</tr>
<tr>
<td></td>
<td>$\phi = 0.001$</td>
</tr>
</tbody>
</table>

These parameters describe an aquifer consisting of large blocks with relatively few, narrow fractures.

As it takes a long time to reach diffusive equilibrium, and there is a large reservoir of native water within the matrix blocks, an ASR system in this aquifer would be problematical. Initially high solute concentrations would take a long time to fall, as the large volume of native water will only slowly be removed through diffusive exchange. Conditioning this aquifer will only ‘flush out’ the surface of the matrix blocks, and successful ASR operation will require the development of a buffer zone within the matrix blocks between the injected water and the native water. The process of developing this buffer zone will be extremely time consuming, and be likely to involve large quantities of water. Figure 6-7 reveals that even after a 360 day conditioning period the solute concentrations of the recovered water will be high. ASR is only likely to be suitable if the water in this aquifer is already of potable quality.
6.2.4. D - ASR behaviour when \( t_{cb} = 1362 \text{ days}, \sigma = 25 \)

<table>
<thead>
<tr>
<th>( \sigma = 25 )</th>
<th>( D_x = 3 \times 10^{-10} \text{ m}^2\text{s}^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t_{cb} = 1362 \text{ days} )</td>
<td>( \phi_m = 0.4 )</td>
</tr>
<tr>
<td>( t_f = 2.18 \text{ days} )</td>
<td>( b = 19 \text{ cm} )</td>
</tr>
<tr>
<td></td>
<td>( a = 6 \text{ mm} )</td>
</tr>
<tr>
<td></td>
<td>( \phi_f = 0.016 )</td>
</tr>
</tbody>
</table>

This aquifer has wide but infrequent fractures, whose volume forms a highly significant volume within the aquifer. It is typical of the Upper Chalk. Although it would take a long time for an ASR system to 'flush out' all the solute mass contained within the matrix blocks, due to the high fracture volumes the total mass diffusing into the fracture water would not be large enough to significantly affect the solute concentrations. It follows that there is the potential for ASR to be developed in this aquifer type.
6.3. **Illustrating the behaviour of ASR systems across ranges of parameter values**

In order to examine the effect of the aquifer characteristics on the development and operation of an ASR system, it is helpful to examine behaviour over a broad range of parameters. Because the DP-Pulse model uses just two parameters to characterise the aquifer, it is possible to view ASR system behaviour in the form of contour plots, with $\sigma$ as the x-axis and $t_{cb}$ as the y-axis. In this section, the recovery efficiencies, conditioning periods and maximum measured solute concentrations are considered.

6.3.1. **Maximum solute concentrations**

By specifying the operational cycle of an ASR system, it is possible to predict the maximum solute concentration that will be abstracted from the well after one operational cycle. This can then be repeated for a number of parameter sets, and a contour plot of the results may be produced. If a conditioning period (as discussed in Section 2.5.2) is included, the effect on solute concentrations can then be visualised across a broad range of parameter values.

The standard operational cycle assumed here is outlined in Table 6-4. This operational cycle was modelled following a number of different conditioning periods (Figure 6-2).

**Table 6-4 A standard annual operational cycle.**

<table>
<thead>
<tr>
<th>Operation</th>
<th>Duration (Days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection</td>
<td>100</td>
</tr>
<tr>
<td>Storage</td>
<td>100</td>
</tr>
<tr>
<td>Abstraction</td>
<td>100</td>
</tr>
<tr>
<td>Dormancy</td>
<td>65</td>
</tr>
</tbody>
</table>
Figure 6-2 Contour plots showing maximum abstracted solute concentrations on a standard annual cycle after 45-day, 90-day, 180-day, 360-day and 720-day conditioning periods ($\Delta T = 1$ day).
These plots can be divided into three regions, as illustrated in Figure 6-2D.

1. Within region 1, in which $t_{cb}$ is approximately greater than 3 times total model duration, the model is essentially controlled by $t_{cf}$ alone. The contours in this area can be described by $t_{cf} = t_{cb} / \sigma^2 = \text{constant}$. Within this region, injected water in the fractures has not significantly interacted diffusively with the water at the centre of the matrix blocks.

2. Within region 2, with low $\sigma$ and $t_{cb}$, both parameters are important.

3. Within region 3, the model is almost entirely controlled by the value of $\sigma$. $t_{cb}$ is sufficiently low, with diffusive equilibrium being reached sufficiently rapidly, that the system essentially acts as a single porosity aquifer, with an effective porosity of $\phi(1 + \sigma)$ i.e. the total porosity. Solute concentrations are controlled by a simple mixing calculation between the fracture and matrix volumes. A high $\sigma$ value indicates relatively large proportions of matrix water, which will maintain high concentration gradients into the fracture waters, forming a strong control over the concentrations of the fracture water for a significantly longer period of time.

6.3.2. Recovery efficiencies

The recovery efficiency obtained on the same annual cycle (Table 6-4) can be illustrated in a similar manner to the maximum solute concentration. For this demonstration two maximum abstracted solute concentrations were chosen. Conditioning periods of 45, 90, 180, 360, 720, 1080 and 14400 days were selected for a maximum abstracted solute concentration of 0.1 (Figure 6-3 and Figure 6-4), and conditioning periods of 45, 90, 180 and 360 days were selected for a maximum abstracted solute concentration of 0.5 (Figure 6-5).
Figure 6-3 Contour plots showing recovery efficiencies with a maximum abstracted solute concentration of 0.1 native solute concentration, and after conditioning periods of 45, 90, 180 and 360 days ($\Delta T = 1$ day).
Figure 6-4 Contour plots showing recovery efficiencies with a maximum abstracted solute concentration of 0.1 native solute concentration, and after conditioning periods of 720, 1080 and 1440 days ($\Delta T = 1$ day).
Figure 6-5 Contour plots showing recovery efficiencies with a maximum abstracted solute concentration of 0.5 native solute concentration, and after conditioning periods of 45, 90, 180 and 360 days ($\Delta T = 1$ day).

As with Figure 6-2, at high $t_{cb}$ values the recovery efficiency is controlled by $t_{cfs}$ while at low $t_{cb}$ values $\sigma$ is the controlling factor.

### 6.3.3. Required conditioning periods

The final contour plot (Figure 6-6) shows the required conditioning period (explained in Section 2.5.3 and Figure 2-4) to produce 100% efficiency on a single standard annual ASR cycle, with a maximum abstracted solute concentration 0.5 of the native solute concentration. This figure again shows the three distinct regions of behaviour.
Figure 6-6 Required conditioning period in days to produce 100% efficiency in relation to a maximum abstracted solute concentration of 0.5 native solute concentration, with a standard annual cycle ($\Delta T = 1$ day).

6.3.4. Variation of recovery efficiency with the maximum concentration

One demonstration of the utility of the method, described in Section 6.1, of defining the parameter space within which an aquifer is defined is to demonstrate how the aquifer parameters will affect the behaviour of an ASR system in a double-porosity aquifer. The sensitivity of the model to the chosen maximum abstracted solute concentration is shown in Figure 6-7. This figure illustrates the variation of recovery efficiency with the maximum concentration for the Lychett Minster Test Site calibrated parameter values (see Chapter 5) and the parameter range characterising the Chalk (as determined through the statistical analysis of reported aquifer characteristics, and the analysis of reported hydraulic conductivities). A conditioning period of 360 days was undertaken prior to the operation of the system, which involved 100 days injection, 100 days of storage and then 100 days abstraction. Increasing the maximum abstracted solute concentration by only a small amount will drastically increase the potential recovery efficiency of the system for all plausible parameter values. The maximum abstracted solute concentration is
strongly controlled by the parameter set chosen, and as such will also have a significant control on the potential of an ASR system.

Figure 6-7 Variation of recovery efficiency with maximum abstracted solute concentration for the bounded Chalk parameter set, as well as the Lychett Minster Test Site calibrated parameter set (Conditioning period of 2360 days, followed by an operational cycle consisting of 100 days injection, 100 days storage and 100 days abstraction).
Chapter 7

Operational Research: Procedures and application
7. Operational Research: Procedures and application

In the previous chapters, this thesis has dealt with the techniques and implementation of ASR, and with a novel model developed to simulate ASR in a double-porosity aquifer. The remainder of this thesis will apply that (DP-Pulse) model in conjunction with Operational Research (OR) methodologies to develop a method for determining the optimal testing regime for a double-porosity system prior to the implementation of an ASR scheme. Before continuing this work however, it is necessary to consider some fundamental ideas from the field of OR. This chapter provides an overview of a subset of OR techniques, and how they may be applied in ASR research. The chapters following look in detail at how the DP-Pulse model can be incorporated into an OR model that allows the simulation of an operational ASR system, and how OR techniques can then be used to develop testing procedures that enable the characterisation of an aquifer prior to the implementation of operational ASR.

7.1. The concept of Operational Research (OR)

Usually the solution to any groundwater problem, from contamination to water resources, has been found through the direct application of hydrogeological techniques. Without consideration of all the (hydrogeological and non-hydrogeological) issues surrounding such a problem it is possible that the solution may fail in a number of ways. Firstly, and possibly most catastrophically, the problem may not be sufficiently defined, and the selected solution may not address all the important issues raised by the problem. In other scenarios, the solution may only be acceptable to a few of the affected parties, possibly affecting other parties in an adverse manner. It is also possible that a chosen solution is not the cheapest (not just in terms of financial cost, but also with regards to environmental costs, public profile, etc.) available solution capable of providing satisfactory results.

The field of OR provides a number of techniques that encourage the user to step away from the problem, and attempt to find a method of solution in a directed manner. These tools prescribe a process that should be followed, encouraging first the determination of the exact nature of the problem, and then highlighting the best way to approach the realisation of a solution.

One prescription for planning, problem solving or decision making, suggested by Rosenhead (1989), incorporates five key stages:

1. Identify objectives, weighting each objective according to importance.
2. Identify all the alternative courses of action.
3. Predict the consequences of possible actions in terms of objectives.
4. Evaluate the consequences on a common scale of value.
5. Select the alternative whose net benefit is highest.

Operational Research incorporates these stages in a series of rigorous systematic decision making frameworks, each tailored to working in a different environment. As most problems can have a number of feasible solutions, the role of OR is to aid the decision-maker in finding the optimal solution. In the real world, however, uncertainty often prevails and a more suitable approach is to find all the solutions that fulfil the requirements satisfactorily, described as ‘satisficing’ solutions. Once the satisficing solutions are determined, various techniques may be applied to determine the optimal one. Through every stage of the situation, including problem definition, determination of all possible solutions and selection of the best solutions, OR techniques can be used to clarify the optimal way to proceed.

Another significant area of OR examines the ‘robustness’ of a decision. Every decision made limits the number of possible future outcomes available to the decision-maker, therefore when choosing it is important to ensure that any decision made does not overly limit future possibilities. A solution that leaves a relatively large number of future options open is said to be robust. Robustness analysis provides an approach to the structuring of problem situations in which uncertainty is high, and where decisions can or must be staged sequentially. It identifies the options in decisions early in the sequence that, relative to other choices will keep open a wide range of options for the future. Robustness analysis and its implementation is discussed more fully in Appendix IX.

7.2. Operational Research theory and its application to hydrogeology

Operational research methodologies have been used for a broad range of hydrogeological applications. The most common use of OR methodologies has been in the implementation of resource management models (Eiger et al., 1994; Kwanyuen and Fontane, 1988; Rogers and Fiering, 1986; Soares and Andrade-Filho, 1988). More in-depth approaches were taken by Sun and Yeh, who applied OR techniques to groundwater modelling practice in general (Yeh and Sun, 1984, Sun and Yeh, 1990a, Sun and Yeh, 1992), and experimental design in particular (Sun and
Yeh, 1990b). Another important body of work develops a framework for hydrogeological decision analysis (Freeze et al., 1990), and applies it to a series of case studies, including groundwater contamination (Massmann et al., 1992), dewatering design (Sperling et al., 1992) and site investigation (Freeze et al., 1992).

Some other applications of OR methodologies are outlined in Table 7-1.

Table 7-1 Selected applications of OR methodologies to groundwater issues.

<table>
<thead>
<tr>
<th>Methodology</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tracer test planning</td>
<td>Cleveland &amp; Yeh, 1990</td>
</tr>
<tr>
<td>Aquifer reclamation</td>
<td>Gorelick et al., 1984</td>
</tr>
<tr>
<td>Groundwater supply protection</td>
<td>Varljen &amp; Shafer, 1993</td>
</tr>
<tr>
<td>Site investigation</td>
<td>Freeze et al., 1992</td>
</tr>
<tr>
<td>Dewatering design</td>
<td>Sperling et al., 1992</td>
</tr>
<tr>
<td>Remediation design</td>
<td>Ahlfeld et al., 1988</td>
</tr>
<tr>
<td></td>
<td>Massmann et al., 1992</td>
</tr>
<tr>
<td></td>
<td>Andricevic &amp; Kitanidis, 1990</td>
</tr>
<tr>
<td>Conjunctive ground and surface water use</td>
<td>Azaiez &amp; Hariga, 2001</td>
</tr>
<tr>
<td></td>
<td>Wong et al., 1997</td>
</tr>
<tr>
<td>Financial examination of remediation costs</td>
<td>Culver and Shoemaker, 1997</td>
</tr>
</tbody>
</table>

7.2.1. The general optimisation problem

To solve an optimisation problem, it is helpful to be able to visualise a conceptual process. Therefore, a general form of the optimisation problem has been developed that may be expressed mathematically as follows.

Find

\[
x = \{x_1, x_2, \ldots, x_n\}
\]  

so as to minimise

\[
F(x)
\]

subject to

\[
g_i(x) \leq 0 \quad i = 1, 2, \ldots, m
\]

and

\[
h_j(x) = 0 \quad j = 1, 2, \ldots, l
\]

Here \(x\) is the set (vector) of control or decision variables, \(F(x)\) is the objective function, \(g_i(x)\) is the set of inequality constraints and \(h_j(x)\) is the set of equality constraints.

7.3. Cycle testing problem: description and formulation

As explained in Section 2.5, and throughout this thesis, before an ASR scheme is implemented an ASR test takes place. This test attempts to characterise the aquifer
in order to allow successful prediction of future behaviour. A typical ASR test consists of a short period of injection, followed by a short period of storage and finally a period of abstraction (e.g. each period consisting of a few days). The solute concentrations in the abstracted water can then be used to calibrate computer models of the ASR scheme. Current ASR methodology, described by Pyne (1995) is to repeat these ‘cycle tests’ until the abstracted solute concentrations are suitably low for operational ASR to begin.

In Section 2.5.4 a process of conditioning the aquifer, as opposed to ‘cycling’ of water was proposed as a more efficient means to prepare a double-porosity aquifer for ASR operation. It is still necessary, however, to complete an ASR test in order to determine the likely necessary length of the conditioning period. By applying the methodologies of OR to the design of this ASR test it is possible to optimise this test. Table 7-2 illustrates some of the factors an OR model of an ASR test will need to take into account. Most of these parameters have a financial value, which will need to be determined before the implementation of a model.

**Table 7-2 Summary of factors involved in the development of an OR model of an ASR test.**

<table>
<thead>
<tr>
<th>Optimisation component</th>
<th>Factors involved</th>
</tr>
</thead>
<tbody>
<tr>
<td>Objective</td>
<td>Design an optimal ASR testing regime to reduce the expense of conditioning the aquifer while still guaranteeing a successful first annual cycle.</td>
</tr>
<tr>
<td>Cost</td>
<td>Start-up costs (e.g. installation, construction, obtaining licence) Water: Provision of potable water for conditioning and injection, and removal of abstracted water. Energy: The cost of electricity to run the pumps, or fuel to power generators. Manpower.</td>
</tr>
<tr>
<td>Benefit</td>
<td>Reduced parameter uncertainty (hence risk). Potable water to supply</td>
</tr>
</tbody>
</table>

The costs given in Table 7-2 are separated out into startup costs and other costs. Startup costs involved in the preparation of the ASR site include the installation and construction costs. For a single ASR site design, however, these are constant and independent of the duration of the tests. An optimisation process that tries to find the
optimal method of implementing ASR, assumes that the ASR site will be constructed, and therefore these costs can be ignored. The variable costs in the system arise from the cost of supplying and injecting the water during the test, the cost of removing and disposing of the water during the test, the cost of supplying and injecting water during the conditioning period as well as the costs of equipment hire and personnel. These costs can be assumed to increase linearly with respect to the pumping duration during both the testing and conditioning procedures.

As an ASR system needs a source of water that is surplus to the local daily requirement, the cost of potable water for injection is not likely to be great. One significant application of ASR is to enable the utilisation of non-potable aquifers. As a result, water removed during the abstraction cycle of the ASR test is likely to be unsuitable for general discharge, and therefore disposal of abstracted water is likely to be a significant cost. This has been borne out with many experiences in the United States (Pyne, 1995). As it is during the abstraction phase of the ASR test that chemical analysis, an additional expense, takes place, it makes sense for the purpose of describing the model to have the cost of abstraction significantly greater than the cost of injection.

7.4. **Examining the appropriateness of current cycle testing procedures for double-porosity aquifers**

The current practice when testing an aquifer prior to the implementation of operational ASR consists of a series of cycle tests (described in Section 2.5.1). The purpose of these cycle tests is to examine the evolution of the interactions between the injected water, the native (matrix) water and the aquifer material. Additionally, within a double-porosity aquifer, this series of cyclical injection stages acts to change the solute concentration distribution in the aquifer, removing solutes from the matrix water, and hence the subsequent impact of the double-porosity nature of the system on the injected water. When the solute concentrations in water removed during the abstraction phase of the cycle tests falls to suitable levels, operational ASR cycling begins.

To examine the suitability of this cycle testing procedure to a double-porosity system it is first necessary to examine the quality of the information provided by the cycle
tests (this section), and subsequently the efficiency of these cycle tests in preparing the aquifer for operational ASR (Section 7.4.1).

To investigate the suitability of the cycle testing procedure to a double-porosity system, the DP-Pulse model was calibrated to the successive test cycles conducted at the Lychett Minster test site (with data from all earlier test cycles being included in each successive calibration). The calibrated parameter value was then plotted against the total duration of the testing procedure, and an indication made of the uncertainty in that calibration. Through examining these plots, it is possible to determine the additional information gained from each subsequent test cycle.

The DP-Pulse model was calibrated to the unweighted test data, and two calibration procedures were carried out, initially calibrating to $t_{cf}$, and subsequently to both $t_{cb}$ and $\sigma$. When calibrating to $t_{cf}$ the value of $\sigma$ was fixed at 40, selected as being a reasonable value for the aquifer under investigation. It should be remembered that at short times, diffusive exchange has not reached deep into the matrix blocks, and therefore only $t_{cf}$ is important, not $t_{cb}$ and $\sigma$ (see Section 3.4.1). The two calibration runs were independent of each other. Calibration to $t_{cf}$ (Figure 7-1 A) shows that the data rapidly indicated a specific parameter value of 0.44 days, reaching a reasonable calibration on the third cycle, or after a cumulative test duration of 50 days. The 95% and 50% confidence bounds3 rapidly narrow, to a minimum after approximately four cycles, or 161 days. Therefore, it is only necessary to complete a relatively short ASR test to determine the value of $t_{cf}$. The calibration to $t_{cb}$ and $\sigma$ (Figure 7-1 B and C), however, takes a lot longer, and a specific value with reasonably narrow confidence bounds is only determined after a long cumulative duration in the testing process. To adequately describe this aquifer, using $t_{cb}$ and $\sigma$, a test of at least 300 days cumulative duration is required.

It can also be seen that later calibrations to $t_{cf}$, $t_{cb}$ and $\sigma$ fall outside the 95% confidence bound of earlier calibrations. This may be for a number of reasons. Firstly, prolonged injection into the aquifer, as in the later test cycles, will be sampling greater volumes of aquifer. Inhomogeneities in the aquifer will result in a general averaging of parameters over a greater volume and hence, possibly, changes in the calibration results. It is also possible that the assumed block geometry does

---

3 95% confidence bound is the parameter region within which a calibration indicates a 95% probability of the true parameter value being within the region.
not adequately describe the aquifer material. This is very likely, as the BGF selected describes identical slabs, which are not likely to be found in nature.

Through examining these results, we can see a few flaws in the conception of this cycle testing methodology when applied in double-porosity aquifers. Whilst the earlier group of tests, up to 50 days, provided a great deal of information about the aquifer, in the form of a well defined $t_{cf}$ value, the intermediary tests provided little extra information. Only the very longest cumulative test durations provided good information about the two parameters, $t_{cb}$ and $\sigma$. 
7.4.1. Comparing the efficiency of different methods of conditioning an aquifer prior to operational ASR implementation

To illustrate the benefits of introducing a conditioning period into the development of an ASR scheme in a DP aquifer, a number of specific scenarios were modelled with the DP-Pulse model. An operational system was modelled as consisting of two periods: a ‘preparation phase’ followed by a continuous ‘operational cycle’. The preparation phase consists of both the ASR testing procedure, and the aquifer conditioning procedure. During this preparation phase, water is injected into the
aquifer with a view to preparing it for an operational ASR scheme, this water is not expected to be returned into supply.

Initially, we shall examine the benefits of a long conditioning period, as opposed to immediate commencement of operational ASR. For periods of 1, 2 and 3 years a continuous injection cycle occurred consisting of 360 days injection, followed by 10 days storage. This was then followed by several years of an annual ASR cycle, consisting of 100 days injection, 100 days storage, 100 days abstraction (100% injected water recovered) and a 60 day dormant period. For comparison, the model was run involving continuous cycling of the example ASR cycle without conditioning. Simulations used the DP-Pulse model and in each case, the overall model run was for fifteen years. Figure 7-2 shows the solute concentrations in fracture water close to the well for each of these model runs, indicating the change in ASR system performance with different preparation regimes.

Figure 7-2 Solute concentrations in water abstracted from the ASR well:
Operational ASR cycling with a varied initial preparation phase ($\sigma = 42$, $t_{cb} = 1087$ days, $\Delta T=10$ days)

Clearly, a prolonged period of injection before implementation of an operational cycle rapidly improves recovered water concentrations. The benefit gained from the initial conditioning period declines as the system operates over a number of years.
The continuous injection vastly improved water quality on abstraction in every case. After one year of continuous injection, the maximum solute concentration of the abstracted water is about 60% native quality, gradually improving with time. Two years continuous injection gave a maximum solute concentration of about 45% native quality, whilst three years continuous injection gives an initial maximum water solute concentration on abstraction of 30% native quality.

7.4.1.1. Conditioning with 'short' duration test cycles

Current practice is to conduct a series of test cycles, of relatively short duration, both to determine how the aquifer is likely to behave during ASR operation, and to prepare the aquifer for ASR implementation. This practice may not be suitable for use in double-porosity aquifers where the diffusive exchange between poor quality matrix water and injected freshwater within the fractures plays a significant role. The injection phase of the test moves water away from the well out into the aquifer. Diffusive exchange of solutes occurs, and solute concentrations in the matrix waters decrease, which is beneficial to the operation of ASR. The subsequent abstraction phase moves water towards the well, and this water which may be of poor quality, will also diffusively exchange solutes with the matrix. As a result, the solute concentrations in the matrix will increase again, limiting the 'conditioning' effect of the aquifer test, and hence potentially decreasing recovery efficiencies.

The efficiency of short duration cycle tests can be indicated by comparison to a proposed alternative of implementing a period of continuous injection (see section 2.5.4). By stipulating the required operational capability of an ASR system on the first operation cycle, it is possible to determine either the number of test cycles required to allow the successful operation of this system, or the minimum duration of continuous injection required, again for the successful operation of the ASR system.

The comparison can take two forms, either comparing the time required for the preparation of the system, or comparing the volume of water injected into the system. The volume of injected water required to condition the aquifer is, in most situations, going to be of most interest. As the DP-Pulse model is invariant with respect to injection rate (Section 3.6), this value can be illustrated by the total period during which injection occurs, assuming that conditioning takes place at the same injection rate as the planned ASR operation.

As the behaviour of a system is dependent on both the operational activities of the ASR system, but also the characteristics of the aquifer, it is necessary to account for
the potential variation in aquifer characteristics. Therefore, the solution will be presented as the total injection duration required to obtain a stated performance of the ASR system on the first operational cycle, plotted against $t_{cf}$, representing the characteristics of the aquifer (again, $\sigma$ is set at 40).

If we consider a short cyclic preparation phase, similar to that currently used for the dual purposes of testing an aquifer’s characteristics as well as preparing it for an operational ASR scheme, and compare it to a preparation phase consisting of continuous injection, we get the results below (Figure 7-3). The cyclic preparation phases consist of a 30 day injection period followed by either a 10 day abstraction period (i.e. 33% injected water is recovered) or a 20 day abstraction period (i.e. 66% of injected water is recovered). The maximum abstractable solute concentration was set at either 0.1 (A,B,C) or 0.5 (D,E,F) and the operational cycle selected was the annual cycle outlined in Table 6-4.

![Figure 7-3 Sum of injection periods required to fulfil requirements on initial operational ASR cycle for different values of $t_{cf}$ ($\sigma = 40$, $\Delta T = 10$ days).](image)

This figure illustrates how, for a broad range of $t_{cf}$ values, abstracting water that has been injected in order to condition the aquifer decreases the efficiency of the conditioning process, by a significant amount. Furthermore:

- When $t_{cf}$ is high, continuous injection can reduce the total injection duration, and hence volume of injected water required to achieve a specified system by up to 50% (compare A with C, and D with F).
• The absolute reduction in conditioning times resulting from continuous injection are greater when the maximum abstracted solute concentration is lower (compare C with F).

From this it is possible to conclude that continuous injection is much more efficient than continuous cycling for preparing an aquifer for ASR operations.

7.4.2. Decreasing benefit with longer test periods

At early times, when diffusion does not penetrate far into the matrix, the model behaviour is characterised by \( t_{cf} \), so only this parameter can be deduced from short-term tests. At later times \( t_{cb} \) and \( \sigma \) are characterising. In order to illustrate the effect of these two time-scales on the Marquardt-Levenberg calibration routine (see Section 3.11.4.2), a data set was produced using the standard DP-Pulse program in simulation mode (see Section 2.4.4 for details of the model formulation, and Appendix VII for instructions on the model use). Gaussian random noise was then added with a specified standard deviation. The DP-Pulse model was then calibrated to the resultant synthetic data, and the confidence levels on the parameters derived were examined. As expected, whether fitting to \( t_{cf} \) or to \( t_{cb} \) and \( \sigma \) the fit improved with time, i.e. the range of the bounds on the fitted parameter described by the confidence levels was reduced.

A series of different synthetic data sets were produced by repeatedly adding gaussian random noise with a specified standard deviation to a single simulated data set. The DP-Pulse model was then calibrated to each synthetic data set in turn, and a standard deviation of the calibrated parameter values (i.e. \( t_{cf} \), or \( t_{cb} \) and \( \sigma \)) was determined from all the individual calibration events.

For the purpose of this test, \( \sigma \) was set to 50, while \( t_{cb} \) was set to 1000 days. A standard cycle of 50 days injection, 50 days storage, 50 days abstraction and 50 days dormancy was used. Random noise with a standard deviation (\( \sigma \)) of 0.05 was added to the solute concentration data, this value having been determined as suitable in Section 4.6.3. When fitting to \( t_{cf} \) (with \( \sigma \) fixed at 50) the standard deviation of the calibrated values fell to 0.14% of the mean value within 150 days, after which it remained relatively constant at around 0.1% (Figure 7-4).

At early times, the standard deviation in the calibrations to \( t_{cb} \) and \( \sigma \) was significantly greater than the mean value, indicating that the fit was extremely poorly constrained. By 600 days the single standard deviation of \( \sigma \) had fallen below 10% of the mean
value, and after 1000 days 1% (Figure 7-5). By contrast, the standard deviation of $t_{cb}$ had fallen below 10% of the mean value after 1150 days, but by 4500 days had still only fallen to 2.5% of the mean value.

![Graph showing change in standard deviation with time](image1)

**Figure 7-4** Change in the standard deviation with time: Calibration to synthetic data produced by adding randomly distributed noise to the results of a DP-Pulse simulation (calibration of $t_{cf}$).

![Graph showing change in standard deviation with time](image2)

**Figure 7-5** Change in the standard deviation with time: Calibration to synthetic data produced by adding randomly distributed noise to the results of a DP-Pulse simulation (calibration of $t_{cb}$ and $\sigma$).

Clearly, calibration to $t_{cf}$ can be undertaken successfully after aquifer tests of short duration. Successful calibration to $t_{cb}$ and $\sigma$ requires that the aquifer test be of sufficiently long duration.

### 7.5. Applying Operational Research methodologies to designing an ASR test.

The previous two sections (Section 7.3 and Section 7.4) detailed the conceptual requirements of an ASR test, as well as discussing the failings of the current test practices. The following sections will readdress the cycle testing problem in greater
detail, and develop a conceptual model for an ASR test that is suitable for use in
double-porosity aquifers, in conjunction with the use of the OR techniques discussed
in Section 7.2.

7.5.1. What are the aims?
To provide structure to the problem of developing an ASR test suitable for use in
double-porosity aquifers, the general form detailed in Section 7.2.1 can be utilised in
conjunction with the DP-Pulse model to provide optimal solutions to a number of
questions.
In this case the methodology will be applied to optimal ASR test design:-
• Outlining the interactions between test duration, conditioning period
duration, aquifer characterisation.
• Considering some of the other aspects involved, including determining the
benefit to be obtained from an observation well.
• Outlining an ideal operational scheme with a high probability of being
able to supply during periods of unexpected demand.
More specifically, there are a number of objectives in the optimisation of a test to
classify the double-porosity characteristics of an aquifer prior to the
implementation of ASR (an ‘ASR test’). These include the maximising of
information gained, minimising the cost of the test, and minimising the time the ASR
test requires. These three optimisations are connected, as maximising the
information gained will be likely to involve increasing the duration of the test and
hence the cost. There are a number of ways of approaching a solution to this kind of
problem.
It is helpful to look at the desired outcome of an ASR test. It may be that the
ultimate goal is to optimally characterise the aquifer. An approach with this goal
would take no account of the use of the aquifer once characterised, and no account of
any preparation required in order to allow that usage. Alternatively, at the end of the
test and preparation periods, the desire may be to have an aquifer that will be
immediately suitable for use for commercially operating ASR. These two different
requirements will, in turn, have different solutions.

7.5.2. What are the controls?
There are actually few controls in any model of an ASR system developed. It is
possible to vary the rate of flow through the well and the pumping pattern (i.e. the
absolute and relative durations of injection, storage, abstraction and dormant periods). For an aquifer with significant double-porosity, a number of cycles to test the aquifer may be useful, the simplest implementation being that of a two cycle testing system, the first indicating a value of $t_{cf}$, the second cycle, designed on the results of the first, giving information about $t_{cb}$ and $\sigma$. It is also possible to introduce extra sets of experimental data through the use of observation wells. The increased benefit of the extra data obtained may reduce the necessary test duration and hence cost of a testing procedure.

If there are no observation wells then, due to the invariance of the DP-Pulse model, varying the rate of injection will not alter the information gained. Variable rates of flow through the well may, however, be important in an ASR testing procedure leading to subsequent commercial operation, as a period of preparation will involve the development of a buffer zone (see Section 2.5.4) and this should be of a scale to cope with the operational cycle. Increased flow rates will allow more rapid development of the buffer zone.

It seems likely that the testing and conditioning of the aquifer should take place on the same scale as the operational cycle, i.e. the preparation processes should involve water flow through an aquifer volume at least as large as that involved in the operational cycle. This may be achieved through a long period of conditioning with low flow rates, or a short period with high flow rates. As the variable velocity function of the DP-Pulse model has only undergone rudimentary testing (Appendix VI) we will concentrate on using identical flow rates to those used in the operational cycle.

The pumping pattern will be the most important control. The approaches will need to examine the relative benefits of a single variable length test cycle and multiple testing cycles, and will also have to account for the varying requirements to condition the aquifer. An OR model should also examine the interrelations between the extra cost of continual injection throughout the year as opposed to the extra time requirements of shorter periods of injection, limited for example to the months of water excess. The conditioning phase may also be broken by one or more periods of abstraction to assess the current condition of the aquifer and improve the calibration of the DP-Pulse model.
Observation wells may be used to increase the quantity and quality of data collected during an ASR test. Extra data may reduce the uncertainty in the calibration and hence justify the cost of installing another well.

7.5.3. Including 'noise' into the optimisation model

Noise is important when the DP-Pulse model is used to calibrate to collected data. It is impossible with the constraints of data collection accuracy to obtain an exact fit of the model and hence exact parameters for use in prediction. There will always be uncertainty, therefore, in model parameters obtained through measurement or simulation. This needs to be incorporated into any optimisation or management model. The easiest way to do this is through some form of sensitivity analysis of the model, giving the bounds of possible behaviour resulting from errors in the initial estimated parameters.

7.5.4. Separating the components of the problem

A comprehensive OR model of the testing and conditioning of an aquifer will need to treat these processes as entirely connected for a number of reasons. Firstly, the testing procedure affects the necessary conditioning period of an aquifer. A long ASR test will perform a certain amount of aquifer 'cleansing', reducing the required conditioning period as a result. The second reason for the connection between the models are the requirements for the solution of an OR model, detailed below. The costs incurred in the ASR testing procedure increase with time, as does the benefit obtained, in the form of reduced parameter uncertainty. The output of such a model is therefore the cost of obtaining a certain amount of data. This by itself cannot be optimised, as there is neither a way of judging the minimum amount of data required, nor an easy way of determining a maximum feasible cost. Optimisation would require a financial value to be placed on the collected data to offset the cost, a requirement that is very difficult to satisfy.

The length of the conditioning period will be influenced by the data obtained during the ASR test, and is likely to reduce with decreasing parameter uncertainty. This potential for decreasing costs with increasing data may provide us with the necessary financial benefit to offset the costs incurred during the testing procedure, allowing a general OR solution. An OR model to optimise the testing of an aquifer should therefore involve the conditioning procedure as an integral component.
Clearly, the problem is complex, and the solution – a comprehensive model - will be difficult to develop.

7.5.5. **Application of OR methodologies to the specific problem of ASR**

Before developing and implementing an OR model, it is worth looking at some of the specific issues related to ASR, and the cycle testing problem discussed in the previous section.

Firstly, when examining the data collected during a cycle test in a double-porosity system, only calibrating $t_{ef}$ will usually be justified, as the test durations are relatively short. As was shown in Section 3.10, as well as in Section 7.4, at early times the model is insensitive to either $t_{cb}$ or $\sigma$, the main control being the combined parameter $t_{cf} = t_{cb}/\sigma^2$. When looking at the system over longer timescales, including conditioning and operation, both $t_{cb}$ and $\sigma$ control the solute concentration changes, and hence it is necessary to examine $t_{cb}$ and $\sigma$ independently.

The final optimisation process will require the application of costs. These were outlined in Table 7-2. The model will only incorporate those costs that depend on time – the cost of water supply and disposal, and the cost of power, as initial ‘start-up’ costs will be similar regardless of scheme design.

Whilst the costs of installation are important, they will need to be examined with respect to the entire OR model. For example, the installation of an observation well will cost a certain amount on top of the other costs of the ASR scheme. Comparison of the startup costs could be undertaken as a separate process if required. For example, in a scenario looking at the potential cost benefits of the installation of an observation well, the optimisation model would be run twice, once with and once without the observation well. If the model run with the observation well indicated a cost reduction larger than the cost of installation and water sampling from the second well, it would be cost effective to install the second well.

**7.6. Summary**

This chapter has provided a first look at some aspects of Operational Research techniques as a tool to aid in problem solving, and at their specific usage in problems of a hydrogeological nature.

The problem of devising a test for determining the applicability of ASR in double-porosity aquifers was described, and the current ‘cycle testing’ methodology was
discussed. The drawbacks to the current methodology were examined empirically, and an alternative methodology, of testing followed by conditioning proposed. Finally, the practicalities of developing an ASR test were examined in detail, and a framework within which the problem could be solved was provided. In the next chapter, the general optimisation problem formulation will be applied to the ASR test problem. This basic illustration has some significant flaws, which are considered towards the end of the chapter, but provides a useful step before developing the OR model in Chapter 10.
Chapter 8

‘Risk Reduction’ methodology: A tool to design an ASR test that will guarantee ‘low-risk’ operation of an ASR system
8. ‘Risk Reduction’ methodology: A tool to design an ASR test that will guarantee ‘low-risk’ operation of an ASR system

In the previous chapter, an ASR test that may be utilised to characterise an aquifer prior to the implementation of an ASR system was discussed in the light of OR techniques of solution determination. The discussion was a general look at how a problem may be defined within a systematic OR approach, and how a solution may then be approached. This chapter aims to take this process further by actually developing a model that is capable of designing an optimal ASR test for application in an ASR scenario. The factors outlined in Table 7-2 will be accounted for, and a coherent and numerically soluble formulation which can result in a tool that can be used to design an optimal ASR test will be produced. The model will be applied to a basic test scenario, and all the potential flaws and limitations of the model will be discussed, along with methods that might be used to overcome these issues.

8.1. The concept of ‘Risk Reduction’

One of the real concerns of any system that plays an important role in a company’s operations, such as a water resource system, is that the operation of that system should have a low risk of failure. This is even more emphasised when the system will require a significant amount of expenditure. Investment in an ASR system, for example, may depend on how probable it is that the investment will show returns, which may also be stated as the magnitude of the risk of failure (i.e. the probability that a scheme cannot be operated as predicted). The ‘Risk Reduction’ allows the risk to be identified and reduced by a significant degree. By optimising cost while maintaining the minimum potential level of risk, reassurance can be gained for the investor.

Frequently, during a cost-benefit analysis of a proposed scheme, the cost of the system is counterbalanced by the potential financial benefit. This is a precarious approach, as supportable definitions of cost and financial benefit are extremely complex to make, depending on both economical and social factors. As an example, it is likely to be extremely damaging to business if a major water resource supply fails, leading to the need for tankered water supplies or the use of standpipes. While there is a definite financial cost that may be determined for this scenario, the social cost in customer dissatisfaction is extremely hard to quantify. From another point of
view, the financial benefit of an assured supply of water at times of peak demand is just as unquantifiable. Risk is often used to embody both the probability of failure and the consequences of failure. As has been stated, it is difficult to quantify the consequences of failure, and therefore within this work the word risk will only describe the probability of failure.

When applying OR techniques, it is possible to offset an increase in cost with a reduction in the risk. To continue to use the ASR test as an example, we could simply state that we wish to 'minimise the cost of an ASR test'. Fulfilment of that statement is simple, as it essentially indicates that no ASR test be carried out, a cheap solution but one that carries a great deal of risk. With the 'Risk Reduction' methodology, the cost of an ASR test should be minimised, while maintaining risk at an acceptably low level.

Within this thesis, the risk is determined to be the probability of a system not performing as required. The model solution requires that a minimum performance is obtained from the system, i.e. that there is minimal risk of failure. The model does not, however, account for the extreme scenario, where characterisation of the aquifer is incorrect due to severely misleading results from high magnitude noise, or large deviation from the assumptions, most notably that of homogeneity of the aquifer. Although the model formulation has been devised to greatly reduce risk, the model should still be used with the same caution that should be applied in the use of any other decision tool.

8.2. Model requirements and description

A robust model of a system should be capable of expansion to encompass all necessary facets of the problem, with all reasoning being consistent and well justified. The 'Risk Reduction' model developed here is designed to have these characteristics. The primary task before model development is that of clearly stating the objective of the work. It is important to clearly define the function of the model. The 'Risk Reduction' model is designed in order to provide a means of determining an ASR testing and conditioning procedure that will result in a system that will, in its first use, provide a suitable ASR system to fulfil criteria defined by the users. This procedure should be selected to be the lowest cost option, while still accounting for uncertainty within the experimental data. The model should produce a solution that outlines the safest option. We specify that a scheme should be 'low risk', which we define to mean that the first operational cycle should produce the required results in
the form of stated quantities of water, with known abstracted solute concentrations, with a very small chance of failure.

The model is formed from three separate stages:-

1. **ASR test design analysis** - Estimation of the potential error in the calibration of the solute transport model (DP-Pulse) to the ASR test data, resulting from noise in the collected experimental data, allowing the determination of a range of potential characteristics to describe the aquifer under test. The error in the calibration, and hence the 'uncertainty' or the range of potential characteristics, is dependent on the protocol of the ASR test, particularly on the duration of the test;

2. **Conditioning period determination** - Determination of the conditioning period necessary to produce the required performance of the ASR system in the first operational cycle with low risk of failure despite the uncertainties in the known aquifer characteristics. The conditioning period will vary according to the aquifer characteristics, and is therefore dependent on the findings of the range determined in the previous stage;

3. **Cost optimisation** - Combining the ASR test and determined conditioning period in order to find the total cost. Varying the length of the ASR test will vary the range of potential aquifer characteristics determined, and hence the calculated conditioning period. The total cost will be optimised, i.e. the combination of ASR test and conditioning period which incur the minimal overall cost will be determined.

The 'Risk Reduction' model optimises the cost. The optimisation algorithm will minimise the total cost, i.e. the sum of the costs incurred during the testing procedure and the cost of the conditioning. Essentially, as we wish to optimise cost, we need to minimise the total pumping duration. This is controlled by the pumping pattern of the initial testing cycle. We will optimise, therefore, with respect to the pattern of pumping during the ASR test.

### 8.3. **Formulation of the optimal ASR testing problem**

The optimisation process described here is a novel application of operational research methodologies. The method is complex, so in order to aid understanding, it is presented here in three ways: here verbally, diagrammatically in Figure 8-1, and mathematically in Section 8.4. It may also be useful to cross-reference these sections with Section 9, in which a basic application of the model is described in full.
8.3.1. Stage I: ASR test design analysis

The ASR test procedure consists of a very simple scenario. A period of injection followed by a period of abstraction of identical duration form a very simple test cycle (\(P_t; \{t_i^t, t_a^t\}; P_t = \text{test pumping cycle}; t_i^t = \text{test injection duration}; t_a^t = \text{test abstraction duration})\). No period of storage is included. An initial estimated \(t_{cf}^{e}\) value (\(t_{cf}^{e}\)) is used for the ASR test model, which should be suitable to describe the aquifer under consideration. Having defined this, and the test and operational cycle, a series of tasks must be carried out:

1) The solute transport model is used to simulate a chosen test scenario, with a specified \(t_{cf}^{e}\) value (\(t_{cf}^{e}\)), in order to produce a set of data (abstracted solute concentrations against time)\(^4\);

2) These data then have a normally distributed random error added to represent the noise (characterised by \(\sigma_d\), the variance of the experimental data similar to that determined in Section 4.6.3) producing a synthetic data set;

3) The solute transport model is then calibrated to this synthetic data set by changing the value of \(t_{cf}^{e}\) (\(\sigma\) is set at a constant, here selected to be 40, as this is representative of the Chalk aquifer being examined). This gives a value of \(t_{cf}^{e}\), which is unique for each synthetic data set;

4) The process of adding error to the data set and subsequently calibrating to \(t_{cf}^{e}\) is repeated a number of times in order to produce, through a Monte Carlo approach, an accurate estimation of the standard deviation of the distribution of \(t_{cf}^{e}\) values (\(\sigma_{td}\)), resulting from the uncertainties introduced by the noise. The standard deviation can then be used to define a probable range of calibrated \(t_{cf}^{e}\) values for each test duration, accounting for the error in the synthetic data set, which can be considered analogous to experimental error;

5) This process is repeated for a number of test durations. The result is a distribution of determined feasible \(t_{cf}^{e}\) values for each test duration.

8.3.2. Stage II: Conditioning period determination

As has been discussed, it is necessary to link the duration (and hence cost) of the conditioning period to the range of aquifer characteristics determined through the analysis of the ASR test, and the inherent uncertainties resulting from inaccuracies in

\(^4\) This is a primary cause of uncertainty in the model, which is discussed in Section 8.6 and addressed in Chapter 10.
the experimental data. This is achieved through the concept of a ‘required conditioning period’ (RCP). This is defined as the minimum length of conditioning required to ensure the maximum abstracted concentration is less than the maximum allowable solute concentration ($C_{\text{max}}$) during the implementation of the first operational ASR cycle, for an aquifer which has known $t_{cb}$ and $\sigma$.

The RCP is dependent on $t_{cb}$, $\sigma$ and hence $t_{cf}$. The RCP is also dependent on the first operational cycle ($P_o$: $t_{t}^{0}, t_{s}^{0}, t_{d}^{0}$); $P_o$ = first operational pumping cycle; $t_{t}^{0}$ = first operational period of storage; $t_{s}^{0}$ = first operational period of dormancy; $t_{d}^{0}$ = first operational injection duration; $t_{a}^{0}$ = first operational abstraction duration). Because of the specification of $P_o$ and $C_{\text{max}}$, the desired recovery efficiency of the system is implicitly stated, and does not need to be treated as a separate parameter.

It is necessary that the RCP account for any uncertainty in the parameter values derived from the ASR test. Therefore, the RCP is determined for the range of $t_{cf}$ values as calculated from the previously completed analysis of the ASR test.

Assuming that, for a single OR model solution, $P_o$ and $C_{\text{max}}$ remain constant, the determined RCP forms a curve, as the duration of the required conditioning period varies according to the aquifer characteristics. The range of aquifer characteristics defined by the first stage results in a range of aquifer characteristics centred on the estimated value $t_{cf}^0$, irrespective of the ASR test design. Varying the ASR test design varies the extent of the range of RCPs around this centre value.

When plotted against $t_{cf}$, again with an assumed $\sigma$, the required conditioning period tends to zero for low values, rises to a maximum and then falls at higher $t_{cf}$ values. This is because when $t_{cf}$ is low, $t_{cb}$ is also small and so the block rapidly comes to equilibrium with the fracture water. When $t_{cf}$ is high, $t_{cb}$ is also high, the matrix blocks are large and so the ratio of block surface area to volume of fracture water is relatively low. As a result, the dilution of the diffusing solutes is greater.

### 8.3.3. Stage III: Cost optimisation

The first stage provided information on a series of different ASR test designs. For each test design, a range of potential aquifer characteristics was determined, resulting from the potential inaccuracies in the solute data collected during the test, and varying according to the test design. Each different test design also has an associated cost resulting from, amongst others, the cost of the injection water, power requirements, and the cost of the data collection.
The second stage used the data from the first stage to determine a range of required conditioning periods, associated with the range of aquifer characteristics determined by the first stage. This extent of this range varies according to the analysis of the uncertainty in the ASR test results carried out in the first stage. Each required conditioning period has an associated cost, resulting from similar costs to the ASR test.

Each ASR test design, with its associated cost, therefore defines a range of required conditioning periods, which in turn define a range of associated costs. There is uncertainty of the ‘true’ aquifer characteristics, however a range has been defined, and therefore in order to minimise risk the longest required conditioning period (and hence highest cost) defined by the range is selected. This cost is then added to the cost of the ASR test to provide an overall cost for the ‘preparation phase’ (i.e. ASR test and indicated RCP combined) which, in this model is analogous to the objective function (Φ) described in Section 7.2.1.

The cost of the preparation phase has now been determined for each ASR test design. This preparation phase encompasses all activities required to ensure (within a known level of risk) a system that will, in its first use, provide a suitable ASR system to fulfil criteria defined by the users – the primary requirement of the model. It is therefore possible to optimise the cost of the preparation phase (Φ) with respect to the ASR test design, \( P^* \).

The structure of the model, wherein the computationally intensive calculations of stages 1 and 2 are conducted before the introduction of actual costs, is useful for the efficient application of the model. It is not possible to characterise costs for a generic model, as each situation will be different. By storing the results of stages 1 and 2, it is possible to rapidly repeat the optimisation process while varying the costs provided in stage 3, thus allowing the easy investigation of multiple scenarios.

In summary, the cost of testing the aquifer increases as the uncertainty in the aquifer characteristics decreases. At the same time, reducing the uncertainty in the aquifer characteristics potentially reduces the required conditioning period. Increasing the duration of the aquifer testing procedure becomes less effective, as the doubly-porous aquifer can only be fully characterised by very long aquifer tests. There is, therefore, an optimal aquifer test duration which can be identified by this model.
Figure 8.1: Deterministic description of the 'Risk Reduction' model for optimal ASK test design.
8.4. Mathematical description of the optimisation process

Firstly, determine the estimated sensitivity of $t_{cf}$ to ASR test length (or more generally, the pumping pattern, $P_t$):

$$\sigma_{tcf}(P, \sigma_{tcf})$$  \hspace{1cm} (118)

$\sigma_{tcf}$ = standard deviation of $t_{cf}$

$t_{cf}^e$ = estimated initial value of $t_{cf}$

$\sigma_d$ = one standard deviation of the actual error in the experimental data

$P_t$ = test pumping pattern: $P_t: \{t_i^e, t_a^e\}$

$t_i = injection duration; t_a = abstraction duration$

It is necessary to evaluate the cost of pumping during each ASR test:

$$C_i(P, c_i, C_a)$$  \hspace{1cm} (119)

$C_i = cost of an individual test; c_i = unit cost of injection; C_a = unit cost of abstraction$

The required conditioning periods for values of $t_{cf}$, i.e. the conditioning period that can guarantee a certain likelihood of success of the ASR system, can be found:

$$t_{c}^{\max}(t_{cf}^e, \alpha, \sigma_d, P_0, P_t, C_{max}) = \max_{\sigma \in [-\sigma_{tcf}, +\sigma_{tcf}]} t_c(t_{cf}^e + \alpha \sigma P_0, C_{max})$$  \hspace{1cm} (120)

Note that $\sigma_{tcf}$ and $t_c$ are both functions with dependences:

$t_c(t_{cf}, P_0, C_{max})$

and

$$\sigma_{tcf}(P, \sigma_d, t_{cf}^e)$$

Where:

$t_c = duration of conditioning; \alpha = constant describing ‘risk level’ – the range of $t_{cf}$ either side of $t_{cf}^e$ selected (for a relatively conservative model $\alpha = 2)$

$C_{max}$ = maximum allowable solute concentration on first operational cycle

$P_0 = operational pumping pattern; P_0: \{t_i^o, t_a^o, t_d^o\}$

$t_s = period of storage; t_d = period of dormancy (for this simple model $t_d = 0)$

The maximising function selects the maximum required conditioning period that exists

The costs for each required conditioning period can be evaluated:

$$C_c(t_c^{\max}, c_i)$$  \hspace{1cm} (121)

$C_c = cost of a conditioning period$

Finally, the objective function, $\Phi$, can then be written
The optimal testing strategy can be determined by minimising the value of \( \Phi \) with respect to the ASR test-pumping pattern, \( P_t \).

The logical order in which the equations should be applied is (122), needing (120) for \( t_c^{\text{max}} \) which in turn needs (118) for \( \sigma_{t_c} \). This would not, however, be efficient in application. The actual method of implementation is described in the following section.

**8.5. Computer implementation of the ‘Risk Reduction’ model**

The implementation of the ‘Risk Reduction’ model is a time-consuming process. A complete run to the final solution of the entire model would take excessive periods of time. One run, for example, could take up to 2 days on an Intel Pentium III 500 MHz machine running Microsoft Windows NT 4. Because of this, the most efficient method of application of the model involves separating the model into three distinct parts. Two of these parts, which perform the functions described in stages 1 and 2 of Section 8.3, are then run a large number of times in order to create large sets of data, which aim to cover the full range of eventualities. The third and final section of the model is then run for each individual cost scenario. As the processing of the data sets has already occurred, this final run will be very rapid, allowing the user to experiment with different parameter values in order to determine sensitivity.

The first section comprises the determination of the estimated sensitivity of \( \sigma_{t_c} \) to ASR test length:

\[
\sigma_{t_c}(P_t, \sigma_{t_c}, t_c)
\]

A set of ideal solute concentration values for a specified ASR test on a specified aquifer are produced. Normally distributed random noise with a specified standard deviation is added to this data set, and then the DP-Pulse model is calibrated to this synthetic ‘noisy’ data. This process will be repeated several times to allow the determination of the standard deviation of \( \sigma_{t_c} \) resulting from the aquifer characteristics, the testing conditions and the standard deviation of the noise in the data set. The entire process will be repeated for different aquifer characteristics \( t_c \), and different testing cycles \( P_t \).
The second process is to determine the required conditioning period for a specified initial operational cycle, maximum abstracted solute concentration and aquifer ($t_{cf}$, with an assumed $\sigma$):

$$t_c (t_{cf}, P_0, C_{max})$$

This process will be described as the 'conditioning determination' process. This will be repeated for different aquifer characteristics and then for different operational cycles and maximum abstracted solute concentrations.

This process is completed by means of a search for the minimum conditioning period that will allow successful operation of the first annual cycle of a selected scheme. As the duration of the conditioning period will have to be an integer multiple of the pulse interval (in DP-Pulse), an optimisation routine is hard to implement. The simplest method is to increase the conditioning period until the most first successful operational cycle is found.

The final section of the model will involve the input of estimated aquifer characteristics and the estimated standard deviation of the noise in the experimental data, the operational cycle, maximum abstracted solute concentrations as well as costs for injection and abstraction. The appropriate information will then be selected from the data sets and a solution found.

### 8.6. Identified problems with the model

This model is flawed in one obvious respect. In order to determine the optimal pumping routine, it is necessary to input estimated values of $t_{cf}$ and $\sigma$. This could limit the practicalities of application, and certainly confidence in the results. Whilst it is possible to obtain rough estimates of the value of $\sigma$, $t_{cb}$ and therefore $t_{cf}$ cannot be obtained without some form of test, either an ASR test or a tracer test. This model is, therefore, not robust. Applying the model to optimal ASR test design produces a solution – a pumping schedule that is dependent on the estimated aquifer characteristics. If the estimated aquifer characteristics are significantly different from the actual aquifer characteristics, the pumping schedule may be different from that which may be necessary. Moreover, within the defined model, if the selected ASR test as determined from the estimated aquifer characteristics is vastly shorter than that actually required to characterise the aquifer, there is no mechanism through which further testing and characterisation of the aquifer can take place.
These problems are addressed in more detail, and potential solutions are provided in Chapter 10.
Chapter 9

‘Risk Reduction’ model use: Initial application of the ‘Risk Reduction’ model
9. ‘Risk Reduction’ model use: Initial application of the ‘Risk Reduction’ model

Initially, we shall examine the simplest application of the Risk-Reduction model. A system consisting of one ASR well, with a test cycle consisting of a single period of injection and abstraction, followed by conditioning of the aquifer up to a suitable standard will be examined.

In the previous chapter, three stages in the solution of the Risk-Reduction model were defined. These stages were:

I  ASR test design analysis;
II Conditioning period determination;
III Cost optimisation.

In the following application of the model, each of these stages will be completed in turn, with detailed analysis of the process as required.

9.1. Stage I - ASR test design analysis

In Section 8.3.1 the method of obtaining a range of potential \( t_{cf} \) values characterising an aquifer through calibration of the solute transport model to a simulated data set was described. This range is characterised by \( t_{cf}^x \) and \( \sigma_{tcf} \). For this example a number of test durations were selected to illustrate the variation in \( \sigma_{tcf} \) with time. The ASR tests consisted of single injection and abstraction periods of identical duration.

In order to describe the ASR tests, half the total duration of the pumping cycles of the test, the ‘half-test duration’, will be stated. This describes the durations of both the injection period and the abstraction period. In this initial investigation, half-test durations of 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 20, 30, 40 and 50 days will be used. It should be restated that no storage occurs between the injection and abstraction periods.

The noise in the solute concentration data introduced by the experimental error was given a standard deviation of 0.05. This is the same as 5% of the difference between the native and injected water solute concentrations (the experimental data was normalised in this way for the determination of the experimental error carried out in Section 4.6.3). The standard distribution of the calibrated \( t_{cf} \) values was determined for a range of \( t_{cf} \) values between 0.01 day, and 3 days. This range was selected as being greater than the possible range that may characterise the Chalk aquifer. (It is worth recalling that at the Lychett Minster test site, for the slab geometry, the
following parameter values were determined: $t_{cb} = 1086$ days and $\sigma = 49.5$, giving $t_{cf} = 0.44$ days.)

Figure 9-1 Change in the accuracy of the $t_{cf}$ calibrated by the DP-Pulse model with increasing aquifer half-test duration. (Simple injection/abstraction test - no storage - single well, $\Delta T = 1$ day, calibration repeated 5,000 times.)

Figure 9-1 shows how, as expected, increasing the duration of the ASR test increases the confidence in the characterisation of the aquifer. When the ASR test is short, a small increase in the ASR test duration creates a large decrease in the standard deviation of the obtained $t_{cf}$ value.

The standard deviation also appears to be sensitive to variation in the initial estimate of $t_{cf}$, $t_{cf}'$. As $t_{cf}$ increases, longer ASR tests are necessary in order to ensure good aquifer characterisation.

It should also be noted that there is a noticeable increase in the determined standard deviation as the half-test duration increases from one to two days when $t_{cf}$ is high. This is an artefact of the model implementation and should be ignored.

9.2. Stage II - Conditioning period determination

Section 8.3.2 discussed the method of determining the required conditioning period to allow successful operation of a specific ASR cycle. In this example, the operational cycle illustrated in Table 9-1 was selected. The maximum solute concentration was 0.5, and the system was required to give a recovery efficiency (defined in Section 2.5.3) of 100%. $\sigma$ was varied according to the range

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characterising the Chalk aquifer ($\sigma = 10$ to 500), as was $t_{cf} (t_{cf} = 0.01$ to 3 days). No prior injection into the aquifer had occurred. A selection of the results obtained is plotted in Figure 9-2.

**Table 9-1 Standard annual operational ASR cycle**

<table>
<thead>
<tr>
<th>Injection</th>
<th>100 days</th>
</tr>
</thead>
<tbody>
<tr>
<td>Storage</td>
<td>100 days</td>
</tr>
<tr>
<td>Abstraction</td>
<td>100 days</td>
</tr>
<tr>
<td>Dormancy</td>
<td>60 days</td>
</tr>
</tbody>
</table>

Figure 9-2 Required conditioning period to successfully complete the annual cycle described in Table 9-1, with 100% efficiency for a maximum solute concentration of 0.5. ($\Delta T=1$ day)

Figure 9-2 illustrates a number of important points:

- At lower $t_{cf}$ values, the required conditioning period is very sensitive to $\sigma$ (the required conditioning period for different $\sigma$ are far apart for $t_{cf} < 0.5$ days);
- At higher $t_{cf}$ values, the required conditioning period is less sensitive to $\sigma$ (the required conditioning period for different $\sigma$ coincide for higher $t_{cf}$);
- The required conditioning period is more sensitive to $t_{cf}$ when $\sigma$ is low.
- The required conditioning period increases with $t_{cf}$ to a maximum, after which it falls again.
9.3. **Stage III - Cost optimisation**

In order to illustrate the application of the ASR test optimisation, a specific scenario will be investigated. The following illustration involves an aquifer whose characteristics are close to those at the Lychett Minster Test Site. Using the operational cycle outlined in Table 9-1, with a requirement of 100% recovery efficiency and a maximum abstracted solute concentration of 0.5. Initial estimates of $t_{cf} = 0.5$ days and $\sigma = 50$ were used. The information displayed in Figure 9-1 and Figure 9-2 are combined in Figure 9-3.

![Diagram](image)

**Figure 9-3** Increasing test durations lead to a decrease in the standard deviation of $t_{cf}$, which in turn restricts the range of required conditioning periods.

The increasing test durations lead to decreasing ranges of $t_{cf}$, outlined by the determined range of two standard deviations either side of $t_{cf}$, and centred on the estimated parameter value. This range restricts the possible required conditioning periods that may be determined. Two standard deviations either side of the value reduce the risk that the actual value will fall outside the defined range of $t_{cf}$ such that there is a 95% chance of success. In this example, in which the $t_{cf}$ ranges all fall below the $t_{cf}$ that produces the maximum required conditioning period, the maximum required conditioning period will always coincide with the uppermost boundary of the range of $t_{cf}$ values. This is not generally true, but will depend on the characteristics of the individual aquifer, the test aquifer duration and the proposed first operational cycle of the ASR system.

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In order to optimise the ASR test with respect to cost we will apply a cost of £100 per day to the injection process, and £200 per day to the abstraction process. The results, consisting of both the determined required conditioning periods for each specific ASR test, and the overall cost of the test and conditioning, are shown in Figure 9-4.

Figure 9-4 Variation in required conditioning period and total cost of ASR testing and conditioning with ASR test duration.

If we first examine the required conditioning periods, we can see an overall decrease in the required conditioning period with increasing test duration. There also a diminishing return, as was seen with the information gained during the ASR testing (9.1). As the ASR tests increase in duration, the required conditioning period decreases as a result of the greater information obtained. The gain, however, becomes less significant as the ASR tests get larger.

Examination of the total costs identify a clear minimum in this scenario, occurring when the ASR test injection and abstraction phases are two days long. When the ASR test is shorter than this, there is not sufficient information to provide a good estimate of the required conditioning period, and as a result the required conditioning period is overestimated. When the ASR test is longer than two days, the reduction in the required conditioning period resulting from the extra information gained (at some extra cost) is not sufficient to markedly reduce the total cost. In this scenario, the total cost is £45,300. The nearest cost identified is £100 more (0.2%). This cost increase is the result of an increase in the duration of the aquifer test of 1 day (i.e. 1
day of injection at £100, and 1 day abstraction at £200), with no resultant decrease in the conditioning period. Through the application of the 'Risk Reduction' model to this scenario, therefore, we have clearly found an optimal ASR test.

9.4. Risk Reduction model discussion

The preceding description of the use of the Risk Reduction model to produce a solution to a single scenario was kept relatively simple in order to maintain clarity and avoid diversion. Through this section, certain aspects of the solution process will be examined in more detail.

9.4.1. The control of $t_{cf}$ on the error determined during Stage I

In Section 9.1, the assumption was made that $t_{cf}$ was one control on the level of the potential error arising during calibration to ASR test data. In order to investigate the truth of this, the confidence in the calibrated value of $t_{cf}$ as a percentage of $t_{cf}$ is illustrated in Figure 9-5. It is apparent from this that there may be no significant effect resulting from variation in the value of $t_{cf}$. This can be examined through the application of a two-tailed Friedman statistical test, a non-parametric test for several related samples.

The following application of the Friedman test will test the hypothesis that variation in $t_{cf}$ affects the confidence in the calibrated value of $t_{cf}$, stated as a proportion of the value of $t_{cf}$ (equation 123).

$$\frac{d\left(\sigma_{tcf}/t_{cf}\right)}{dt_{cf}} \neq 0$$  \hspace{1cm} (123)

Table 9-2 illustrates the results from the test and shows that as there is an 11.6% probability that the null hypothesis is true, that $t_{cf}$ does not exert a significant effect. As this is not a sufficiently high probability to discount the stated hypothesis, it will be necessary to continue to define $t_{cf}$ in the application of the 'Risk Reduction' model.

Table 9-2 Results of the Friedman statistical test.

<table>
<thead>
<tr>
<th></th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>14</td>
</tr>
<tr>
<td>Chi-Square</td>
<td>10.224</td>
</tr>
<tr>
<td>Degrees of freedom</td>
<td>6</td>
</tr>
<tr>
<td>Asymptotic significance</td>
<td>0.116</td>
</tr>
</tbody>
</table>
9.4.2. Implication of errors resulting from the DP-Pulse model formulation on Stage I

In Chapter 2.4.4 two major constraints on the range of model parameters acceptable for use with the DP-Pulse model were described. The first, equation 106, indicated that for dispersion to be negligible, a sufficient condition was that \( t_{cf} \) be less than \( t_\alpha/3 \). When the ASR test is short and \( t_{cf} \) large this constraint is not met. Table 9-3 lists the minimum aquifer half-test durations that may be accurately described by the DP-Pulse model under this constraint.

**Table 9-3 Minimum half-test durations ensuring negligible dispersion.**

<table>
<thead>
<tr>
<th>( t_{cf} ) (Days)</th>
<th>Shortest acceptable aquifer half-test duration (Days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.0</td>
<td>4.50</td>
</tr>
<tr>
<td>2.5</td>
<td>3.25</td>
</tr>
<tr>
<td>2.0</td>
<td>3.00</td>
</tr>
<tr>
<td>1.5</td>
<td>2.25</td>
</tr>
<tr>
<td>1.0</td>
<td>1.50</td>
</tr>
<tr>
<td>0.5</td>
<td>0.75</td>
</tr>
<tr>
<td>0.1</td>
<td>0.15</td>
</tr>
</tbody>
</table>
A second limitation arises from the error analysis. Section 3.6 described the potential errors that arise from the discretisation of the system into cells of uniform concentration. If we treat the system as having an infinite matrix, an acceptable assumption considering the relative brevity of the ASR tests, we found that the error varied as the number of annuli varied. For a maximum of 1% error, \( N > 33t_c/t_a \), while for a 5% error, \( N > 13t_c/t_a \). As a result, this also affects the minimum acceptable half-test duration. Table 9-4 lists the minimum aquifer half-test durations that may be accurately described by the DP-Pulse model under this constraint, with a \( \Delta T \) of 1 day.

### Table 9-4 Minimum half-test durations ensuring maximum errors of 1% and 5% with a \( \Delta T \) of 1 day.

<table>
<thead>
<tr>
<th>( t_c ) (Days)</th>
<th>Shortest acceptable aquifer half-test duration (Days)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Maximum error of 5%</td>
</tr>
<tr>
<td>3.0</td>
<td>3.12</td>
</tr>
<tr>
<td>2.5</td>
<td>2.85</td>
</tr>
<tr>
<td>2.0</td>
<td>2.55</td>
</tr>
<tr>
<td>1.5</td>
<td>2.21</td>
</tr>
<tr>
<td>1.0</td>
<td>1.80</td>
</tr>
<tr>
<td>0.5</td>
<td>1.27</td>
</tr>
<tr>
<td>0.1</td>
<td>0.57</td>
</tr>
</tbody>
</table>

When \( t_c \) is high, the possible error in the solute concentrations during the shorter ASR tests will be over 5%. This potential error could be overcome through the use of shorter pulse intervals, with a \( \Delta T \) of 0.1 days, the shortest acceptable half-test duration giving an error of 1% is less than 1 day for all the illustrated values of \( t_c \). Unfortunately, this dramatically increases computational time. A single model run of 10 days duration, with a pulse interval of 0.1 days takes 30 milliseconds on an Intel Pentium 500MHz processor running Windows NT 4. This model run must be completed about 16 times for each calibration cycle and that repeated a 1000 times for the Monte Carlo process. The resulting total model duration is 316 seconds. Section 3.11.1 described how the DP-Pulse model simulation duration increased rapidly with time. To calculate the error in the calibration to a test with a half-test duration of 50 days and a pulse interval of 0.1 days would take approximately 9 hours.
9.4.3. Distribution of calibrated $t_{cf}$ values in Stage I

During the completion of Stage I, it is necessary to characterise the range of values of $t_{cf}$ determined through calibration of the DP-Pulse model to the simulated data set. Describing the characterisation as a normal distribution, centred about the mean calibrated $t_{cf}$ value, completed this characterisation. It is necessary to check that this distribution of values is truly normal. In order to conduct this check, Stage 1 of the Risk Reduction model was calculated for a number of different parameter sets, and all the calibrated $t_{cf}$ values were recorded.

We can examine the normality of the calibrated $t_{cf}$ values by applying a number of different statistical tests for normality, including the Kolmogorov-Smirnov One-Sample Test, the Shapiro-Wilks test and the Anderson-Darling test. Lindley & Scott (1995) indicate that normality tests become increasingly sensitive with large sample sizes, such that even minimal divergence from normality will indicate a non-normal distribution. The indicated normality tests have therefore been applied to a randomly selected sub-set of the 5000 calibrated values determined in Section 9.1. Table 9-5 outlines the results obtained in each test for a set of 100 calibrated values (an asymptotic significance of greater than 0.05 indicates that the distribution can be described as normal). We can see that, on the whole, the distributions fit a standard normal distribution. There is, however, some a divergence from the normal distribution at the high and low values (see Figure 9-7, Figure 9-9 and Figure 9-11).

Table 9-5 Results of three normality tests on the range of calibrated $t_{cf}$ values
(Half test duration = 5 days, sample size = 100).

<table>
<thead>
<tr>
<th>$t_{cf}$ (Days)</th>
<th>0.1</th>
<th>0.5</th>
<th>3.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Asymptotic significance</td>
<td>Kolmogorov-Smirnov</td>
<td>&lt;0.15</td>
<td>0.0664</td>
</tr>
<tr>
<td></td>
<td>Shapiro-Wilks</td>
<td>0.4412</td>
<td>0.0570</td>
</tr>
<tr>
<td></td>
<td>Anderson-Darling</td>
<td>0.4549</td>
<td>0.0598</td>
</tr>
</tbody>
</table>

To further prove this normality, the distributions of the calibrated $t_{cf}$ values were plotted on a series of histograms (Figure 9-6, Figure 9-8 and Figure 9-10) and probability plots (Figure 9-7, Figure 9-9 and Figure 9-11) alongside a standard normal distribution, with the same mean and standard deviation.
Figure 9-6 Probability plot of the distribution of \( t_{cf} \) values calibrated to artificially created data from an ASR test consisting of five days injection followed by five days abstraction. \( (\sigma_d = 0.05, t_{cf} = 0.1 \text{ days}, \Delta T = 1 \text{ day}) \)

Figure 9-7 Probability plot of the distribution of \( t_{cf} \) values calibrated to artificially created data from an ASR test consisting of five days injection followed by five days abstraction. \( (\sigma_d = 0.05, t_{cf} = 0.1 \text{ days}, \Delta T = 1 \text{ day}) \)
Figure 9-8 Probability plot of the distribution of $t_{cf}$ values calibrated to artificially created data from an ASR test consisting of five days injection followed by five days abstraction. ($\sigma_d = 0.05$, $t_{cf} = 0.5$ days, $\Delta T = 1$ day.)

Figure 9-9 Probability plot of the distribution of $t_{cf}$ values calibrated to artificially created data from an ASR test consisting of five days injection followed by five days abstraction. ($\sigma_d = 0.05$, $t_{cf} = 0.5$ days, $\Delta T = 1$ day.)
Figure 9-10 Probability plot of the distribution of $t_{cf}$ values calibrated to artificially created data from an ASR test consisting of five days injection followed by five days abstraction. ($\sigma_d = 0.05, t_{cf}^e = 3.0 \text{ days}, \Delta T = 1 \text{ day}.$)

Figure 9-11 Probability distribution of $t_{cf}$ values calibrated to artificially created data from an ASR test consisting of five days injection followed by five days abstraction. ($\sigma_d = 0.05, t_{cf}^e = 3.0 \text{ days}, \Delta T = 1 \text{ day}.$)
We can see that the calibrated $t_{cf}$ values are approximately normally distributed. If the noise is correctly described by the statistical analysis, a level of known control can be applied to the risk in the model. For example, using:

$$\pm \sigma_{cf} / \sqrt{n}$$

(124)
to define the range of potential $t_{cf}$ values will define the risk as 4.6%, where $n$ is the number of calibrations of $t_{cf}$ that have taken place. For the completion of this work it is, however, sufficient that the range of calibrated $t_{cf}$ values is largely encompassed by the 'normal distribution'. As a result, the absolute value of risk is not known, but it is possible to state that the use of two standard deviations ($\alpha=2$ in Equation 124) to describe the range of potential $t_{cf}$ values will reduce the risk to a low level. The normal distribution encompasses approximately the same range of $t_{cf}$ values as can be found within the calibration data set, and so for the purposes of the 'Risk Reduction' model, the distribution is close enough to normal such that it is sufficient to describe the range of calibrated $t_{cf}$ values.

**9.4.4. Convergence of the variance in the calibrated values of $t_{cf}$**

It is important to ensure that the calibration of the DP-Pulse model to the simulated noisy data set is repeated for a sufficient number of realisations to successfully achieve convergence in the value of $\sigma_{cf}$ determined. To confirm that sufficient realisations were taking place, the calculation of Stage I of the model solution process was repeated for a number of different scenarios. For each successive realisation, the standard deviation of $t_{cf}$ was determined, and plotted in Figure 9-12. Initially, the determined variance of $t_{cf}$ is unstable (the first 10 sequentially calculated variances of the calibrated $t_{cf}$ values of series A range between 3.86 and 4.87 days$^2$). It can be seen that after roughly 100 realisations, a reasonable approximation to the standard deviation had been determined (between 95 and 105 sequentially calculated variances values in the same series range between 3.80 and 3.83 days$^2$). Using 5,000 realisations will ensure a good approximation of the standard deviation in $t_{cf}$ (the standard deviation over 10 results is 3.67 days$^2$).
Figure 9-12 Standard deviation in calibrated $t_{cf}$ values, resulting from noise in the solute concentration data during ASR testing after successive realisations of Stage 1 of the Risk Reduction model ($\Delta T = 1$ day).

9.4.5. Description of the required conditioning period determined in Stage II

The curve describing the required conditioning period is a distinctive shape (e.g. Figure 9-2). As $t_{cf}$ increases from 0 days, the required conditioning period increases. If we consider $t_{cf}$ as it is defined in equation 23, we can see that by maintaining $\phi_D$ and $\alpha$, as $D_A$ tends to infinity then $t_{cf}$ tends to zero. This implies that diffusion happens at such a rate that the matrix is rapidly ‘flushed’, approaching injected solute concentrations. As a result the required conditioning period is short. As $D_A$ tends to zero, $t_{cf}$ increases towards infinity. In this case, diffusion is so slow that effectively no solutes diffuse from the matrix into the fracture, so the matrix water remain at the native solute concentration while the injected water maintains the injected solute concentration. Conditioning periods are again short as a result.

With regard to the operational research application of this curve, we can derive further information. When combined with the range of $t_{cf}$ values, centred about the estimated $t_{cf}$ produced by the Stage II of the Risk Reduction model solution, we obtain a defined range of required conditioning periods. We then wish to select the highest required conditioning period within this range. If the entire range of $t_{cf}$ is less than the $t_{cf}$ at the curve maximum (Figure 9-13A), the highest required conditioning period...
period will be that produced by the highest $t_{cf}$ value in the range. If the entire range of $t_{cf}$ is greater than the $t_{cf}$ at the curve maximum (Figure 9-13C), the highest required conditioning period will be that produced by the lowest $t_{cf}$ value in the range. Finally, if the $t_{cf}$ at the curve maximum falls within the range of $t_{cf}$ described by Stage II of the Risk Reduction model solution, the highest required conditioning period will equal the maximum (Figure 9-13B).

![Graph showing how the required conditioning period varies with time](image)

Figure 9-13 Sketch of how the required conditioning period varies with time, showing the impact of uncertainty in the value of $t_{cf}$ for three distinct cases (A, B and C).

It is important to note that the required conditioning period has been determined for an aquifer in which no prior injection has taken place. This approximation is a limitation as it is clear that any testing involving injection of water into the aquifer will affect the solute concentrations within the aquifer, leading to shorter required conditioning periods. If the system were to account for these potential benefits during the ASR testing procedure, it would become necessary to describe the required conditioning period for each selected ASR test procedure. This would require a large amount of computer time, and is not possible within the resources of this work. Potential methodologies for including the conditioning effect of the ASR test will be discussed and applied to a selected example in Section 10.4.
9.4.6. Discussion of the limitations in the described implementation of the Risk Reduction model

The integer nature of the current problem is clearly illustrated in Figure 9-4. Both the conditioning period and the ASR test regime must consist of integer multiples of the selected pulse interval, in this case 1 day. This results in the ‘step-wise’ nature of the falling required conditioning period illustrated. The loss of resolution resulting from this method of implementation will result in a loss of resolution in the solution. The current model will find the cheapest ASR test and conditioning period that result in a low risk of the system failing to meet the stated requirements, and be determined through this integer approach. As the integer nature of the model restricts the ability of the model to represent the flexibility of a real-life scenario, a non-optimal test may be selected by the optimisation routine.

There are two possible methods that may ameliorate this problem. The first would be to reduce the chosen $\Delta T$, which would have the disadvantage of greatly increasing computational requirements. The second method involves approximating the results of Stage I and Stage II of the Risk Reduction model solution process with some form of mathematical formulation. This is discussed further in Section 10.1.

9.5. Determining the sensitivity of the ‘Risk Reduction’ model

In Section 5.2 the calibration of the DP-Pulse model to the Lychett Minster data was submitted to an uncertainty analysis. The purpose of such an analysis is to quantify both the quality of a model calibration and the reliability of any predictions. With this OR model, we are dealing with hypothetical scenarios, and therefore a comprehensive uncertainty analysis is not appropriate. Instead, a sensitivity analysis will be conducted in such a way as to identify the parameters that exert a strong influence over the model findings.

In order to test the sensitivity of the ‘Risk Reduction’ model it is necessary to vary a number of parameters. These are listed below:

- the cost of groundwater supply and injection;
- the cost of groundwater abstraction and disposal;
- the error in the experimental data;
- the effect of changing the estimated value of $t_{df}$;
- the effect of changing the estimated value of $\sigma$. 


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• the maximum abstracted solute concentration;
• the desired recovery efficiency.

The model will additionally be sensitive to $\sigma_d$, which may be altered to vary the inherent risk in the scheme. This variable will not, however, be examined here. The costs of groundwater injection and abstraction will only have an effect if the relative differences between them are varied. For example, if groundwater abstraction and disposal are vastly more expensive than supply and injection, the optimal system will involve a short ASR testing cycle, with an emphasis on over-conditioning the aquifer in order to guarantee low-risk operation. If groundwater supply is a greater expense, then extensive testing of the aquifer in order to minimise the conditioning period will be optimal.

Increasing the noise added to the solute concentration data will reduce the reliability of the ASR testing procedure, encouraging a dependence on extensive conditioning to ensure low-risk operation. Decreasing the noise will have an opposite effect.

Changing the estimated values of $t_c$ and $\sigma$ will largely affect the overall cost of the testing/conditioning procedure, and may also change the optimal procedure.

In order to investigate these sensitivities a series of model runs were performed. The different groups of selected parameters are outlined in Table 9-6. The outcome of these model runs (both required conditioning periods and total costs) are illustrated and discussed below.

At this point, it is worth noting that variations in recovery efficiency are accomplished by varying the initial operational ASR cycle, $P_0$.

**Table 9-6 Parameter values selected for sensitivity analysis of the ‘Risk Reduction’ model.**

<table>
<thead>
<tr>
<th>Group</th>
<th>Cost of groundwater supply and injection (£)</th>
<th>Cost of groundwater abstraction and disposal (£)</th>
<th>Standard deviation of synthetic noise in solute concentrations</th>
<th>Maximum abstracted solute concentration</th>
<th>Recovery efficiency (%)</th>
<th>$t_c$ (Days)</th>
<th>$\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ST</td>
<td>100</td>
<td>200</td>
<td>0.05</td>
<td>0.5</td>
<td>100</td>
<td>0.5</td>
<td>50</td>
</tr>
<tr>
<td>A</td>
<td>100</td>
<td>100</td>
<td>0.05</td>
<td>0.5</td>
<td>100</td>
<td>0.5</td>
<td>50</td>
</tr>
<tr>
<td>B</td>
<td>200</td>
<td>100</td>
<td>0.05</td>
<td>0.5</td>
<td>100</td>
<td>0.5</td>
<td>50</td>
</tr>
<tr>
<td>C</td>
<td>100</td>
<td>200</td>
<td>0.10</td>
<td>0.5</td>
<td>100</td>
<td>0.5</td>
<td>50</td>
</tr>
<tr>
<td>D</td>
<td>100</td>
<td>200</td>
<td>0.01</td>
<td>0.5</td>
<td>100</td>
<td>0.5</td>
<td>50</td>
</tr>
<tr>
<td>E</td>
<td>100</td>
<td>200</td>
<td>0.05</td>
<td>0.5</td>
<td>100</td>
<td>1.0</td>
<td>50</td>
</tr>
<tr>
<td>F</td>
<td>100</td>
<td>200</td>
<td>0.05</td>
<td>0.5</td>
<td>100</td>
<td>0.1</td>
<td>50</td>
</tr>
<tr>
<td>G</td>
<td>100</td>
<td>200</td>
<td>0.05</td>
<td>0.5</td>
<td>100</td>
<td>0.5</td>
<td>100</td>
</tr>
<tr>
<td>H</td>
<td>100</td>
<td>200</td>
<td>0.05</td>
<td>0.5</td>
<td>100</td>
<td>0.5</td>
<td>10</td>
</tr>
<tr>
<td>I</td>
<td>100</td>
<td>200</td>
<td>0.05</td>
<td>0.5</td>
<td>50</td>
<td>0.5</td>
<td>50</td>
</tr>
<tr>
<td>J</td>
<td>100</td>
<td>200</td>
<td>0.05</td>
<td>0.1</td>
<td>100</td>
<td>0.5</td>
<td>50</td>
</tr>
</tbody>
</table>

*Note: ST identifies the standard against which other scenarios are compared.*
Figure 9-14 Variation in required conditioning period and total cost of ASR testing and conditioning with ASR test duration. (Sensitivity analysis - varying injection and abstraction costs – Cases A, B and ST.)

Figure 9-14 illustrates the effect of varying the costs of injection and abstraction. Within the range examined, the optimal test duration is not sensitive to the cost of injection. The optimal test duration is, however, sensitive to the cost of abstraction. The total cost of testing and conditioning is very sensitive to both the costs of injection and abstraction.
Figure 9-15 Variation in required conditioning period and total cost of ASR testing and conditioning with ASR test duration. (Sensitivity analysis - varying synthetic noise – Cases C, D and ST.)

Figure 9-15 shows that varying the standard deviation of the synthetic noise has a small effect on the optimal testing regime. Small magnitude noise (D – standard deviation of noise^2 = 0.01) produces the same optimal test as the standard (standard deviation of noise = 0.5). If there is little noise (i.e. experimental sampling is very accurate, and the aquifer homogenous, example D – standard deviation of noise = 0.01) a shorter ASR test is optimal, while if the noise is of high magnitude (C – standard deviation of noise = 0.1) a longer aquifer test is optimal.

Varying the noise has a large effect on the overall cost of the testing and conditioning process, as increased accuracy when testing leads better refinement of the aquifer characteristics, and hence allows shorter and cheaper conditioning periods.

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5 The noise referred to here is defined by the standard deviation, e.g. a standard deviation of 0.1 means the noise has a standard deviation of 0.1 x (Native solute concentrations-Injected solute concentrations) (see Section 4.6.3).
Figure 9-16 Variation in required conditioning period and total cost of ASR testing and conditioning with ASR test duration. (Sensitivity analysis - varying $t_{cf}$ - Cases E, F and ST.)

Figure 9-16 shows that varying $t_{cf}$ has an effect on the length of the optimal ASR test. It also has a large effect on the overall cost of testing and conditioning. With a high $t_{cf}$ (Case E - $t_{cf} = 1$ day) it is optimal to have a shorter test, as the large $t_{cf}$ value means an increase in test duration results in a relatively small increase in the information gained about the aquifer. A low $t_{cf}$ (Case F - $t_{cf} = 0.1$ days) also has a longer test, as it is easier to fully characterise the aquifer within a reasonable period of time. Variations in the total cost of testing and conditioning the aquifer arise from increases in the required conditioning period for higher $t_{cf}$ values.
Figure 9-17 Variation in required conditioning period and total cost of ASR testing and conditioning with ASR test duration. (Sensitivity analysis - varying \( \sigma \) - Cases G, H and ST.)

Figure 9-17 shows that varying \( \sigma \) can have a large effect on the total cost and also impacts on the optimal ASR test. When \( \sigma \) is low (Case H - \( \sigma = 10 \)), the required conditioning periods are low, so the reduced conditioning period resulting from improved characterisation becomes insignificant with respect to the increased costs of the testing. When \( \sigma \) is high (Case G - \( \sigma = 100 \)), an increase in test duration results in a relatively small increase in the information gained about the aquifer, and so short ASR tests are optimal.
Figure 9-18 Variation in required conditioning period and total cost of ASR testing and conditioning with ASR test duration. (Sensitivity analysis - varying maximum solute concentration, $m$, and recovery efficiency – Cases I, J and ST.)

Figure 9-18 shows that varying the maximum solute concentration has a large effect on both the total cost and the optimal ASR test. When the maximum solute concentration is low and the recovery efficiency is high (Case J – maximum relative abstracted solute concentration = 0.1, recovery efficiency = 100%), the required conditioning periods are high, so the decrease in the length of the conditioning period resulting from improved characterisation becomes significant with respect to the increased costs of the testing. When recovery efficiencies are low, and the maximum solute concentration is high (Case I – maximum relative abstracted solute concentration = 0.5, recovery efficiency = 50%) there is a reduction in the conditioning period, and a hence reduction in the length of the optimal ASR testing regime.

9.6. Conclusions of the sensitivity analysis

A number of conclusions can be drawn from the sensitivity analysis:

- The cost of injection does not affect the optimal test duration, only the total cost of testing and conditioning.
- Varying the magnitude of the synthetic noise has little effect on the optimal ASR test duration, doubling the magnitude of the noise increases the optimal test...
duration by one day. If the experimental sampling is very accurate a shorter ASR test is optimal.

- Varying the magnitude of the synthetic noise has a large effect on the overall cost of the testing and conditioning process, with increased accuracy when testing leading to shorter, and hence cheaper conditioning periods required to guarantee low-risk operation of the ASR system.

- Varying $t_{cf}$ has a significant effect on the length of the optimal ASR test, increasing $t_{cf}$ from 0.1 days to 1 day decreases the optimal test duration from 6 days to 1 day. Although the increased $t_{cf}$ would mean that a shorter test could characterise the aquifer, at higher $t_{cf}$ values the required conditioning period is less sensitive to variation in $t_{cf}$, and therefore a shorter test is optimal. It also has a large effect on the required conditioning period, which is longer for higher $t_{cf}$ values, and therefore on the overall cost.

- Varying $\sigma$ can have a large effect on both the total cost and the optimal ASR test. When $\sigma$ is less than 10, the required conditioning periods are low (generally less than 100 days, depending on $t_{cf}$), so the reduced conditioning period resulting from improved characterisation becomes insignificant with respect to the increased costs of the testing. When $\sigma$ is greater than 50, an increase in test duration results in a relatively small increase in the information gained about the aquifer, and so short ASR tests of the order of 1 day duration are optimal.

- Decreasing the maximum abstracted solute concentration from 0.5 to 0.1 can increase the total cost by a factor of 10, and as a result good characterisation of the aquifer by the ASR test is optimal, and the optimal ASR test is significantly longer (9 days longer). When the maximum abstracted solute concentration is low, the required conditioning periods are high, so the decrease in the length of the conditioning period resulting from improved characterisation becomes significant with respect to the increased costs of the testing.

- When recovery efficiencies are reduced to 50%, there is a reduction in the conditioning period of about 38%, and also a reduction in the length of the optimal aquifer-testing regime.
Chapter 10

Further developments of the ‘Risk Reduction’ model
10. Further developments of the ‘Risk Reduction’ model

The previous two chapters have, respectively, described the formulation of the Risk Reduction model, and implemented it in a simple hypothetical situation in order to demonstrate the use of the model. Within this chapter, a number of scenarios will investigate different facets of a potential ASR system. This exercise will serve to both identify the potential benefits of different forms of ASR test, and to illustrate how the ‘Risk Reduction’ model may be developed to examine almost any potential requirement.

Initially, two scenarios will be discussed: the incorporation of a period of storage into the ASR test, and the use of observation wells to increase the quantity of data collected. After the Risk Reduction model is used to quantify the potential benefits of each variation to the standard test previously applied, close examination of the implications of the solutions will be undertaken. Subsequently a final scenario, incorporating a number of variations in the methodology will be described. These variations form a response to a number of the criticisms of the current model implementation that have been raised in the text.

The description of the application of the Risk Reduction model that follows will be somewhat reduced from the description of the previous section. It is hoped that the reader will refer back to the previous chapter where clarification on process is provided.

10.1. Including a period of storage in the ASR test

All previous discussions have discounted the inclusion of a period of storage in the middle of the ASR test. The duration of the ASR test has been shown to play an important role on controlling the quality of the calibration of the DP-Pulse model. It therefore seems possible that introducing a storage period, which would also increase the duration of the ASR test, could serve to increase the information obtained for relatively little cost. In order to investigate this hypothesis, a storage period was introduced to the ASR test during the implementation of the Risk Reduction model. This storage period, of a fixed length, was applied between the injection and abstraction phases of the ASR test.

In order to determine the effect of this storage period, the results from the Stage 1 process (determining the potential error in the determination of $t_{cf}$ when calibrating to the ASR test) were compared with those from ASR tests with no storage period over
a range of \( t_{cf} \) values. The results when \( t_{cf} = 1 \) day are summarised below in Figure 10-1 and Appendix I illustrates the same results for a range of \( t_{cf} \) values.

![Figure 10-1 Comparing the standard deviation of the calibrated values of \( t_{cf} \) resulting from ASR tests with different storage periods (\( t_{cf} = 1.0 \) days, \( \Delta T = 1 \) day, standard deviation of the random distribution of noise = 0.05).](image)

From examining Figure 10-1:

- The inclusion of a period of storage in the ASR testing procedure reduced the confidence in the characterisation of the aquifer.
- The detrimental effect of including a storage period was most notable in short ASR tests, but still present in longer duration ASR tests.

Caution should be applied when utilising this result however. Although a period of storage has been shown to decrease the information obtained about the double porosity nature of an aquifer during an ASR test, geochemical interactions do take place. It may, therefore, still be necessary to include a period of storage in an ASR test in order to determine potential geochemical interactions that may take place during operation of the ASR system.

10.1.1. Why does a period of storage decrease the information obtained during an ASR test?

The results indicate that that the inclusion of a period of storage in an ASR test, rather than improving the resulting characterisation, is in fact detrimental to the calibration process. To explain this, it is necessary to examine the abstracted solute
concentrations produced by the model for two scenarios. The model was run with $t_{cb}$ values of 1000, 1250 and 1500 days, and a $\sigma$ value of 50 (giving $t_{cf}$ values of 0.4, 0.5 and 0.6 days). The model was then set up for a single day of injection followed by a single day of abstraction with either no storage period, or one of 50 days. The abstracted solute concentrations produced by the model are illustrated in Figure 10-2.

![Figure 10-2 Comparison of abstracted solute concentrations from an ASR test consisting of 1 day injection followed by one day abstraction, with and without a storage period of 50 days ($t_{cb} = 1250$ days, $\sigma = 50$, $\Delta T = 0.1$ days).](image)

During the storage period, diffusion occurs from volumes of high solute concentrations to volumes of low solute concentrations – in the illustrated example this diffusion is from the matrix to the fracture. As a result, the solute concentrations in the fracture approach equilibrium with the matrix. It is clear that there is a significant difference in the abstracted solute concentrations, linked to the length of the storage period, for all examined values of $t_{cf}$. When a storage period is included in the ASR test cycle the range of abstracted solute concentrations during the abstraction process is much narrower. As expected, after a period of storage all of the abstracted solute concentrations are closer to the native solute concentrations.

For the purposes of the automated calibration, it is the sensitivity of the abstracted relative solute concentrations to $t_{cf}$ that is important. Figure 10-2 shows that when there is no storage period, the abstracted solute concentrations are more sensitive to variations in $t_{cf}$. Within the range of $t_{cf}$ selected, the maximum difference between
abstracted solute concentrations when there is no storage period is 0.0411, or 18.4%. With a 50-day storage period the maximum difference is 0.0127, or 1.44%.

Inclusion of a storage period into the ASR test procedure allows more time for the water in the fracture to approach equilibrium with the water in the matrix. If the storage period were infinitely long, the solute concentration of the fracture water would be at total equilibrium with the matrix water. As the end solute concentration in this scenario would be entirely controlled by \( \sigma \) (i.e. the ratio of matrix to fracture porosities) and not by \( t_{cb} \) (which controls the time for equilibrium to be reached), this scenario would be totally insensitive to variations in \( t_{cb} \). The shorter the storage period, therefore, the more sensitivity to \( t_{cb} \) increases. As a result of this increased sensitivity, when there is no storage period the abstracted solute concentrations are more sensitive to variations in \( t_{cf} \).

### 10.2. Use of an observation well

It is standard practice in the development of ASR sites to include at least one observation well. These wells are important for a number of reasons, including the determination of accurate hydraulic characteristics of the aquifer. In addition to these requirements, the observation wells may be used for the purposes of characterising double-porosity behaviour. As a result, it is necessary to investigate the potential of observation wells within the 'Risk Reduction' model, within which they may increase the benefits of an ASR test, and hence reduce the required conditioning period. As well as the selection of whether to install one or more observation wells, it is necessary to examine the placement of these wells.

During an ASR test a second set of data may be collected from an observation well, illustrating the result of flow through the aquifer. If this second data set is also included in the calibration, the characterisation of the aquifer may be more successful. For a comparison, rather than compare the results of the entire 'Risk Reduction' model, it is simpler to compare the results of Stage 1 of the solution. As long as the range of calibrated \( t_{cf} \) values does not encompass the maximum required conditioning period (see Section 9.4.5), we can assume that if the standard deviation of the calibrated \( t_{cf} \) values is smaller for a specific test cycle, that the required conditioning period will be shorter. As such we can determine whether there is any benefit to be gained from the installation of an observation well, and if so we can determine at what distance from the ASR well it should be.
A full analysis of the benefits of installing an observation well would require the full implementation of the model. The optimal cost of a system with an observation well would then be compared to the optimal cost of a system without an observation well. If the cost benefit gained through the implementation of an ASR well, and hence better characterisation of the aquifer, is greater than the cost of installing such a well, then the use of the observation well would be optimal. It should also be noted that it would be necessary to include the increased costs of sampling the extra well in the analysis. This approach to the problem is site specific, as the cost of well installation will vary from one location to another. The methodology applied here is more generic, and suited to identifying if there are any potential benefits to the use of an observation well.

For the initial analysis a series of model runs were completed with different \( t_{cf} \) values and observation wells at different distances from the ASR well (i.e. in different annuli). Calibration of \( t_{cf} \) was undertaken using data from both the observation well, and the ASR well itself. In order to equate each annulus with a distance, it must be remembered that water in the fracture moves a distance of one annulus in one pulse interval. In this comparison, the annulus will be in that location defined by the distance injected water will travel in one day. The results for when \( t_{cf} = 1 \) day are shown in Figure 10-3, and results for a range of \( t_{cf} \) values are given in Appendix III.

Figure 10-3 Comparing the standard deviation of calibrated values of \( t_{cf} \) resulting from ASR tests with different observation wells. (\( t_{cf} = 1.0 \) days, \( \Delta T = 1 \) day, standard deviation of the random distribution of noise = 0.05.)
A number of things are apparent from the above figure, which immediately suggests there may be significant benefit to be gained from the use of an observation well.

- As expected, when the ASR test does not lead to injected water interacting with the annulus within which the observation well is located (e.g. when the observation well is located in annulus 50, and the aquifer half-test duration is 10 days), there is no improvement in the characterisation of the aquifer.
- Consistently, the greatest improvements occurred when the observation well was situated closer to the ASR well.

To understand this improvement it is useful to refer back to Section 10.1.1 discussing the introduction of a storage period into the ASR test. It was found that the introduction of a storage period significantly decreased the change in solute concentrations occurring during the ASR test. For the purposes of the analysis this impacted on the quality of the data obtained from the test. In this scenario, if the observation well is within the zone influenced by the ASR test, additional data is added to the calibration routine, without affecting the quality of the data from the ASR well. This data will to some extent aid in the characterisation of the aquifer. If the observation well is situated closer to the ASR well, then the change in concentration resulting from the ASR test will be greater and as a result the additional data obtained will be of greater benefit.

In certain situations (e.g. observation well in annulus 10, half-test duration of 20 days) the fit is less good despite the additional data. This is likely to be a result of the limited variation of the data with time in the observation well, in a similar manner to the way a period of storage influences the calibration described in Section 10.1.1.

In conclusion we can say that the inclusion of an observation well in the ASR testing system can be useful. We can also say that, in general, the observation well should be close to the ASR well. It is also noticeable that at early times, the greatest information was obtained when the observation well was very close to the well (i.e. in the second annulus), but that at greater times, greater resolution of \( t_{cf} \) was achieved when the observation well was further from the ASR well.

It is necessary to remember when applying this model that the observation well is necessary for purposes other than aiding in the characterisation of the aquifer, for example the measurement of drawdown. The potential gain in aquifer
characterisation achieved by placing an observation well in a specific location may be offset by other requirements.

10.3. **Final development of the model – A two cycle ASR test**

It has been noted in Chapter 8 that the model is not truly robust. Poor initial identification of the value of $t_{cf}$ prior to the implementation of the model has the potential to create a misleading scenario, with potentially costly benefits. One solution to this problem is to develop a system in which the AST test consists of two cycles. The first test cycle is a generic cycle, implemented regardless of the known characteristics of the aquifer. After completion of the first test, the DP-Pulse model can be calibrated to the collected data, providing a value of $t_{cf}$ which may then be used to determine the optimal duration of the second test.

In this final implementation of the model, two further possible improvements that have been mentioned within the text will be described. The first of these improvements involves approximating the results of both Stage 1 and Stage 2 with a mathematical formula, or 'response function'. If the data can be successfully represented by a response function, the error arising from the integer nature of the problem (described in Section 9.4.6) can be removed.

The second improvement to the Risk Reduction model will be to incorporate the ASR test scenario into the determination of the RCP. The process of testing the aquifer will have some effect on the aquifer. Injection of water with low solute concentrations will, to some extent, reduce the solute concentrations of the matrix waters and as a result will reduce the RCP for the aquifer. Due to computational limitations, all the currently completed work has treated this effect as insignificant, and hence used the RCP for a ‘pristine’ aquifer. A more comprehensive methodology would have to account for this effect. Unfortunately, this requires recalculation of the RCP for each individual ASR test, which will impact considerably on the computational demand of the model.

The following section describes the use of the response function within the model in further detail. Subsequently, the failure of the single cycle model will be illustrated in a quantitative manner, and the two cycle methodology will be applied.
10.3.1. Approximating the solutions to Stages 1 and 2 of the Risk Reduction model with ‘Response Functions’

As was mentioned in Section 9.3, the method of solution developed for the ‘Risk Reduction’ model is an integer problem. The solutions to both Stage 1 and Stage 2 are determined for an integer multiple of the pulse interval, $\Delta T$ (e.g. an ASR test may consist of 10 days injection followed by 10 days abstraction, modelled with a $\Delta T$ of 1 day). As a result, the resolution of the standard deviation in $t_{df}$ and of the required conditioning period are limited to $\Delta T$. Decreasing $\Delta T$ in order to increase the resolution leads to a large increase in the computational time requirement of the model.

It is possible, instead of calculating individual values for the standard deviation and required conditioning period, to approximate the curves (as illustrated in Figure 9-1 and Figure 9-2) with a mathematical formula – a ‘response function’.

Figure 10-4 illustrates a number of approximations to the results from Stage 1 of the Risk Reduction model solution. Calibrations were completed using the Sigmaplot automatic ‘fit curve’ calibration tool. The best solution was that produced by the modified three-parameter exponential decay solution (equation 125).

$$y = a \exp \left[ \frac{b}{x + c} \right]$$ (125)

Figure 10-5 illustrates two approximations to the required conditioning period model. The best solution was that produced by a standard log normal solution (equation 126).

$$y = a \exp \left\{ -0.5 \left[ \frac{1}{b} \ln \left( \frac{x}{x_0} \right) \right]^2 \right\}$$ (126)
Figure 10-4 Approximations to the solution of Stage 1 of the Risk Reduction model \( t_{cf} = 0.5 \) days, \( \Delta T = 1 \) day).

Figure 10-5 Approximations to the required conditioning period \( \sigma = 50, \Delta T = 1 \) day)

By using the selected equations, it is possible to repeat the optimisation model without the integer limitation. The resultant costs are illustrated in Figure 10-6.
Figure 10-6 Costs of testing and conditioning an aquifer determined through approximation of Stages 1 and 2 of the Risk Reduction model with Response Functions ($t_{cf} = 0.5$, $\sigma = 50$, cost of injection = £100/day, cost of abstraction = £200/day).

The optimal ASR test according to this model is 2.81 days. This is not greatly different from the value of 2 days obtained in an equivalent integer model in Section 9.3.

One possible advantage of this approximation method is that it may be possible to reduce the density of data required in the determination of the required conditioning period. As this is the most intensive section of the model, computationally, it may be possible to achieve reasonable approximations whilst reducing the number of data points on the curve. Figure 10-7, for example, illustrates how the approximation to the required conditioning period when $\sigma = 50$ changes as the total number of data points falls. In order to ensure there is no bias, the data points are evenly distributed across the range.

This method may be used to considerably reduce the necessary number of model realisations used to produce the curve describing the required conditioning period.
Figure 10-7 Approximating the required conditioning period with a ‘log normal’ curve using different data densities (σ = 50).

10.4. Including two cycles in the ASR test

10.4.1. The failure of a single cycle ASR test

The major identified flaw in the previously described form of the ‘Risk Reduction’ model was the lack of robustness. In order to show that the single test cycle approach has the potential to seriously mislead the user, a simple scenario will be examined. This scenario will illustrate that a poor initial estimate of \( t_{cf} \) may not only lead to extra costs, due to unexpectedly long conditioning periods, but also that the poor initial estimate can result in higher costs than would have been encountered had the initial estimate been correct.

Figure 10-8 shows the required conditioning period (RCP) for a specified value of \( \sigma = 50 \), with no prior test period accounted for. The maximum required conditioning period, 516 days, occurs when \( t_{cf} \) is between 1.3 and 1.5 days. The minimum required conditioning period occurs when \( t_{cf} \) is low. When \( t_{cf} = 0.1 \), the RCP is 117 days.
Running the optimisation model with an estimated $t_{cf}$ value of 0.1 days indicated an optimal ASR test of 6 days, and a required conditioning period of 148 days. Assuming that the cost of injection = £100 / day and the cost of abstraction = £200 / day), the estimated cost of preparing an ASR system prior to any activities taking place, with an estimated $t_{cf}$ value of 0.1 days is £16,600.

Repeating the run with an estimated $t_{cf}$ value of 1.5 days indicates an optimal ASR test of 1 day, and a required conditioning period of 516 days. Again, assuming that the cost of injection = £100 / day and the cost of abstraction = £200 / day), the estimated cost of preparing an ASR system prior to any activities taking place, with an estimated $t_{cf}$ value of 1.5 days is £51,900.

It is clear that estimating that an aquifer is characterised by $t_{cf} = 0.1$ days, when the actual aquifer is characterised by $t_{cf} = 1.5$ days, will lead to significant underestimation of costs. In this scenario, costs will be underestimated by £35,300.

In an operational situation, it is likely that the model would be recalibrated after the ASR test. Remembering that the aquifer is really characterised by a $t_{cf}$ value of 1.5 days, the 5-day test indicated by the incorrect $t_{cf}$ value of 0.1 days, when applied to the real system, would lead to a calibration of $t_{cf}$ to within 25% of the true value. By delineating two standard deviations either side of the actual aquifer parameter and determining the resulting required conditioning period we can obtain a new total
cost, accounting for the incorrectly selected ASR test, and the subsequently affected required conditioning period. The resulting cost of testing and conditioning the system would total £53,100. This total cost is £1,200 more than it would have been had initial predictions of $t_{cf}$ been correct. Therefore, not only was the total cost underestimated by £35,300, but the initial incorrect selection of $t_{cf}$ also raised the total cost by a further £1,200.

Clearly there is a problem with the application of this model in situations where the aquifer characteristics are almost totally unknown.

10.4.2. Selecting the duration of the first 'generic' ASR test cycle in a two cycle model

It is possible that, prior to the implementation of any ASR test, the aquifer can be regarded as wholly uncharacterised (although an initial estimate can be made using the characterisation of different aquifers completed in Chapter 6). It therefore does not make sense to develop an ASR test that is dependent on the aquifer. Instead an optimal first cycle test is one that may reasonably characterise any aquifer.

Figure 9-1 (reproduced below) illustrated how the standard deviation in the calibration of $t_{cf}$ decreased as the test duration increased.

![Figure 9-1 Change in the accuracy of the $t_{cf}$ calibrated by the DP-Pulse model with increasing aquifer half-test duration. (Simple injection/abstraction test - no storage - single well, $\Delta T = 1$ day, calibration repeated 5,000 times.)](image-url)
An ASR test consisting of two days injection, followed by two days abstraction, resulted in one standard deviation of the calibrated value of \( t_{cf} \) being less than 25% of the actual value. Whilst this accuracy is not particularly high, this test procedure is sufficient to provide an indication of the characteristics of any otherwise untested aquifer. The test is also of sufficiently short duration that it may be carried out within one working week, and this has practical implications for the implementation of any ASR test.

Using this information, therefore, we can develop an ASR test that consists of two test 'cycles'. The first cycle will consist of two days injection, followed by two days abstraction, regardless of the actual aquifer characteristics. This test will be used to provide an initial estimate of the aquifer characteristics, in order to allow the optimisation of the second cycle and conditioning process, according to the 'Risk Reduction' methodology described above.

### 10.4.3. Implementation of a two-cycle ASR test

In a two-cycle ASR test situation, the initial testing procedure will have some effect on the resultant required conditioning period. Although in this implementation the cycle tests will be short, and hence the effect on the conditioning period small, it is worth incorporating the conditioning effect of the tests as an illustration of how flexible the model can be. The effect of this primary ASR test on the aquifer system will therefore need to be incorporated into the model when the required conditioning period is determined. The second cycle may also, depending on its duration, have a significant effect: this will also be incorporated.

As a result of incorporating the effects of the testing procedures, however, there is a significant increase in the computational burden – the required conditioning period will have to be determined for possible \( t_{cf} \) value, and for each potential ASR test regime. As a result, it is sensible to incorporate the methods for approximating the description of Stages 1 and 2 of the Risk Reduction model with response functions, as described in Section 10.3.1. This enables the model to be completed with fewer determinations – most notably of the required conditioning period.

Figure 10-9 illustrates how incorporating the cycle testing procedure reduces the required conditioning period. An initial ASR test cycle consisted of two days injection, followed immediately by two days abstraction. A second ASR test cycle of variable, but identical, injection and abstraction duration was then performed. Each of these curves describing the required conditioning period may be
approximated by a log normal curve (see Section 10.2, equation 126 and Figure 10-5). Although generally a fairly good approximation, as $t_{cf}$ increases the approximation diverges slightly from the data. This should be remembered during the interpretation of any results obtained using the approximation.
Figure 10-9 Required conditioning period to successfully complete the annual cycle described in Table 1, with 100% efficiency and a maximum solute concentration of 0.5 ($\Delta T = 1$ day). Prior testing (2 days injection and 2 days abstraction followed by a second test cycle) incorporated in the model.

Figure 10-10 Change in the accuracy of the $t_{cf}$ calibrated by the DP-Pulse model with increasing ASR test duration. (Two-cycle injection/abstraction test, first injection period = 2 days, first abstraction period = 2 days, no storage, single well, $\Delta T = 1$ day, calibration repeated 1,000 times, standard deviation of noise in solute concentrations = 0.05).
In combination with the values produced by Stage 1 of the model, illustrated in Figure 10-10, the RCP can be combined with the financial cost of injection and abstraction to produce the results shown in Table 10-1. The cost of injection was specified to be £200 per day, whilst the cost of abstraction was £100 per day.
Table 10-1 Optimisation of the two-cycle ASR test. (Cost of injection = £200 / day, cost of abstraction = £100 / day.)

<table>
<thead>
<tr>
<th>$t_{cf}$ (Days)</th>
<th>0.1</th>
<th>0.5</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test Duration (Days)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>£34,732</td>
<td>£88,593</td>
<td>£102,231</td>
<td>£103,052</td>
<td>£100,266</td>
</tr>
<tr>
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<td>£96,607</td>
<td>£114,165</td>
<td>£116,063</td>
<td>£110,856</td>
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</table>

Optimal second test cycle

<table>
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<th>$t_{cf}$ (Days)</th>
<th>0.1</th>
<th>0.5</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optimal test duration</td>
<td>7 days</td>
<td>4 days</td>
<td>1 day</td>
<td>0 days</td>
<td>1 day</td>
</tr>
<tr>
<td>Total cost of both test cycles and subsequent conditioning</td>
<td>£29,932</td>
<td>£86,361</td>
<td>£101,909</td>
<td>£103,052</td>
<td>£98,923</td>
</tr>
</tbody>
</table>

It can be seen that for the lower $t_{cf}$ values an optimal ASR test exists. The long durations of these ASR tests, when compared to Figure 9-14 of Section 9.4.2 (a single ASR test cycle), is a result of the incorporation of the conditioning effect of the ASR test. For a $t_{cf}$ value of 0.5 days, the total injection duration of 4 days and abstraction duration of 4 days reduces the required conditioning period from 447 days to 426 days. For greater values of $t_{cf}$ (i.e. $t_{cf} > 0.5$ days and $t_{cf} < 3.0$ days), the reduction in the required conditioning period produced by the extra characterisation of the aquifer resulting from the longer ASR test is not as large. This is because the actual aquifer parameter, $t_{cf}$, is such that the required conditioning period is near a maximum, regardless of the accuracy of the characterisation, and as testing is less efficient at conditioning an aquifer, continuous injection is the most efficient method.
of preparing the aquifer. When $t_{cf}$ is high (e.g. $t_{cf} = 3$ days) the indicated optimal second ASR test cycle is one day long. This may be a result of the fact that as $t_{cf}$ increases, the required conditioning period falls, and so the maximum conditioning period is again constrained by the accuracy of the aquifer characterisation. Alternatively this result may be caused by the increasing error in the approximation of the required conditioning period as $t_{cf}$ increases (seen in Figure 10-9).
Chapter 11

Summary and discussion
11. **Summary and discussion**

Before drawing conclusions concerning the work undertaken in this thesis, it is worth returning briefly to each of the topics discussed in turn, and summarising the more important findings.

11.1. **The DP-Pulse model: Capabilities and limitations**

The DP-Pulse model simulates the advection and diffusion processes that occur in double-porosity media. The model discretises the velocity of advective flow into a series of instantaneous pulses. The formulation of the model produces two parameters, $t_{cb}$ and $c_r$, which characterise the aquifer. In addition the fracture/matrix geometry is specified through the use of the block geometry function (BGF).

The model has a number of distinctive features:

- The pulsed formulation allows the reversal of the direction of flow. This ability has not previously been possible with an analytical model.
- Because dispersion is treated as negligible, the model is invariant with respect to both flow geometry and pumping rate.
- The low parameterisation of the model allows easy and unique calibration, rapid and comprehensive sensitivity analyses and simple result visualisation techniques (contour plots).
- The relative simplicity of the model allows for simple adaptation and incorporation into more complex (e.g. operational research) models.

The model was successfully verified against a simple analytical code, DP1D, and the calibration against the experimental data from the Lychett Minster Test Site validated the model for use in simulating ASR systems.

Previous attempts to simulate ASR systems, and analyse ASR test results, in double-porosity rocks have relied upon complex numerical models, specifically using the SWIFT code, which require a high level of parameterisation. Frequently it is not possible to specify the aquifer characteristics with any certainty. As a result, uncertainty in the model simulations, and hence limitation of their use in decision making processes is high.

The DP-Pulse model, with its low parameterisation, may be calibrated to experimental data in order to characterise an aquifer with ease. As the calibration is unique, the degree of confidence in the calibration can easily be determined. This
makes the DP-Pulse model a very useful tool, for both characterising an aquifer and simulating processes within that aquifer.

The complexity involved in the application of numerical models also restricts their flexibility in predictive modelling. For example, Section 2.5.4 introduces the required conditioning period, which is then evaluated in Section 6.3.3. Evaluation of this value (a non-linear problem) requires that the model is capable of recognising the maximum abstracted solute concentration in a specific cycle. The model must also be capable of varying the length of the conditioning period so as to ensure that the conditioning period is kept to a minimum, whilst ensuring that the maximum abstracted solute concentration does not increase beyond the maximum abstractable solute concentration. Incorporating this feature into a numerical (proprietary) code would be complex. Incorporating this facility into the DP-Pulse model is a relatively simple task.

It must be established, however, that the DP-Pulse model has limitations:

- The current model is not capable of dealing with non-conservative solutes. It would, however, be possible to incorporate any change in solute concentrations (e.g. production, decay) that displays linear behaviour in the formulation.
- Although the model is invariant with respect to flow rate, it has already been stated that this is dependent on the actual flow rate (but not flow direction) remaining constant. An assumption enabling variations in the relative flow rate has been incorporated into the code, but has not undergone full error analysis.

Error analysis of the effect of discretising the velocity on the accuracy of the DP-Pulse model (Section 3.6) indicated low sensitivities to everything but the duration of the simulation and the pulse interval:

- Simulations of short periods of time required short pulse intervals to maintain an acceptable level of error. Longer simulations produced acceptable results with larger time steps. This allows simulations of long periods of time to be completed with a large pulse interval, thus reducing the size and duration of the model run.
- Increasing the acceptable error dramatically increased the maximum acceptable pulse interval, allowing rapid model run times. This may be useful when considering trends of behaviour, as opposed to simulating actual systems where accuracy becomes more important.
• The maximum acceptable time step was insensitive to $\sigma$, and only slightly sensitive to $t_{cb}$. Over a range of $t_{cb}$ values from 31 to 31,622 days, the maximum acceptable pulse interval only varies by a factor of two.

11.2. **Lychett Minster: The test site and experimental data**

The Lychett Minster Test Site is an ASR test scheme in Dorset, UK. The borehole penetrates the Upper Chalk, an important aquifer with highly double porous properties. Extensive testing indicated a transmissivity of 172 m$^2$/d and a storage coefficient of $2.5 \times 10^{-4}$. A series of injection and abstraction cycles of varying duration were undertaken to characterise the aquifer with a view to scope the possibility of establishing an operational ASR scheme in the area.

Calibration of the DP-Pulse model to the data from Lychett Minster highlighted a number of features:

- Assuming a slab geometry, $t_{cb} = 1086 (\pm 63)$ days, $\sigma = 49.5 (\pm 1.6)^6$
- The calibrated parameters were well constrained by the complete testing cycle.
- The early stages of the testing cycle were only successful in constraining $t_{cf} \approx 0.44$ days.

Plotting the aquifer at the Lychett Minster Test Site on the contour plots in Section 6.1 illustrated that at early times, solute concentrations in the abstracted water would be high. A conditioning period of at least one year would have been required to obtain a peak solute concentration of 50% native water solute concentrations in the abstracted water, on a typical annual ASR cycle working at 100% efficiency.

From this simple approach, therefore, we can see that, with respect to the conservative solutes, ASR is feasible in the Chalk aquifer at the Lychett Minster site, but that it would require a significant amount of preparation prior to operation.

11.3. **ASR experience in the UK and abroad**

ASR has been widely and successfully applied across the US and to a lesser extent the world. In the UK a major question has arisen over the implications of double-porosity behaviour for the successful implementation of ASR in UK aquifers, most

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$^6$ Range of uncertainty for 50% confidence interval
notably the Chalk. It was believed that diffusion of solutes from the matrix into the fracture could significantly reduce recovery efficiencies for long periods.

It has been illustrated in Section 6.1 that although recovery efficiencies are impacted by double-porosity behaviour, fully operational schemes of the type described in Figure 6-6 may be implemented after between 100 and 600 days conditioning. The increase in expense resulting from this necessary conditioning may be viewed as reasonable in comparison to the cost of alternative forms of water resource management (e.g. surface reservoirs).

Current methodology of ASR testing prior to ASR implementation has worked well in the US, as aquifers there do not have a significant double-porosity. Section 7.4 illustrated the limitations of the standard cycle testing procedure when applied at the Lychett Minster Test Site. The early cycles successfully characterised $t_{cf}$ while determination of $t_{cb}$ and $\sigma$ could not be completed with confidence until many more cycles had been undertaken. As a result, test cycles 3-8 provided little useful information about the behaviour of conservative solutes.

It is apparent that significant testing will be required to fully characterise the aquifer, and therefore predict the operational behaviour of an ASR system.

11.4. Developing an optimal ASR test: the ‘Risk-Reduction’ model

A series of models using operational research techniques were developed to identify an optimal ASR test, based on the ‘Risk-Reduction’ model. This model was designed to provide an ASR testing and conditioning methodology that would result in successful operation of a specified ASR system on the first operational cycle with a low risk of failure. The increased benefit of testing was quantified through the method of simulating how well the data collected would allow characterisation of an aquifer. ‘Required conditioning periods’ were determined certain operational ASR scenarios, for a broad range of probable aquifer characteristics. All groundwater modelling was undertaken using the DP-Pulse model. As increased testing durations allowed better characterisation of the aquifer, the increased cost was offset against the reduction in the required conditioning period resulting from better knowledge of the aquifer characteristics.

This ‘Risk Reduction’ model was applied to a number of different scenarios, all with a single test cycle and a single well, in order to test its sensitivity. It was found that:
• The unit cost of injection does not affect the optimal test duration, only the total cost of testing and conditioning.

• Varying the noise in the solute data has some effect on the optimal testing regime. Increasing the noise increases the optimal test duration.

• Varying the noise in the solute data has a large effect on the overall cost of the testing and conditioning process, with increased accuracy when testing leading to shorter, and hence cheaper, conditioning periods required to guarantee low-risk operation of the ASR system.

• Varying $t_{cf}$ has an effect on the length of the optimal ASR test. It also has a large effect on the overall cost of testing and conditioning. When $t_{cf}$ is greater than 1 day, the model will choose the shortest test duration simulated. A low $t_{cf}$ has a longer optimal test (with $t_{cf} = 0.1$ days, a half test duration of six days was optimal), however this is unlikely for UK aquifers. Variations in the total cost of testing and conditioning the aquifer arise from increases in the required conditioning period for higher $t_{cf}$ values.

• Varying $\sigma$ has a large effect on both the total cost and the optimal ASR test. When $\sigma$ is less than 10, the required conditioning periods are low (generally less than 100 days, depending on $t_{cf}$), so the reduced conditioning period resulting from improved characterisation becomes insignificant with respect to the increased costs of the testing. When $\sigma$ is greater than 50, an increase in test duration results in a relatively small increase in the information gained about the aquifer, and so short ASR tests of the order of 1 day duration are optimal.

• Varying the maximum allowable solute concentration in the abstracted water has a large effect on both the total cost and the optimal ASR test. When the maximum solute concentration is low, the required conditioning periods are high (up to several years), so the decrease in the length of the conditioning period resulting from improved characterisation becomes significant with respect to the increased costs of the testing.

• When recovery efficiencies are low, there is a small reduction in the conditioning period, and a reduction in the length of the optimal aquifer-testing regime.

The OR model was then applied to two different scenarios, the inclusion of an observation well, and the inclusion of a period of storage in the middle of the ASR test:
• Inclusion of an observation well in the ASR testing system can be useful. In general the observation well should be close to the ASR well.

• The inclusion of a period of storage in the ASR testing procedure reduced the confidence in the characterisation of the aquifer. The effect of including a storage period was most notable in short ASR tests, but still present in longer duration ASR tests.

One major flaw in the ‘Risk Reduction’ model was noted – there was sensitivity to the initial estimate of \( t_{cf} \), a quantity that is hard to determine without completing a tracer test.

### 11.5. Improving the ‘Risk-Reduction’ model

The sensitivity of the Risk-Reduction model to the initial estimate of \( t_{cf} \) was considered a significant flaw. In order to overcome this a development to this approach was proposed, in which a standard initial 2-day injection, 2-day abstraction test would be carried out. This test would be sufficient to characterise most aquifers to within 25% of the actual parameter values. This reduces the possibility of failure due to poor initial estimation of the aquifer parameters, and increases the robustness of the model. Further improvements included methods of interpolating data, to reduce the need for comprehensive simulation across all possible characteristic parameters, and the incorporation of the ASR test period into the ‘required conditioning period’. This revealed a number of results:

- For the lower \( t_{cf} \) values (\( t_{cf} < 1.5 \) days) optimal ASR tests exist.
- For greater values of \( t_{cf} \) (i.e. \( t_{cf} > 1.0 \) days and \( t_{cf} < 3 \) days), the reduction in the required conditioning period produced by the extra characterisation of the aquifer resulting from the longer ASR test is not sufficiently large to justify the extra testing. This is because the actual aquifer characteristics are such that the required conditioning period is near a maximum, regardless of accuracy of the characterisation, and as testing is less efficient at conditioning an aquifer, the model indicates a concentration on continuous injection.
- When \( t_{cf} \) is high (\( t_{cf} > 3 \) days) there is an optimal second test cycle. This is a result of the fact that as \( t_{cf} \) increases, the required conditioning period falls, and so the maximum conditioning period is again constrained by the accuracy of the aquifer characterisation.
Chapter 12

Conclusions and further work
12. Conclusions and further work

12.1. Conclusions

A semi-analytical model enabling the simulation of diffusion processes and reversible advective flow in double-porosity aquifers was developed. The model is characterised by the block shape and two transport parameters: a block diffusion time, $t_{cb}$, and a porosity ratio, $\sigma$. For times much less than the time for diffusion across a matrix block, only a single parameter, the 'fracture diffusion time', $t_{cf}$, is needed to characterise double-porosity diffusion.

The model assumes negligible mechanical dispersion, which has the consequence that the flow geometry is of no importance for ASR simulation. Furthermore, for the simulation of ASR operations, where injection and observation are at the same point, the assumption makes the model results invariant with respect to the pumping rate. These observations are of general importance in double-porosity modelling and tracer testing.

The low parameterisation of the DP-Pulse model makes it a powerful tool for the simulation of the processes occurring within a double-porosity aquifer. The simplicity of the model structure easily allows adaptation to a variety of different uses, and incorporation into other computer models. In this thesis the model has been integrated firstly with an automated calibration routine, and subsequently with a series of optimisation models based on operational research techniques.

The DP-Pulse model was successfully verified against an analytical advection-diffusion model, DP1D. An analysis of the possible error inherent in the formulation of the DP-Pulse model was completed. The DP-Pulse model was then calibrated with experimental data collected from the Lychett Minster Test Site.

The calibration to the data characterised the Upper Chalk aquifer, in Lychett Minster. By assuming values for the apparent diffusion coefficient, and the matrix porosity, these results can be interpreted to give the physical characteristics of the aquifer.

Calibration of the DP-Pulse model to the cumulative data set over increasing numbers of test cycles showed a rapid determination of the value of $t_{cf}$, with little improvement over a relative error in the calibration of 5% after 4 cycles, taking a total of 66 days. Successful determination of both $t_{cb}$ and $\sigma$ only took place in the later cycles; for example, the relative error in $t_{cb}$ reduced to 6% after 9 cycles when
the total test time reached 632 days (i.e. the total test duration amounted to about 60% of $t_{ch}$).

<table>
<thead>
<tr>
<th>Slab Geometry</th>
<th>Calculated aquifer characteristics</th>
<th>Sphere Geometry</th>
<th>Calculated aquifer characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calibrated parameters</td>
<td>$b = 16.8$ cm</td>
<td>$r = 154$ cm</td>
<td></td>
</tr>
<tr>
<td>$\sigma = 49.5$</td>
<td>$a = 2.7$ mm</td>
<td>$\phi_f = 0.008$</td>
<td></td>
</tr>
<tr>
<td>$t_{ch} = 1086$ days</td>
<td>$\phi_m = 0.4$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$t_{cf} = 0.44$ days</td>
<td>$D_f = 3 \times 10^{-10}$ m$^2$s$^{-1}$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Where $2b$ is the fracture spacing, $a$ is the fracture aperture and $\phi_f$ the fracture porosity.

Assumed Parameters

| $r = 154$ cm |
| $\phi_f = 0.003$ |

Calculated aquifer characteristics

$$a = 2.6$ mm 
$$r = 154$ cm 
$$\phi_f = 0.003$$

Where $r$ is the sphere radius and $a$ is the ratio of the fracture volume to the fracture surface area and $\phi_f$ the fracture porosity.

From this it is possible to conclude that in the Upper Chalk, tracer tests of a few days duration are sufficient only to characterise the rate of diffusive interaction between the fracture and matrix porosities. In order to fully characterise the aquifer, including determination of the fracture separation, tracer tests of much longer durations are required. Very fast tests only reveal the fracture (kinematic) porosity while very slow tests reveal only the total (accessible) porosity.

Were the sole purpose of this test the characterisation of the diffusive interaction between the fracture and matrix porosities these results reveal flaws in the conception of this aquifer-test methodology. Whilst the earlier group of tests, up to 50 days, provided a great deal of information about the aquifer, in the form of a well defined $t_{cf}$ value, the intermediary tests provided little extra information. Only the very longest cumulative test durations provided full information about the aquifer.

It is important that both experimentation on and modelling of double-porosity media are undertaken with due regard to the characteristic times involved. With tracer tests it will often be possible to control some of these values; for example, through the test distance, pumping rates and choice of tracer. However, it will often be the case that the long-term behaviour of a system cannot be accurately determined via short-term observations or tests, such as those conducted in the laboratory.

Current standard ASR practices were outlined, and their limitations and inefficiencies were discussed. The need for a ‘conditioning period’ consisting of an extensive period of continuous injection of water into the aquifer prior to the implementation of an ASR system in a double-porosity aquifer was identified.

It was determined that ASR in the UK Chalk aquifer was practical, but that double-porosity effects played an important role in controlling the efficiency of ASR.
operations. It was also determined that ASR in the UK Chalk aquifer would require significant periods of preparation time, of the order of one to five years, involving continuous injection, to obtain recovery efficiencies of 80% to 100%. These times were determined by assuming a desired reduction the solute concentrations of abstracted water of 50% to 90% relative to native groundwater. Additionally, these conclusions only apply to the behaviour of the conservative solutes in a double-porosity system. It is important, however, to consider these durations in terms of the operational life of the ASR system, and in comparison to the potential time required for the installation of an alternative water resource management system.

With a view to determining the optimal ASR test for a double-porosity aquifer prior to the implementation of an ASR system, a number of operational research methodologies were considered. A model, called the ‘Risk Reduction’ model and incorporating the DP-Pulse code, was developed to identify the optimal (with respect to cost) combination of ASR cycle test and conditioning period, ensuring successful operation of the ASR system on the first cycle with a quantifiably low risk of failure. This model applied artificial noise to data from model simulations, in order to produce synthetic ‘experimental data’. Monte Carlo methods were then used to determine the ability of specific ASR tests to characterise an aquifer. The model also determined the ‘required conditioning period’ that would result in the successful completion of a specified ASR cycle in the first year of operation.

By offsetting the increased cost of testing with a reduced required conditioning period from better aquifer characterisation, this model successfully identified optimal ASR test durations for a simple case. The model was very sensitive to:

- The cost of groundwater supply and injection;
- The relative costs of groundwater abstraction and disposal;
- The error in the experimental data;
- The true and estimated value of $t_{cr}$;
- The maximum abstracted solute concentration;
- The desired recovery efficiency.

The model was also slightly sensitive to:

- The effect of changing the estimated value of $\sigma$.

The Risk-Reduction model was then used to examine the relative benefits of including a storage period in the ASR test, and the use of an observation well. It was concluded that :-
• An observation well could be of benefit, if it was sufficiently close to the injection well to be impacted by the changing solute concentrations resulting from the injection phase of the ASR test.

• The incorporation of a period of storage was detrimental to the ability of the ASR test to characterise an aquifer under all the investigated test conditions.

There are three main flaws in the presented basic ‘Risk Reduction’ model. Firstly, there is a dependency on the initial estimate of the aquifer characteristics. As a result, the model is not robust and can be misleading if initial estimates are wrong. The model does not account for the conditioning effect of the ASR test, which may significantly reduce the required conditioning period, and finally the discrete nature of the model prevents good resolution of the solution.

A two-cycle test model was introduced which addressed the flaws in the basic ‘Risk Reduction’ model. This model showed the capacity to successfully, and robustly, identify an optimal ASR test cycle.

12.2. Implications for ASR in the Chalk aquifer

The primary conclusion of this work is that the cyclical storage of potable water in a non-potable Chalk aquifer is feasible. This finding is of some significance for the future of ASR in the UK. There are however, a number of findings that may influence the potential applicability of ASR in UK Chalk aquifers.

Although it is possible to gain a reasonable understanding of the parameter \( t_{cf} \), which can be thought of as describing how the surface of the fracture interacts with the fracture water, this is insufficient to fully describe a double porosity aquifer for the purpose of determining the potential success of an ASR system. In order to be able to simulate the solute transport processes associated with the doubly porous nature of the medium, it is necessary to be able to characterise the matrix blocks, described by the parameters \( t_{cb} \) and \( \sigma \).

Current aquifer testing methodology takes the form of a series of short cycles of injection and abstraction. The initial tests allow the determination of \( t_{cf} \), however full aquifer characterisation will not be possible until the duration of the test is of the order of \( t_{cb} \). Little is learned from the cycle tests carried out after characterisation of \( t_{cf} \), but of much shorter total duration than \( t_{cb} \). In order, therefore, to successfully simulate ASR in a double porosity aquifer without extended testing, other means of parameter determination, such as fracture mapping or tracer testing (using tracers...
with high tracer diffusion coefficients) need to be considered. Alternatively, it would be possible to determine a likely maximum expense of the development of a system, given the understood geology, which would potentially limit the need for testing prior to conditioning.

Given the large uncertainty in the potential conditioning requirement of an ASR system prior to investigation, it may be difficult to obtain sufficient momentum to begin testing an ASR system in the Chalk. It should be noted, however, that the general conclusion of this work is that ASR is feasible in most cases, although significant investment in the form of extended injection of potable water may be required.

Due to the uncertainties, and the potential costs, it is important to look at the potential benefit of an ASR system at a location, prior to investigating the ground conditions. As an example, the selected location should have a suitable demand for water, as well as a ready supply of water for recharge, and a suitable means for distribution. If the infrastructure is already suited to the implementation of ASR, it is likely that there will be a significant benefit to ASR development, outweighing the potential costs and uncertainties.

Alternative means of water resource management to ASR are also known to have major limitations. Surface reservoirs are expensive, and the planning and authorisation process may take many years before construction begins. Care should be taken to look at the potential costs and benefits of each form of resource management to ensure that the correct selection is made.

### 12.3. Further work

There are a number of potential directions further work could take. Firstly, the novel parameterisation of the model allows for the delineation of plausible characteristics of an aquifer. Whilst a brief overview on a method of identifying the bounds on the aquifer parameters has been outlined, lack of data has resulted in this work being at best a cursory examination. Collation of unpublished tracer test results, and a progressive nationwide aquifer characterisation through the use of tracer tests would allow this parameter delineation to be more comprehensive, and provide greater confidence in the conclusions.

The DP-Pulse model is currently in a very basic form. It may be possible to include a number of other important processes that can occur during groundwater flow, including dispersion, decay and sorption. The latter two would be relatively simple,
while the former would be difficult. It may also be possible, though a complex problem, to develop the pulsed velocity concept into a two or three dimensional model.

The ‘Risk Reduction’ model has been shown to be useful in identifying optimal ASR testing and conditioning regimes prior to the operational implementation of an ASR scheme. The model has also been shown to be useful in identifying the potential of ASR in the UK Chalk aquifer. Further work building on from this thesis could follow a number of courses.

Despite its’ limitations, the basic ‘Risk Reduction’ model could prove very useful as a research tool for preliminary investigation of the possible benefits of certain practices during the testing and conditioning of an aquifer prior to ASR implementation. These practices could include the use of expensive, but highly accurate, solute measurement techniques, or the installation and location of one or more observation wells. Provision of a complete set of data, across all parameter ranges, would be time consuming and computationally intensive. Once completed, however, this data would provide a useful basis for further research. The model could further be used with this data to assess the cost implications of using different water sources, and even to examine the overall viability of an ASR scheme. The latter use would, however, require some financial value to be placed on an operational ASR system.

The methodologies within the ‘Risk Reduction’ model could be applied to a number of different applications. ASR schemes have been implemented for many different purposes, most notably to provide a resource at times of either unexpected demand or drought. The ‘Risk Reduction’ methodology could be used to develop a system that can provide a supply in these eventualities. Risk could be determined according to predictions of the likelihood of any such eventuality, and a system developed such that except in the most unpredictable of scenarios supply can be maintained.
Chapter 13

References
13. References


National Rivers Authority (NRA), 1994. Groundwater modelling and modelling methodology. NRA R&D Note 295/19/A.


Chapter 14
Glossary
14. Glossary

ARR
Artificial recharge and recovery is the storage of water in a suitable aquifer through a well during times when water is available, and recovery of the water from the same or different wells during times when it is needed.

ASR
“Aquifer Storage Recovery may be defined as the storage of water in a suitable aquifer through a well during times when water is available, and recovery of the water from the same well during times when it is needed” (Pyne, 1995).

ASR test
The testing procedure carried out prior to ASR operations or conditioning, designed to characterise the aquifer. This test may or may not be a cycle test as defined below.

Conditioning period
The pre-operational preparation of an aquifer for ASR operations, consisting of a period of constant sacrificial injection of potable water.

Cycle testing
The current standard practice is to test an ASR scheme before operational implementation by performing a number of cycles, of short duration, involving injection and abstraction. These cycles are designed to improve the aquifer over time, while also giving data for the determination of the characteristics of the aquifer.

Double-porosity aquifer
An aquifer type in which two significant porosities occur, a primary intergranular porosity, and a secondary fracture porosity. Flow occurs within the secondary, fracture porosity, but no significant flow occurs within the granular porosity. (Aquifer types with significant flow in both primary and secondary porosities are generally referred to as dual permeability media.)

Preparation phase
The period during which both ASR testing and conditioning take place.

Recovery efficiency
“The percentage of water volume stored that is subsequently recovered while meeting a target water quality criterion in the recovered water” (Pyne, 1995).
Appendix I. Uncertainty analysis – Full results for Section 5.2.1.

An analysis of the uncertainty of the DP-Pulse model of the Lyckett Minster test site ASR cycle tests was carried out in Section 5.2.1. The following figures illustrate the findings of this analysis. In each figure, a pair of parameter sets are illustrated along with the calibrated Lyckett Minster parameters. The parameter sets were chosen so as to display different forms of sensitivity. Parameter sets A95, A50, B95 and B50 have similar $t_{cf}$ values, so they illustrate the effect of variations of $t_{cb}$ and $\sigma$, without great change in $t_{cf}$. Parameter sets C50, C95, D50 and D95 have very different $t_{cf}$ values. They illustrate the effect of variations of $t_{cb}$ and $\sigma$, as well as $t_{cf}$.

Figure I-1 Sensitivity analysis - Comparison of parameter groups A95 and B95 with the calibrated parameter group, Lyckett Minster Test Site data. ($\Delta T = 1$ day, slab geometry.)
Figure I-2 Sensitivity analysis - Comparison of parameter groups C95 and D95 with the calibrated parameter group, Lychett Minster Test Site data. (£T = 1 day, slab geometry.)

Figure I-3 Sensitivity analysis - Comparison of parameter groups E95 and F95 with the calibrated parameter group, Lychett Minster Test Site data. (£T = 1 day, slab geometry.)
Figure I-4 Sensitivity analysis - Comparison of parameter groups G95 and H95 with the calibrated parameter group, Lychett Minster Test Site data. ($\Delta T = 1$ day, slab geometry.)

Figure I-5 Sensitivity analysis - Comparison of parameter groups A50 and B50 with the calibrated parameter group, Lychett Minster Test Site data. ($\Delta T = 1$ day, slab geometry.)
Figure I-6 Sensitivity analysis - Comparison of parameter groups C50 and D50 with the calibrated parameter group, Lychett Minster Test Site data. ($\Delta T = 1$ day, slab geometry.)

Figure I-7 Sensitivity analysis - Comparison of parameter groups E50 and F50 with the calibrated parameter group, Lychett Minster Test Site data. ($\Delta T = 1$ day, slab geometry.)
Figure I-8 Sensitivity analysis - Comparison of parameter groups G50 and H50 with the calibrated parameter group, Lychett Minster Test Site data. ($\Delta T = 1$ day, slab geometry.)
Appendix II. Comparing the standard deviation in $t_{cf}$ resulting from ASR tests with different storage periods for a range of $t_{cf}$ values. (Full results for Section 10.1.)

Figure II-1 Comparing the standard deviation in $t_{cf}$ resulting from ASR tests with different storage periods ($t_{cf} = 0.1$ days, $\Delta T = 1$ day, standard deviation of the random distribution of noise$^7 = 0.05$).

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$^7$ Noise is relative to native water solute concentrations.
Figure II-2 Comparing the standard deviation in $t_{cf}$ resulting from ASR tests with different storage periods ($t_{cf} = 0.5$ days, $\Delta T = 1$ day, standard deviation of the random distribution of noise = 0.05).

Figure II-3 Comparing the standard deviation in $t_{cf}$ resulting from ASR tests with different storage periods ($t_{cf} = 1.0$ days, $\Delta T = 1$ day, standard deviation of the random distribution of noise = 0.05)
Figure II-4 Comparing the standard deviation in $t_{cf}$ resulting from ASR tests with different storage periods ($t_{cf} = 3.0$ days, $\Delta T = 1$ day, standard deviation of the random distribution of noise = 0.05)
Appendix III. Comparing the standard deviation in $t_{cf}$ resulting from ASR tests with different observation well positions for a range of $t_{cf}$ values. (Full results for Section 10.2)

![Graph](image)

Figure III-1 Comparing the standard deviation in $t_{cf}$ resulting from ASR tests with different observation wells. ($t_{cf}^* = 0.1$ days, $\Delta T = 1$ day, standard deviation of the random distribution of noise = 0.05.)
Figure III-2 Comparing the standard deviation in $t_{cf}$ resulting from ASR tests with different observation wells. ($t_{cf} = 0.5$ days, $\Delta T = 1$ day, standard deviation of the random distribution of noise = 0.05.)

Figure III-3 Comparing the standard deviation in $t_{cf}$ resulting from ASR tests with different observation wells. ($t_{cf} = 1.0$ days, $\Delta T = 1$ day, standard deviation of the random distribution of noise = 0.05.)
Figure III-4 Comparing the standard deviation in $t_{cf}$ resulting from ASR tests with different observation wells. ($t_{cf} = 3.0$ days, $\Delta T = 1$ day, standard deviation of the random distribution of noise = 0.05.)
Appendix IV. A mathematical description of the pulsed double-porosity model, DP-Pulse.

Based on work by Barker (described in Appendix X) and Fretwell (1999), revised by the author.

IV.I. Introduction

This document provides the mathematical description of a new type of double-porosity model. The model has already found application to aquifer storage recovery and to periodic elution of solutes due to a fluctuating water table.

The model has much in common with some mixing-cell models but adds matrix exchange.

A full analytical solution is developed: the solutions take a form of summation over Green's functions. Implementation must be via a computer programme so the model is best described as a semi-analytical model.

A qualitative description of the model is followed by a mathematical definition and the solution of the equations.

IV.II. Description

The fundamental assumption in the model which permits an analytical solution is that water moves in a series of instantaneous pulses, separated by a period of time called the pulse interval. It is assumed that each jump involves the same volumetric movement of water and that volume of water defines the cells of the system. For linear flow those cells might be cubes while for cylindrical flow to and from a well they would be concentric cylinders. When a pulse occurs, water in the fissures of one cell is replaced by water from a neighbouring cell. This approximation becomes a better assumption as the pulse interval gets smaller.

IV.III. Assumptions

The model assumptions are summarised here:

Steady state flow conditions are established instantaneously so the movement of water can be considered 'piston' flow.

There is no water movement in the rock matrix.

The fissures remain locally at a uniform but changing concentration - there is full mixing.

Mechanical dispersion is negligible.
Movement of solutes within the matrix is described by Fick's second law and characterised by an 'apparent' diffusion coefficient.
Density effects on the flow are negligible.
Cells have the same fissure volume.
Solute concentrations through the matrix are initially uniform.

**IV.IV. Model Description**

We focus on a single cell consisting of fissure and rock matrix. As water flows through the fissure system, mass enters and leaves the fissure component of the cell. It is convenient to envisage this as a source (or sink) term in the mass balance equation so neighbouring cells don't need to be considered explicitly.

The model is best described and the mathematics developed for a specific matrix geometry but this is generalised later. The geometry adopted is that of parallel identical slabs of matrix separated by a uniform fissure (Figure IV-1). The unit considered here extends from the centre of one matrix slab across to the centre of a neighbouring block. The fissures have an aperture of $a$ while the blocks have a (total) thickness of $2b$.

**Figure IV-1 A set of model cells. Each cell extends from a fracture to the centres of the two neighbouring matrix blocks. (Slab geometry.)**

**IV.V. Mathematical Formulation**

The concentrations within the fissure and matrix for a cell will be denoted by $c_f(t)$ and $c_m(z,t)$, respectively.
Equating change of mass per unit area in the fissure with the sum of the diffusive flux and the source gives

\[
\frac{\partial \tilde{c}_f}{\partial t} = 2D_E \frac{\partial \tilde{c}_m}{\partial z} \bigg|_{z=0} + aS(t)
\]

where \(a\) is the fissure aperture, \(D_E\) is the effective diffusion coefficient and \(S(t)\) is the mass produced per unit volume per unit time.

We assume that the initial concentration in the fissure is zero:

\[
\tilde{c}_f(0) = 0
\]

Within the matrix mass balance is described by the diffusion equation:

\[
\frac{\partial \tilde{c}_m}{\partial t} = \frac{\partial^2 \tilde{c}_m}{\partial z^2}
\]

where \(D_A\) is the apparent diffusion coefficient.

As there is no diffusion across the centre of a matrix block (by symmetry):

\[
\frac{\partial \tilde{c}_m}{\partial z} \bigg|_{z=b} = 0
\]

At the matrix fracture interface the matrix and fracture water concentrations are assumed equal:

\[
\tilde{c}_m(0, t) = \tilde{c}_f(t)
\]

We assume that the initial concentration in the matrix is independent of position within the matrix.

\[
\tilde{c}_m(z, 0) = \tilde{c}_{m0}
\]

We introduce dimensionless time and distance variables given by

\[
\tau = \frac{D_A t}{b^2}
\]

and

\[
\zeta = \frac{b - z}{b}
\]

So (3) becomes

\[
\frac{\partial \tilde{c}_m}{\partial \tau} = \frac{\partial^2 \tilde{c}_m}{\partial \zeta^2}
\]

Taking Laplace transforms gives

\[
p \tilde{c}_m - \tilde{c}_{m0} = \frac{d^2 \tilde{c}_m}{d \zeta^2}
\]

where \(p\) is the transform variable. Using, (4), (5) and (6), this has the solution
\[ \bar{c}_m(z, p) = \frac{c_{m_0}}{p} + \left[ \bar{c}_f(p) - \frac{c_{m_0}}{p} \right] \frac{\cosh q \zeta}{\cosh q} \]  

(11)

where

\[ q = \sqrt{p} \]  

(12)

The derivative at the surface of the matrix block is

\[ \frac{d\bar{c}_m}{d\zeta} \bigg|_{\zeta=1} = \left[ \bar{c}_f(p) - \frac{c_{m_0}}{p} \right] q \tanh q \]  

(13)

We now return to the equation for transport in the fracture. Transforming to dimensionless distance and time and taking Laplace transforms gives

\[ p\bar{c}_f - c_{f_0} = \sigma \frac{d\bar{c}_m}{d\zeta} \bigg|_{\zeta=1} + \bar{S}'(p) \]  

(14)

where

\[ \sigma = \frac{2bD_E}{aD_A} \]  

(15)

can be regarded as the ratio of matrix to fracture storage since \( D_E/D_A \) is an effective matrix (diffusion) porosity. (We have introduced a modified source term

\( S'(\tau) = \beta S(t)/D_A \) but, as will become evident later, we do not need to use this transformation.)

Inserting (12) into (13) and rearranging gives the Laplace transform for the concentration in the fracture:

\[ \bar{c}_f(p) = \frac{\bar{S}'(p) + c_{f_0} + \sigma c_{m_0}B(q)}{p\left[1 + \sigma B(q)\right]} = \left[ \bar{S}'(p) + c_{f_0} - c_{m_0} \right] \bar{G}(p,q) + \frac{c_{m_0}}{p} \]  

(16)

where

\[ B(q) = \frac{\tanh q}{q} \]  

(17)

and

\[ \bar{G}(p,q) = \frac{1}{p\left[1 + \sigma B(q)\right]} \]  

(18)

**IV.VI. Discrete source term**

To move towards our original problem with transport in the matrix we now consider the source term as a series of instantaneous injections of mass into the fracture for the cell under consideration.

\[ S(t) = \sum_i \Delta c_i \delta(t - t_i) \]  

(19)
This causes a jump in concentration of $\Delta c_i$ at time $t_i$. Substituting into (16)

$$
\bar{c}_f(p) = \sum_i \Delta c_i \exp(-p \tau_i) + c_{f_0} - c_{m_0} \overline{G}(p, \sigma) + \frac{c_{m_0}}{p} \tag{20}
$$

We can now formally give the solution in time:

$$
c_f(\tau) = \sum_i \Delta c_i G(\tau - \tau_i, \sigma) + (c_{f_0} - c_{m_0}) G(\tau, \sigma) + c_{m_0} \tag{21}
$$

where, from (18), the Green's function $G$ is given by an inverse Laplace transform:

$$
G(\tau, \sigma) = \begin{cases} 0 & \tau \leq 0 \\
\mathcal{L}^{-1} \left\{ \frac{1}{p^2 + \sigma B(\sqrt{p})} \right\} & \tau > 0 
\end{cases} \tag{22}
$$

**IV.VII. Concentration in the matrix**

The result for the matrix is given by (9) and (19)

$$
\bar{c}_m(p, \zeta) = \frac{c_{m_0}}{p} + \left[ \sum_i \Delta c_i \exp(-p \tau_i) + c_{f_0} - c_{m_0} \right] \overline{G}(p, \sigma) \frac{\cosh q \zeta}{\cosh q} \tag{23}
$$

and the formal solution in time:

$$
c_m(\tau, \zeta) = c_{m_0} + \sum_i \Delta c_i G(\tau - \tau_i, \zeta, \sigma) + (c_{f_0} - c_{m_0}) g(\tau, \zeta, \sigma) \tag{24}
$$

where

$$
g(\tau, \zeta, \sigma) = \begin{cases} 0 & \tau \leq 0 \\
\mathcal{L}^{-1} \left\{ \frac{\cosh q \zeta}{p[1 + \sigma B(\sqrt{p}) \cosh q]} \right\} & \tau < 0
\end{cases} \tag{25}
$$

The average concentration in the matrix is obtained by taking the average of that result across a matrix block to give

$$
\langle \bar{c}_m(p) \rangle = \frac{c_{m_0}}{p} \left[ 1 - B(q) \right] + \bar{c}_f B(q) \tag{26}
$$

Combining, (26) with (21) gives the combination $\overline{G}(p)B(q)$ but this can be separated:

$$
\overline{G}(p, q) B(q) = \frac{B(q)}{p[1 + \sigma B(q)]} = \frac{1}{\sigma p} \overline{G}(p, \sigma) \tag{27}
$$

so

$$
\langle \bar{c}_m(\tau) \rangle = c_{m_0} + \frac{1}{\sigma} \left\{ \sum_i \Delta c_i [H(\tau - \tau_i)G(\tau - \tau_i, \sigma) + (c_{f_0} - c_{m_0})] - G(\tau, \sigma) \right\} \tag{28}
$$

$$
H(\tau) = \begin{cases} 0 & \tau \leq 0 \\
1 & \tau > 0 
\end{cases} \tag{29}
$$

**IV.VIII. Comments on the Green's functions**
The Green’s function $G(r, \sigma)$ decreases from unity to $1/(1 + \sigma)$ as time increases:

$$\lim_{t \to 0} G(t, \sigma) = 1$$  \hspace{1cm} (30) \\
$$\lim_{t \to \infty} G(t, \sigma) = \frac{1}{1 + \sigma}$$  \hspace{1cm} (31)

For small times

$$G(r, \sigma) \approx \exp(\sigma^2 r) \text{erfc}(\sigma \sqrt{r})$$  \hspace{1cm} (32)

For large $\sigma$ this becomes

$$G(r, \sigma) \approx \frac{1}{\sigma \sqrt{\pi t}}$$  \hspace{1cm} (33)

(Note that in both (32) and (33) $r$ and $\sigma$ only appear in the grouping $\sigma^2 r$ which represents a new dimensionless time. See the later section on diffusion times.) The Green’s function $g(r, \zeta, \sigma)$ also increases from zero to $1/(1 + \sigma)$ as time increases:

$$\lim_{t \to 0} g(t, \zeta, \sigma) = 0$$  \hspace{1cm} (34) \\
$$\lim_{t \to \infty} g(t, \zeta, \sigma) = \frac{1}{1 + \sigma}$$  \hspace{1cm} (35)

For small times

$$g(r, \zeta, \sigma) \approx \text{erfc}\left(\frac{1 - \zeta}{2\sqrt{r}}\right)$$  \hspace{1cm} (36)

**IV.IX. Generalisation of block geometry**

The function $B(q)$ introduced above has been previously defined for a number of different matrix geometries by Barker (1985a, 1985b) where it was described as a 'block geometry function' (BGF). It can be defined for blocks of any specified geometry and for mixtures of blocks of a variety of shapes and sizes. However, only simple cases have been used, normally slabs, cylinders and spheres. Block geometry functions for some simple cases are discussed in Section 3.5. Barker (1988) provided a single formula for those three recognising that they are all 'spheres' of different dimensions and generalising to a sphere of any dimension.

Each geometry is associated with a characteristic length which is the ratio of block volume to block area in contact with the fractures. That length generalises or replaces $b$ in equation 7 and the square of that length divided by the (apparent) diffusion coefficient gives a characteristic time for diffusion through a block, $t_{cb}$ (see below).

**IV.X. Diffusion times**
Diffusion of solutes through saturated porous media is a slow process in which distance of diffusion increases as the square root of time. Typically diffusion over a distance of 1 mm takes about one hour, over 1 cm about a day, 10 cm about 6 months and 1 m about 50 years.

The diffusion coefficients and block sizes do not appear separately in the model but in combination as $b^2/\kappa$. This parameter can be regarded as a characteristic time for diffusion across a matrix block and will be represented by $t_{cb}$. It will normally have values in the range of months to decades.

While the porosity ratio, block diffusion time and block shape fully describe the behaviour of a double-porosity system, another parameter, $t_{cf}$, alone is characteristic of 'short-term' behaviour. This is the characteristic time for 'significant' diffusion between the fractures and the matrix, $t_{cf}$. The time $t_{cf}$ can be thought of as the time for diffusion through a volume of water in the matrix equal to the volume of water in the fracture in a single cell.

Water in a fracture with aperture of about 1 mm will approach equilibrium with a volume of about five times as much water (e.g., 14 mm at 30% porosity) in one day. It should therefore move roughly 80% of the way from its initial concentration to that of the matrix water in about one day. From the asymptotic behaviour characterised by equations (32) and (33), it is evident that the fracture diffusion time can be defined in terms of the block diffusion times through

$$t_{cf} = \frac{t_{cb}}{\sigma^2}$$

so the quantity $\sigma^2 \tau$ represents the dimensionless time $t/t_{cf}$.

### IV.XI. Multiple cell model

This section introduces an implementation of the mathematical model, described above as a cell model. Figure IV-1 illustrates the movement of water through the model.

Let $c^n(t)$ be the concentration in the fracture in cell $n$ at time $t$. This is given by

$$c^n(t) = c^n(0) + \sum_{i \in [t_{cb}]} \Delta c^n_i G((t - t_i)/t_{cb}) \quad n = 1, \ldots, N$$

where $t_i$ is the time of movement and $t_{cb}$, is the characteristic block diffusion time.

The concentration jumps are given by
\[ \Delta c_i^n = \begin{cases} 
\lim_{t \to t_i} [c^{n-1}(t) - c^n(t)] & v > 0 \\
0 & v = 0 \\
\lim_{t \to t_i} [c^{n+1}(t) - c^n(t)] & v < 0 
\end{cases} \]  

(39)

where the concentrations at the ends of the model

- \( C^0(t) \) = concentration in cell 0
- \( C^{N+1}(t) \) = concentration in cell N + 1

must be specified as boundary conditions.
Appendix V. Comparison of a Dual-Domain Mass Transfer model with a true double-porosity model

There are two types of model that are commonly used to simulate double-porosity behaviour. The two conceptual models are different in the way in which they treat the immobile water system formed by the matrix blocks.

The first conceptual model, here referred to as the ‘Diffusive Model’, is more physically correct in the way it describes double-porosity behaviour. Flow occurs through a fracture network and is described by standard advection-dispersion equations. The fracture network is adjoined by a second system, the matrix blocks, within which no flow occurs. Diffusion within the matrix blocks is described by Fick’s second law, and exchange between the matrix and fracture systems by Fick’s first law. This form of model, typified by SWIFT amongst others, can get very complex. As well as the usual aquifer specification parameters, it is necessary to completely describe the matrix system.

The second type of double-porosity model is described here as a ‘Dual-Domain Mass Transfer model’ (D-D-M-T model). In this model, advection-dispersion equations describe the flow through a fracture system. This fracture system is joined to a cell in which no flow occurs. Unlike the ‘Diffusive Model’, the D-D-M-T model describes the matrix block as a fully mixed volume of water. Solute exchange between the matrix and fracture waters is characterised by an ‘exchange coefficient’, $\alpha$. Models of this type, including PHREEQC, are much simpler to use, requiring less specificity about the aquifer. The over-simplification of the double-porosity system can, however, lead to errors in the simulation. The source of these errors is discussed below.

V.I. Behaviour of the ‘Diffusive Model’

If we consider the ‘Diffusive Model’ with an infinite slab of matrix, with a fracture on either side, we can visualise the changing solute concentration of the matrix waters resulting from diffusion of solutes into and out of the fracture waters. As the solute concentration in the fracture water varies and diffusion occurs into a matrix block, the solute concentration across the matrix block moves out of equilibrium. The time taken for a matrix block to then return to equilibrium will be of the order of $t_{eb}$. As an example of this, if we were to describe a system in which fracture and matrix had the same solute concentration – referred to as the native solute
concentration, and briefly reduce the solute concentration of the fracture water to zero, solutes would diffuse out of the matrix into the fracture water and we would obtain the situation in Figure V-1.

Figure V-1 Solute concentration profile through the matrix a short time after a change in fracture water concentrations (Diffusive Model).

Returning the solute concentration of the fracture water to the native solute concentration will start diffusion of the solute back into the matrix (Figure V-2).

Figure V-2 Solute concentrations profile through the matrix after fracture water concentrations return to the native solute concentration (Diffusive Model).

Finally, by reducing the fracture solute concentrations to zero again, we can generate a solute concentration profile as in Figure V-3.

Figure V-3 Solute concentration profile through the matrix after fracture water concentrations are reduced to 0 for a second time (Diffusive Model).
It is apparent from this illustration that the matrix block ‘remembers’ the variations in the solute concentration of the fracture water over time. Under certain conditions this ‘memory’ will affect the fracture water solute concentrations and hence the results produced by a diffusive model.

V.II. Formulation of the Dual-Domain Mass Transfer model, and the Diffusive Model

In order to determine how important diffusion within a matrix block is, we need to determine the sensitivity of $\alpha$. To do this we describe both the D-D-M-T model and the diffusive model:

The D-D-M-T model is normally (Berkowitz, 1994):

\begin{equation}
\theta_{mo} R_{mo} \frac{\partial C_{mo}}{\partial t} = \alpha (C_{im} - C_{mo}) - \bar{v}_l \frac{\partial C_{mo}}{\partial l} + D_l \frac{\partial^2 C_{mo}}{\partial l^2} \tag{1}
\end{equation}

and

\begin{equation}
\theta_{im} R_{im} \frac{\partial C_{im}}{\partial t} = \alpha (C_{no} - C_{im}) \tag{2}
\end{equation}

$\theta_{im}$ = immobile porosity; $\theta_{im}$ = mobile porosity;
$R_{im}$ = retardation coefficient in the immobile volume; $R_{mo}$ = retardation coefficient in the mobile volume;
$C_{im}$ = immobile concentration; $C_{mo}$ = mobile concentration;
$D_l$ = dispersion coefficient; $v_l$ = flow velocity; $l$ = flow length;
$t$ = time.

Whilst the diffusive model can be stated:

\begin{equation}
\frac{\partial C_f}{\partial t} = \frac{2D_E}{a} \frac{\partial C_m}{\partial Z} \bigg|_0 - \bar{v}_l \frac{\partial C_f}{\partial l} + D_l \frac{\partial^2 C_f}{\partial l^2} \tag{3}
\end{equation}

$C_m$ = matrix concentration; $C_f$ = fracture concentration;
$D_l$ = dispersion coefficient; $D_E$ = effective diffusion coefficient;
$v_l$ = fracture flow velocity; $l$ = distance in fractures;
$t$ = time; $a$ = aperture width; $Z$ = distance into block.

and:
\[
\frac{\partial C_m}{\partial t} = D_A \frac{\partial^2 C_m}{\partial x^2}
\]  
(4)

In order to compare the two models, it is necessary to compare the exchange term in the D-D-M-T model with the diffusion term in the diffusion model. The solute concentration of the fracture is set to vary with time according to a sine function, with an angular frequency of \( \omega \), and an amplitude determined by the constant \( A \). We vary the concentration in the fractures (mobile phase) according to equation 5:

\[
C_{mo}(t) = Ae^{i\omega t}
\]  
(5)

Assuming the solute concentration of the immobile phase (matrix volume) behaves as:

\[
C_{im}(t) = Be^{i\omega t}
\]  
(6)

Then from equations 1, 4, 5, and 6:

\[
i\omega B = \alpha_{im}(A - B)
\]  
(7)

And from equations 2, 4, 5, and 6 we find:

\[
- Exchange = \left( \frac{\alpha_{mo}i\omega}{\alpha_{im} + i\omega} \right) Ae^{i\omega t}
\]  
(8)

Where

\[
\alpha_{mo} = \frac{\alpha}{\theta_{mo} R_{mo}} \quad \alpha_{im} = \frac{\alpha}{\theta_{im} R_{im}}
\]  
(9,10)

Similarly, applying the changing fracture concentration to the Diffusive model we get:

\[
C_f(t) = Ae^{i\omega t}
\]  
(11)

\[
C_m(t) = C_{mo}e^{i\omega t}
\]  
(12)

Let

\[
\lambda^2 = \frac{i\omega}{D_A}
\]  
(13)

Then

\[
- Exchange = \sigma i\omega B(\lambda b) Ae^{i\omega t}
\]  
(14)

Where

\[
B(x) = \frac{\tanh x}{x}
\]  
(15)

and
\[
\sigma = \frac{2bD_e}{aD_A}
\]  

(Note that \(B(\alpha)\) is the Block Geometry Function, and \(\sigma\) is the porosity ratio as described in Chapter 2.4.4.)

We want to examine two aspects of the concentration change in the matrix, the magnitude of the exchange, and its period (or rather the angular frequency). By equating these two 'exchange' formulae, we can compare the two models and determine the parameters which could result in equivalent behaviour in both models.

By equating the real and imaginary parts of the exchange terms, we obtain:

\[
\alpha = \omega \theta_{im} R_{im} \frac{P^+(\tau)}{P^-(-\tau)}
\]

\[
\alpha_{im} = \frac{\theta_{mo} R_{mo}}{\theta_{im} R_{im}} = \frac{P^+(\tau)}{\sigma}
\]

where \(R\) is the retardation coefficient and

\[
P^+(\tau) = \frac{\tau}{2} \left( \frac{\sinh \tau \pm \sin \tau}{\cosh \tau - \cos \tau} \right)
\]

\[
\tau = \sqrt{2\omega t_{cb}} = \sqrt{4\pi t_{cb}/T}
\]

Where \(t_{cb}\) is the characteristic block time as described in Chapter 2.4.4, and \(T\) is the period.

If each model is to have identical parameters characterising the aquifer, we need to ensure that \(\theta_{im}/\theta_{mo}=\sigma\). From equation 15 we can see for this to be the case when there is no retardation \((R_{im}=R_{mo}=1)\) and \(P^+(\tau)\) equals unity. If \(T > 10t_{cb}\), then the difference between the parameters from each model, i.e. the error, is less than 1%:

\[
P^+(\tau) - 1 < \frac{1}{100}
\]

The behaviour is shown for specific parameter values in Figure V-4. We can see that for low \(t_{cb}\) values, \(P^+(\tau)\) remains close to a value of 1, whether we vary \(T\) or \(t_{cb}\).

Thus, for low \(t_{cb}\), the amplitude of the solute concentration change in the matrix of a mixing-cell model is insensitive to the period of the solute concentration change in the fracture. At high \(t_{cb}\) values the \(P^+(\tau)\) is very sensitive to the period of the solute concentration change in the fracture as well as to \(t_{cb}\).
We can draw several conclusions:

- When equating the period of solute concentration change in the matrix block, aquifers characterised by a low \( t_{cb} \) value will have low sensitivity to the period of the change of solute concentrations in the fracture. As a result it is relatively unimportant to correctly define the period of the change of solute concentrations in the fracture. Both the D-D-M-T model and the standard Diffusive model will have equivalent parameter values.

- When equating the period of solute concentration change in the matrix block, aquifers characterised by a high \( t_{cb} \) value will have high sensitivity to the period of the change of solute concentrations in the fracture. As a result it is important to correctly define the period of the change of solute concentrations in the fracture. In order to obtain a good match between the Diffusive and the D-D-M-T models, the selected matrix and fracture porosities will not be equivalent between the two models.

From (17) we can obtain the exchange term \( \alpha \):

\[
\frac{\alpha}{\omega \delta_{m} R_{m}} = \frac{\sinh \tau + \sin \tau}{\sinh \tau - \sin \tau}
\]  

(22)
Varying $\theta_m$, $\theta_{mo}$ and $t_{cf}$ can show how sensitive the mixing-cell model will be to variation in $\alpha$. Figure V-5 illustrates the variation in $\alpha$ with changing $\theta_m$ and $\theta_{mo}$, while Figure V-6 shows the sensitivity to $t_{cf}$.

Figure V-5 Variations in $\alpha$ with changing $\theta_m$ and $\theta_{mo}$.

Figure V-6 Variations in $\alpha$ with changing $t_{cf}$.

Again, several conclusions can be drawn
Figure V-5 shows that when the mobile porosity is low (lines A and B) $\alpha$ is insensitive to the immobile porosity. When the immobile porosity is high (lines C and D), $\alpha$ is slightly more sensitive. When using a mixing-cell model the accuracy of the immobile porosity measurements are relatively unimportant.

- Comparing lines A and C or B and D clearly show that $\alpha$ is extremely sensitive to variations in the mobile porosity. When using a mixing-cell model, the accuracy of the measurement of mobile porosity is very important.
- Figure IV-6 shows high sensitivity of $\alpha$ to $t_{cf}$, therefore this parameter needs to be well characterised when using a mixing-cell model.
- Both Figure V-5 and Figure V-6 show a decreasing sensitivity of $\alpha$ to $T$, as $T$ increases.

V.III. Conclusions on the feasibility of using a mixing-cell model to approximate double-porosity behaviour.

With a periodic $C_f$ it is possible to approximate the amplitude of change in $C_m$ in a double-porosity model with a mixing cell model. As long as $t_{cf}$ is small (<0.1 day), and the period, $T$, is large (>100 days), the $T$ of the $C_f$ is relatively unimportant. With larger $t_{cf}$ values, to ensure a good approximation the parameters characterising the aquifer in the mixing-cell model ($\theta_m$ and $\theta_{mo}$) may not be equal to the equivalent parameter in the double-porosity model, i.e. $\theta_m/\theta_{mo} \neq \sigma$.

It is also possible to approximate the frequency of the change in $C_m$ in a double-porosity model with a mixing cell model. As long as $T$ is small, however it is essential to accurately identify both the mobile porosity and $t_{cf}$.

It is possible, therefore, to use a mixing-cell model to approximate double-porosity behaviour within certain bounds. A mixing-cell model can be successfully calibrated to experimental data from a double-porosity system. It is, however, more difficult to ensure accurate predictions of behaviour from a mixing-cell model. Figure V-4 shows the large sensitivity of $\alpha$ to the period of the variation in $C_f$. Thus a model calibrated to experimental data would provide a value of $\alpha$ specific to that particular test. To use that calibrate value to predict behaviour under a different period would result in large errors in the results. These errors would, however, decrease if both the test and the predictive model had large periods ($T>100$ days).

A likely expansion of the work would use Fourier analysis to determine a set of frequencies that combine to produce a likely ASR pumping pattern. This methodology could then look at sensitivities across the range of frequencies required.
Equating the frequency of solute change would be difficult for short $T$, and as any the Fourier analysis of any pumping pattern is likely to result in some short $T$, this scenario will need to be investigated carefully.

Alternatively, it would be possible to replace the Block Geometry Function in either the DP-Pulse or the DP1D model with something of the form of equation 1, as discussed in Barker (1985a). This would allow the use of the D-D-M-T double-porosity approximation with these models, allowing direct comparison of the two.

\[ B(x) = \frac{\alpha'}{\alpha' + x^2} \]  

(1)
Appendix VI. Relating the geometrically invariant DP-Pulse model to real scenarios

A major control on the results from the ASR model is the size of the pulse interval ($\Delta T$) used. Careful consideration must be made of the implications of variations in this value. In the current model the flow regime is geometrically invariant, and hence only times are specified, i.e. the duration of injection/abstraction and the pulse interval. To simplify consideration of the implications of this and the meaning of variation in $\Delta T$ we will first look at the linear model.

VI.I. Linear model

In setting up a model run we specify $P_T$ (the set of times that define the pumping pattern), $\Delta T$ and $N$ (the number of annuli). These parameters are sufficient to provide all the required information, provided we only look at the injection/abstraction well.

The model in this form is invariant with respect to the physical geometry of the system. This invariance is very useful in that it allows us to model a system without knowing aquifer geometries or fracture network patterns. There may be some cases, however, when some knowledge of the geometry will be useful. The invariant model can only tell us concentrations at the well, so watching how the solute concentrations vary at (absolute) distances from the well is not possible. By specifying one more parameter, either velocity, $V$, the length of the system, $x$, or the width of a cell, $\Delta x$, we can outline all the physical flow parameters.
Table VI.1 - Parameters used to specify advective flow when interpreting the geometrically invariant DP-Pulse model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
<th>Error analysis</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_t$</td>
<td>Time since start of model run</td>
<td>Specified through the model setup parameters.</td>
<td></td>
</tr>
<tr>
<td>$\Delta T$</td>
<td>Pulse interval (period between pulses)</td>
<td>Error analysis: Reducing both $\Delta T$ and $\Delta x$ (hence increasing $N$) will decrease the error. Velocity ($V$): Changing $\Delta T$ whilst maintaining $\Delta x$ will change the velocity. Application of this involves reading the results at the same $n$ for different runs with different $\Delta T$ values.</td>
<td></td>
</tr>
<tr>
<td>$N$</td>
<td>Number of cells</td>
<td>$N = t_t / \Delta t$</td>
<td></td>
</tr>
<tr>
<td>$n$</td>
<td>Specific cell</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Delta x$</td>
<td>Cell width (1-D only)</td>
<td>Error analysis: Reducing both $\Delta T$ and $\Delta x$ (hence increasing $N$) will decrease the error. Velocity ($V$): Changing $\Delta x$ whilst maintaining $\Delta T$ will change the velocity. Application of this may involve reading the results at the same $t$, value, generally that of the advective front, and obtaining the shape of the solute pulse. Comparison with other model runs with different values of $\Delta x$ but at the same time, $t$, will be interesting.</td>
<td></td>
</tr>
<tr>
<td>$V$</td>
<td>Velocity</td>
<td>$V = \Delta x / \Delta T$</td>
<td></td>
</tr>
</tbody>
</table>

The model can therefore be defined through the use of a number of different parameter sets including:

- $t_t$ and $\Delta t$ ($N = t_t / \Delta T$ can be derived from these)
- $x$, $\Delta x$, and $V$ (again $N$ can be derived)

Essentially, as well as specifying $\Delta T$ and $t_t$, which are required by the DP-Pulse model, either $\Delta x$ or $x$ is required to define the model geometry. From these, all parameters $N$, $V$ etc. can be determined.

VI.II.  Cylindrical model

Determining the position of a point within the annular (cylindrical flow) model may also be completed by the same method as for the one-dimensional model, although it must be remembered that, due to the annular nature of the model, ‘$\Delta x$’ will change in a known manner with distance from the well.

A more useful method of determining positions from the geometrically invariant model is to equate the volume flow to a the fracture porosity within the aquifer:

$$Qt_t = \theta_f \pi r^2$$  \hspace{1cm} (1)

Where:

- $Q$ is the rate of injection of water into the aquifer;
- $\theta_f$ is the fracture porosity;

and $r$ is the radius of the front of the injection water from the injection well.

VI.III.  Determining pumping rate
Varying the pumping rate in the double-porosity model is not a simple matter. The current coding of the model does not allow for variation of $\Delta T$ or $\Delta x$ during a model run. Whilst $\Delta x$ is fixed for a model run, $\Delta T$ could be varied. This process is, however, computationally expensive, as every time $\Delta T$ changes all Green’s functions have to be recalculated.

Another potential method of varying the rate is to allow the water to ‘skip’ cells, thereby allowing relative increases in flow rate. For example, water flowing at a rate of ‘1’ would pass from cell 1 to cell 2, then to cell 3 and so on (see Figure VI-1A) Water flowing at a rate of ‘2’ would only pass through half of the cells, so flowing from cell 1 to cell 3, and on to cell 5 (see Figure VI-1B)

![Figure VI-1 Changing the rate of flow in the DP-Pulse model by stepping over cells.](image)

This method works for the one-dimensional model, although the error in the model is likely to increase. For the annular model, however, there are a number of concerns. Firstly, due to the annular nature, the front clearly does not move forward at a constant rate. Secondly as the cells are of equal volume by definition, they are not of equal width. These concerns have not been addressed by this work.
Appendix VII. DP-Pulse model use

This section was taken from a note provided with the first released version of the DP-Pulse model, enclosed with this volume on a compact disk. A general overview of the model concept is provided, along with sufficient information to allow simple applications of version 1 of the model.

DP-Pulse Version 1

John Barker & Tim Wright

UCL

June 2000

DP-Pulse models injection of water to and abstraction from a well in a double-porosity media.

A double-porosity media is formed of blocks of a small grained highly porous media (high porosity ($\phi$), low hydraulic conductivity ($K$)), separated by relatively large fractures (low $\phi$, high $K$). Within the matrix block, groundwater flow is negligible due to the small pore throats, and so groundwater flow occurs within the fractures. ASR therefore injects water into the fractures, within which it will come into direct contact with the native water within the matrix blocks and diffusion of solutes will occur (Figure VII-1). This causes the solute concentrations in the abstracted water to behave in a different manner to those in an equivalent single porous media. In general, abstracted solute concentrations from an ASR system in a double-porosity aquifer will be higher than those from a single porosity aquifer.
Matrix

Fracture

Fluid flow through high permeability fractures

Diffusion from high to low solute concentrations

Figure VII-1: Fluid flow and diffusion in double-porosity media

Although the model formulation is invariant with respect to flow geometries, it is possible to visualise flow as being either 1-D linear or 2-D radial. In the linear case water flows in a series of pulses from one cell to another (Figure VII-2a). In the radial case flow passes radially out from a central point (Figure VII-2b). In the extreme case, the flow may be anisotropic in 3 dimensions (Figure VII-2c).

A – 1D Linear flow   B – 2D Radial flow

Equal Volume Cells

Groundwater Flow

C – 3D Anisotropic flow

Figure VII-2: Model invariance to flow geometry
Outline description
This code simulates reversible solute transport through a double-porosity medium with a specified input concentration. It outputs the concentration in the fractures for a specified set of times at the point of injection.

Version 1 assumes:
- Dispersion is negligible.
- The input concentration is piecewise constant.

The user creates a data file DP_PULSE.DAT in the same directory as the executable file DP_PULSE.EXE and the output appears in a file called DP_PULSE.OUT.

Processes simulated
Fracture water:
- Reversible advection
- Diffusion exchange with matrix.

Matrix water:
- Diffusion according to Fick's second law

Mathematical formulation
In order to describe the formulation of the model we will discuss the case of radial flow in a medium formed from slabs of matrix.
Figure VII-3: Injection of water with varying solute concentrations and rates into a confined fractured aquifer.

The model provides a solution to the standard advection-diffusion equations.

Diffusion within matrix according to Fick's second law:

\[
\frac{\partial C_m}{\partial t} = D_A \frac{\partial^2 C_m}{\partial z^2}
\]

With the boundary conditions:

\[
C_m(r,\pm b, t) = C_f(r, t)
\]
\[
C_m(r, z=0) = C_m(0)
\]
\[
\left. \frac{\partial C_m}{\partial z} \right|_{z=b} = 0
\]

Diffusion into the fracture is according to Fick's first law. For the radial case, the problem can be stated:

\[
\frac{\partial C_f}{\partial t} + \frac{Q(t)}{2\pi a N_f} \frac{\partial C}{\partial r} = \frac{2D_E}{a} \left. \frac{\partial C_m}{\partial z} \right|_{z=b}
\]

With the boundary conditions:

\[
C_f(r_0,t) = C_{in} \quad Q > 0
\]
\[
C_f(r,t) = C_m(0) \quad r \to \infty
\]

In the solution, the parameters are combined into two groups, \( t_{cb} \) and \( \sigma \) (defined below).

The concentration in the fracture in cell \( n \) at time \( t \):

\[
c^n(t) = c^n(0) + \sum_{i \in [t_i < t]} \Delta c^n_i G[(t-t_i)/t_{cb}, \sigma] n = 1, \ldots, N
\]

where

\( t_i \) is the time of movement (pulse time);

\( t_{cb} \) is the characteristic 'block' diffusion time (see below).

The concentration jumps are given by

\[
\Delta c^n_i = \begin{cases} \lim_{t \to t_i^-} [c^{n-1}(t) - c^n(t)] & v > 0 \\ 0 & v = 0 \\ \lim_{t \to t_i^+} [c^{n+1}(t) - c^n(t)] & v < 0 \end{cases}
\]

The Green's function, \( G \), is given by an inverse Laplace transform:
$G(\tau, \sigma) = \begin{cases} 
0 & \tau \leq 0 \\
L^{-1}\left\{p^{-1}\left[1 + \sigma B(\sqrt{p})\right]^{-1}\right\} & \tau > 0 
\end{cases}$

$p$ is the transform variable; is the effective matrix to fracture porosity ratio

The function $B$ is the ‘block geometry function’ (BGF).

**Characteristic features of the model**

a) The matrix/fracture porosity ratio, for the case of the slab model (see Figure VI-1):

$$\sigma = \frac{2b\phi}{a}$$

b) The characteristic time for diffusion across a matrix block.

$$t_{cb} = \frac{b^2}{D_a}$$

In general, $b$ is the ratio of block volume to block area.

$t_{cb}$ is 5.08 times the time for the average concentration in a block to reduce by 50% due to diffusion into fracture water held at zero concentration.

Note: $t_{cf}$ and $\sigma$ combine to produce the characteristic time for diffusion from a fracture

$$t_{cf} = \frac{a^2}{4D_\phi} = \frac{a^2}{4D_a\phi^2} = \frac{t_{cb}}{\sigma^2}$$

This is 1.69 times the time for the time for the concentration in a fracture to drop by 50% due to diffusion into infinite matrix blocks.

c) The Block Geometry Function (Barker 1985a,b, Barker *et al.* 2000)

For the slab model:

$$B(x) = \frac{\tanh x}{x}$$

For a spherical geometry

$$B(x) = \frac{\coth x}{x} - \frac{1}{3x^2}$$
Table VII.1 Parameters used to characterise the aquifer

<table>
<thead>
<tr>
<th>SYMBOL</th>
<th>DESCRIPTION</th>
<th>DIMENSIONS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$</td>
<td>Fissure aperture (full width of a single fissure).</td>
<td>L</td>
</tr>
<tr>
<td>$b$</td>
<td>Matrix block vol./area (e.g. half slab thickness).</td>
<td>L</td>
</tr>
<tr>
<td>$B$</td>
<td>Block Geometry Function</td>
<td></td>
</tr>
<tr>
<td>$C_f$</td>
<td>Solute concentration in the fracture water</td>
<td>ML$^{-3}$</td>
</tr>
<tr>
<td>$C_m$</td>
<td>Solute concentration in the matrix water</td>
<td>ML$^{-3}$</td>
</tr>
<tr>
<td>$C_{mb}$</td>
<td>Solute concentration in the matrix water at $t=0$</td>
<td>ML$^{-3}$</td>
</tr>
<tr>
<td>$c^n(t)$</td>
<td>Concentration in fracture water in cell $n$</td>
<td></td>
</tr>
<tr>
<td>$D_a$</td>
<td>Apparent diffusion coefficient</td>
<td>L$^2$T$^{-1}$</td>
</tr>
<tr>
<td>$D_e$</td>
<td>Effective diffusion coefficient</td>
<td>ML$^2$T$^{-1}$</td>
</tr>
<tr>
<td>$n$</td>
<td>Cell number</td>
<td>-</td>
</tr>
<tr>
<td>$N$</td>
<td>Total number of cells</td>
<td>-</td>
</tr>
<tr>
<td>$N_f$</td>
<td>Number of fractures</td>
<td>-</td>
</tr>
<tr>
<td>$Q(t)$</td>
<td>Flow from well at time $t$</td>
<td>L$^3$T$^{-1}$</td>
</tr>
<tr>
<td>$r$</td>
<td>Radius from well</td>
<td>L</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
<td>T</td>
</tr>
<tr>
<td>$t_{cb}$</td>
<td>Characteristic block diffusion time</td>
<td>T</td>
</tr>
<tr>
<td>$t_{cf}$</td>
<td>Characteristic fracture time</td>
<td>T</td>
</tr>
<tr>
<td>$z$</td>
<td>Distance into matrix block</td>
<td>L</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Matrix porosity</td>
<td>-</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Ratio of matrix porosity to fracture porosity</td>
<td>-</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Dimensionless time $= t/t_{cb}$</td>
<td>-</td>
</tr>
<tr>
<td>$\Delta T$</td>
<td>Pulse interval</td>
<td>T</td>
</tr>
</tbody>
</table>

Data input (File: DP_PULSE.DAT)

Example data set. Take particular attention of the order and the notes given below

Demonstration run

```
30 1000 2   sigma, tcb, ngeom
0.5 0.5   vratio, sratio
0 1 1   start time, npattem, pulse interval
5 5 5 5 0.5   nrepeat, tinj, tstor, tdorm, tabst, concin
1   initconc
5   number of mid-pulse concentration readings
1 2 3 4 5   times of mid-pulse concentration readings
end
```

(1) ngeom specifies the Block Geometry – 1=slab, 2=mixture of two slab sizes, 3=sphere, 4=mixture of two sphere sizes

(2) vratio = volume ration of two block geometry sizes; sratio = size ratio of two block geometry sizes. If ngeom=1 or 3 this line is ignored.

(3) npattem – number of pumping patterns (following lines)

(4) nrepeat = number of times pumping pattern is repeated; tinj = injection duration; tstor = duration of period of no flow; tabst = abstraction duration; tdorm = duration of period of no flow; concin = solute concentration of injected water.

(5) initconc = initial concentration
1. The first record (line) provides a brief description of the run.
2. Each parameter value should be given in the form of a number
3. Parameters must be input in the correct order (see example below).
4. If 'E' format is used for input, include the decimal point.
5. All units should be consistent.

**Selection of pulse interval**

DP-Pulse approximates continuous flow with a series of instantaneous pulses: as the pulses become closer together, the approximation to the actual situation improves. It is important, therefore, to choose a suitably small pulse interval ('pulse interval').

However, the size of the program is proportional to the square of the number of pulse intervals, so computer memory and processor speed can rapidly become a limitation on the model and a compromise must be made.

We are continuing to research the implications of large pulse intervals in terms of the incurred error, but we have two simple equations to guide the choice of the pulse interval. Having chosen a value using these equations, the user is encouraged to experiment with the pulse interval. The model automatically determines the number of cells required from the input data set.

For an error of less than 1%:

\[
\frac{t}{\Delta t} > \frac{66t_{cf}}{t}
\]

where \( t \) is the length of time simulated by the model and \( \Delta t \) is the pulse interval.

For an error of less than 10%:

\[
\frac{t}{\Delta t} > \frac{25t_{cf}}{t}
\]
Appendix VIII. Calibration of data from the Boynton Beach ASR scheme, Florida.

In December 1991 an ASR well was constructed at Boynton Beach, Florida for the City of Boynton Beach. The open section of this well, from 804 feet to 909 feet below ground level, penetrated the confined artesian Floridian Aquifer system. This consists of the Suwannee Limestone and the Avon Park Limestone. The Suwannee Limestone is a fossiliferous biomicritic limestone, and the Avon Park Limestone is a finely fragmented fossiliferous limestone.

After development, a step pumping test determined injection transmissivities of the open zone to be between 63 and 120 m²/d. During the recovery after the test, a transmissivity of 18 m²/d was measured. An overall transmissivity for the section of open well was estimated to be 87 m²/d.

Commencing on October 21st, 1992, a series of cycle tests were completed to evaluate the operational potential of the ASR system and to determine the initial water quality response. The times of injection and abstraction during the first fifteen cycle tests are outlined in Table VIII-1. The solute concentrations were measured and the chloride results are illustrated in Figure VIII-1.

![Figure VIII-1 Chloride solute concentrations from four Cycle Tests at the Boynton Beach ASR site.](image-url)
Table VIII-1 Cyclic pumping regime for the Boynton Beach ASR site.

<table>
<thead>
<tr>
<th>Cycle No.</th>
<th>Action</th>
<th>Start time</th>
<th>Stop time</th>
<th>Duration (Days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Injection</td>
<td>21/10/92 15:01</td>
<td>03/11/92 07:44</td>
<td>12.7</td>
</tr>
<tr>
<td>1</td>
<td>Abstraction</td>
<td>03/11/92 11:15</td>
<td>10/11/92 08:10</td>
<td>6.9</td>
</tr>
<tr>
<td>2</td>
<td>Injection</td>
<td>11/11/92 00:08</td>
<td>22/12/92 09:09</td>
<td>41.4</td>
</tr>
<tr>
<td>2</td>
<td>Abstraction</td>
<td>23/12/92 10:40</td>
<td>08/01/93 10:10</td>
<td>16.0</td>
</tr>
<tr>
<td>3</td>
<td>Injection</td>
<td>25/01/93 08:53</td>
<td>07/03/93 08:00</td>
<td>41.0</td>
</tr>
<tr>
<td>3</td>
<td>Abstraction</td>
<td>15/03/93 14:05</td>
<td>06/04/93 08:00</td>
<td>21.7</td>
</tr>
<tr>
<td>4</td>
<td>Injection</td>
<td>20/04/93 13:50</td>
<td>07/05/93 09:20</td>
<td>16.8</td>
</tr>
<tr>
<td>4</td>
<td>Abstraction</td>
<td>14/05/93 08:10</td>
<td>28/05/93 08:10</td>
<td>14.0</td>
</tr>
<tr>
<td>5</td>
<td>Injection</td>
<td>01/06/93 10:00</td>
<td>27/07/93 08:45</td>
<td>55.9</td>
</tr>
<tr>
<td>5</td>
<td>Abstraction</td>
<td>02/11/93 10:30</td>
<td>06/12/93 07:55</td>
<td>33.9</td>
</tr>
<tr>
<td>6</td>
<td>Injection</td>
<td>24/02/94 14:00</td>
<td>21/04/94 08:20</td>
<td>55.8</td>
</tr>
<tr>
<td>6</td>
<td>Abstraction</td>
<td>16/06/94 00:00</td>
<td>25/07/94 07:12</td>
<td>39.3</td>
</tr>
<tr>
<td>7</td>
<td>Injection</td>
<td>25/07/94 11:23</td>
<td>07/09/94 08:35</td>
<td>43.9</td>
</tr>
<tr>
<td>7</td>
<td>Abstraction</td>
<td>09/01/95 00:00</td>
<td>13/02/95 12:54</td>
<td>35.5</td>
</tr>
<tr>
<td>8</td>
<td>Injection</td>
<td>20/04/95 14:40</td>
<td>05/05/95 08:45</td>
<td>45.8</td>
</tr>
<tr>
<td>8</td>
<td>Abstraction</td>
<td>05/06/95 13:30</td>
<td>03/07/95 08:30</td>
<td>27.8</td>
</tr>
<tr>
<td>9</td>
<td>Injection</td>
<td>27/09/95 08:27</td>
<td>30/10/95 08:55</td>
<td>33.0</td>
</tr>
<tr>
<td>9</td>
<td>Abstraction</td>
<td>21/11/95 09:26</td>
<td>20/12/95 08:50</td>
<td>29.0</td>
</tr>
<tr>
<td>10</td>
<td>Injection</td>
<td>18/01/96 09:15</td>
<td>04/03/96 08:44</td>
<td>46.0</td>
</tr>
<tr>
<td>10</td>
<td>Abstraction</td>
<td>24/04/96 10:09</td>
<td>22/05/96 08:25</td>
<td>27.9</td>
</tr>
<tr>
<td>11</td>
<td>Injection</td>
<td>04/06/96 09:00</td>
<td>08/07/96 08:51</td>
<td>34.0</td>
</tr>
<tr>
<td>11</td>
<td>Abstraction</td>
<td>04/12/96 10:13</td>
<td>31/12/96 09:14</td>
<td>27.0</td>
</tr>
<tr>
<td>12</td>
<td>Injection</td>
<td>03/01/97 09:30</td>
<td>14/02/97 07:14</td>
<td>41.9</td>
</tr>
<tr>
<td>12</td>
<td>Abstraction</td>
<td>06/05/97 13:30</td>
<td>16/06/97 09:04</td>
<td>40.8</td>
</tr>
<tr>
<td>13</td>
<td>Injection</td>
<td>19/06/97 11:05</td>
<td>24/07/97 08:55</td>
<td>34.9</td>
</tr>
<tr>
<td>13</td>
<td>Abstraction</td>
<td>14/01/98 13:50</td>
<td>23/02/98 08:30</td>
<td>39.8</td>
</tr>
<tr>
<td>14</td>
<td>Injection</td>
<td>23/02/98 09:10</td>
<td>10/04/98 08:55</td>
<td>46.0</td>
</tr>
<tr>
<td>14</td>
<td>Abstraction</td>
<td>10/04/98 12:35</td>
<td>20/08/98 08:50</td>
<td>131.8</td>
</tr>
<tr>
<td>15</td>
<td>Injection</td>
<td>12/11/98 09:00</td>
<td>04/02/99 09:10</td>
<td>84.0</td>
</tr>
<tr>
<td>15</td>
<td>Abstraction</td>
<td>02/04/99 10:30</td>
<td>03/06/99 07:54</td>
<td>61.9</td>
</tr>
</tbody>
</table>

The shape of the solute concentration curves at early times (Cycle 1 illustrated) differs markedly from those obtained at the Lychett Minster Test Site (illustrated in Figure 4-12). At Lychett Minster the chloride solute concentrations increasing rapidly at the start of recovery, and then approached a maximum asymptotically. The early results from Boynton Beach show the concentrations staying low at the start of recovery, and rising rapidly later on. This indicates a change in the relative importance of the processes occurring. At Lychett Minster, the dominant processes controlling conservative solute concentrations were advection and diffusion between the fracture and matrix waters. Dispersion was found to be relatively unimportant. It is likely that at Boynton Beach the dominant controls are advection and mechanical dispersion, with double-porosity diffusion playing a smaller role.

An attempt was made to calibrate the DP-Pulse model to the data from Boynton Beach using the automated calibration routine. The time data input to the calibration model can be seen below (Table VIII-2). The initial parameter estimates were $t_{cb} =$
1000 days, \( \sigma = 50 \). A pulse interval of 1 day was used, and a slab geometry provided a better calibration than the sphere geometry.

**Table VIII-2** Pumping-cycle times input for the semi-analytical model

<table>
<thead>
<tr>
<th>Cycle</th>
<th>Injection</th>
<th>Storage</th>
<th>Abstraction</th>
<th>Dormancy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12.7</td>
<td>0.1</td>
<td>6.9</td>
<td>0.7</td>
</tr>
<tr>
<td>2</td>
<td>41.4</td>
<td>1.1</td>
<td>16.0</td>
<td>16.9</td>
</tr>
<tr>
<td>3</td>
<td>41.0</td>
<td>8.3</td>
<td>21.7</td>
<td>14.2</td>
</tr>
<tr>
<td>4</td>
<td>16.8</td>
<td>7.0</td>
<td>14.0</td>
<td>4.1</td>
</tr>
<tr>
<td>5</td>
<td>55.9</td>
<td>98.1</td>
<td>33.9</td>
<td>80.3</td>
</tr>
<tr>
<td>6</td>
<td>55.8</td>
<td>55.7</td>
<td>39.3</td>
<td>0.2</td>
</tr>
<tr>
<td>7</td>
<td>43.9</td>
<td>123.6</td>
<td>35.5</td>
<td>66.1</td>
</tr>
<tr>
<td>8</td>
<td>45.8</td>
<td>0.2</td>
<td>27.8</td>
<td>86.0</td>
</tr>
<tr>
<td>9</td>
<td>33.0</td>
<td>22.0</td>
<td>29.0</td>
<td>29.0</td>
</tr>
<tr>
<td>10</td>
<td>46.0</td>
<td>51.1</td>
<td>27.9</td>
<td>13.0</td>
</tr>
<tr>
<td>11</td>
<td>34.0</td>
<td>149.1</td>
<td>27.0</td>
<td>3.0</td>
</tr>
<tr>
<td>12</td>
<td>41.9</td>
<td>81.3</td>
<td>40.8</td>
<td>3.1</td>
</tr>
<tr>
<td>13</td>
<td>34.9</td>
<td>174.2</td>
<td>39.8</td>
<td>0.0</td>
</tr>
<tr>
<td>14</td>
<td>46.0</td>
<td>0.2</td>
<td>131.8</td>
<td>84.0</td>
</tr>
<tr>
<td>15</td>
<td>84.0</td>
<td>57.1</td>
<td>61.9</td>
<td>0.0</td>
</tr>
</tbody>
</table>

The calibration identified a \( t_{cb} \) value of 228 days, and a \( \sigma \) value of 6. The DP-Pulse model was then run with the calibrated parameters. The output is shown in Figure VII-2.

![Graphs showing relative solute concentration over time for different cycles](image)

**Figure VIII-2** Comparison of Boynton Beach data to calibrated DP-Pulse model
(Slab geometry; Pulse interval = 1 day; \( t_{cb} = 228 \) days; \( \sigma = 6 \))
The calibration does not fit the data well. It appears, as has been previously suggested, that advection and dispersion are the dominant processes, and that double-porosity diffusion is not as significant a factor.
Appendix IX. A broader overview of Operational Research Methodologies

This thesis has implemented Operational Research (OR) methodologies in a highly quantitative manner. The use of OR in this manner is well documented throughout the literature, and was discussed in Chapter 7. An alternative perspective is the use of OR methodologies to aid in the implementation of a method of working and problem solving in an interpersonal manner. This qualitative use of the theories is becoming more common, with, for example, trained mediators being used in confrontational situations. This section of the thesis summarises some of these developments. The majority of this chapter is drawn from the book “Rational analysis for a problematic world” (Rosenhead, 1989).

IX.I. Cognitive mapping and SODA (Strategic Options Development and Analysis)

Many issues, most notably those with a component of environmental impact, arouse strong feelings on all sides. Any attempt to reconcile these concerns can be fraught with difficulty, and will frequently leave one or more of the groups feeling unrepresented. The result of this can be the situation in which the exact nature of the problem remains concealed, with involved parties viewing the question as having only a right or wrong answer whilst failing to consider any form of compromise. For example, groundwater abstraction, leading to dewatering of natural wetlands may be commercially necessary to farmers, but unacceptable to environmental groups. In such cases, the debate may simply turn into a battle over whether the farmer has a right to abstract, and fail to consider possible alternatives such as alternative supplies of water and localised artificial recharge.

Strategic Options Development and Analysis (SODA) is a technique most usefully applied in the solution of a ‘messy’ problem: one in which not only is the solution unknown, but the question being asked is unclear. It is helpful in confrontational situations, where it becomes necessary to ensure that all parties are heard in the debate. It involves bringing together two sets of skills on the part of the OR consultant in order to facilitate discussion between a group of parties. These skills are:
• The skills of a facilitator required to get a team to work together efficiently and effectively.
• The skills required to construct a model of, and appropriately analyse, the issues which each member of the team wishes to address.

Although an understanding of the situation and knowledge of terminology used in the scenario is important, it is essential that the OR consultant is as interested in designing and managing problem solving workshops as in research and analysis of the problem characteristics.

As with most OR techniques, SODA uses a contingent and cyclic approach to working on the problem, choosing to view the situation from a number of points of view and looking for ways to progress the analysis of the system rather than heading directly towards a solution. The entire process could be viewed as a facilitative device, providing not a solution, but a means of arriving at a solution. SODA has proved useful in situations involving a group of people with differing, possibly opposing, points of view, who all need to agree to a "best" plan of action.

Implementation of SODA requires an initial consultation with each of the parties individually, during which a cognitive map should be designed. This map should illustrate the facts, assumptions, procedures and objectives for the individual. An example is shown in Figure IX-1, in which a water company describes the thinking behind its desire to install an ASR system.

![Diagram](image)

Figure IX-1  Example cognitive map
The cognitive maps produced by each party involved are combined into one model of the situation by the facilitator who then applies appropriate analytical techniques to illustrate similarities in desires, differing assumptions and alternate methods offered by different parties. A workshop at which all interested ‘stakeholders’ should be present is then arranged. At the workshop the facilitator initially describes the cognitive map developed, giving overviews of key goals, interrelated problems, key options and key assumptions. During this process there is little discussion. This ‘first pass’ has two purposes: firstly to indicate that all views have been taken on board, and secondly to begin the process of participants accepting alternative views. A second pass, which is protracted with discussion, should be spent extending the map, elaborating on individual positions and identifying further requirements (e.g. modelling) to the analysis of the problem. The aim of this process should be to either achieve a solution to the problem, or to determine opportunities for further analysis. SODA is a very generalised technique, providing not a solution, but a means of arriving at a solution. The technique is of most use when combining ideas and desires amongst a disparate group of people and finding the best means by which to progress. The facilitator is required to illustrate the problem in clear terms and attempt to introduce a true perspective of each party’s perception of the issues. The situation in which different parties have different desires often arises in hydrogeology and so it could be a useful technique if applied as a means for improving interactions between interested parties. A client, for example, may want the cheapest solution to a contamination problem, a consultancy either the cheapest or the most innovative, whilst the Environment Agency might require the most effective solution. Use of SODA may clarify the desires of each party, and lead to a proposed direction of action, preventing undesired confrontation and non-cooperation.

IX.II. Soft Systems Methodology

Soft systems methodology (SSM) is a useful technique when dealing with problems that have a definable formulation but no obvious solution. Similarly to SODA, SSM is an approach to problem solving rather than a solution provider, giving direction to a group of people who wish to investigate a problem with the view of improving a situation.
SSM involves a seven stage process (Figure IX-2), which may cycle continuously if desired. This cycle may be entered at any stage and repeated, continuously improving the situation, until all parties are satisfied.

**Figure IX-2** Seven stage procedure for SSM. (After Rosenhead, 1989.)

These 7 stages are described below.

- **Stage 1 & 2** involve finding out how to express the problem in a useful and productive manner.
- **Stage 3** involves formulating root definitions of relevant systems in the problem, defining which parties are involved and how, what the system does (how the system transforms the current situation), the Weltanschauung\(^8\) of the system and constraints acting upon it.
- **Stage 4** requires the construction of conceptual models of the problem.
- **Stage 5** involves comparisons between the models and reality.
- **Stage 6** involves using differences between the models and reality to define changes which could bring about possible improvement in the problem situation.

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\(^8\) From the German, 'worldview'. The perception of the world, as defined by previous experience and current circumstance. An individuals Weltanschauung, for example, would be influenced by family, education and the media.
These changes may be to make life approach the model solution, or move away from it, but it is important to ensure that they are both practically and culturally feasible in order for them to be implemented.

- **Stage 7** requires enacting the changes highlighted during stage 6.

Once stage 7 is complete, and the changes have had an affect on the problem situation, the whole process can be repeated if required, continuing improvement of the system.

SSM is a useful method where the problem is reasonably well defined but as yet the solution is unknown. Often a case arises where a group of people combine to discuss a situation, be it the cleanup of a contamination site or the best use of academic funds. Whilst all involved people have an idea of what the situation is, there is no clear solution. Through an iterative process of reviewing the situation and the solution, a conclusion should be arrived at which satisfies all people involved.

An example problem that could be aided by this approach could be the development of Environmental Protection Zone methodology. Whilst the current system is recognised as being too simplistic to accurately simulate real life, an improved methodology would have to incorporate many factors including the accuracy of the modelling, the cost of the data requirements and practicability of application. Recognition of all involved parties would include the environment agencies, who have to determine and implement the zones, the water companies and local industries, who will all have to be aware of the vulnerability of a locality. Obtaining a larger view of the problem and the Weltanschauung of the system would require taking into account public perception, giving a means of explaining clearly and simply the procedure embodied in the methodology, and also consulting lawyers to ensure a method that would be easily enforceable in court. Use of SSM could lead to a coherent strategy for producing a ‘satisficing’ solution.

### IX.1.1. The Strategic Choice Approach

The Strategic Choice Approach (SCA) is a management method for dealing with a problem involving many options and a large amount of uncertainty. It is designed for use in a dynamic decision making process, i.e. one where the decision makers are under a certain amount of pressure due to time constraints. SCA defines three fields of uncertainty, and categorises questions that arise according to these:

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9 See Chapter 7.
1. Uncertainties pertaining to the working environment (UE);
2. Uncertainties pertaining to related decision fields (UR);
3. Uncertainties pertaining to guiding values (UV).

SCA describes four modes of thought involved in the decision making process. As with the other procedures discussed so far, these modes ideally form a cycle, involving continual reassessment of the problem under consideration. In normal conversation, however, it is likely that the flow from one mode to another will involve feedback loops as suggestions by one party inspire responses from another.

The first mode is a shaping process, in which the problem is formulated. Consideration is given as to whether the problem as specified is comprehensive of all important facets, or alternately whether the problem could be broken down into more manageable components. Once the problem has been defined, focus points are decided for urgent consideration (i.e. those affected by the time constraints) and the central points of most importance are highlighted.

While functioning in the second, designing mode, the decision makers are concerned with the possible courses of action available to them. It is important to consider all possible options, removing those that are unfeasible with a systematic approach, involving decision matrices and logic trees. The third mode functions when comparing the feasible options created during the third mode. A series of important areas for comparison are chosen and the options are quantified in each area. The minimum and maximum (e.g. lowest cost/highest cost) options are then highlighted.

Finally, the choosing mode is used. The obvious non-optimal options are removed and the rest are analysed, highlighting the importance of and the type of uncertainty (UR/UV/UE). These uncertainties are then quantified, describing how much a possible solution to the uncertainty would exacerbate or eliminate the risk involved in this option (here ‘robustness’ should be considered, see later) hopefully with the result of highlighting an optimal course of action.

Hydrogeology suffers greatly from uncertainty, including the exact parameters describing rocks and groundwater flow (UE), the predicted behaviour of parties involved in any situation (UR) and how the public will react to any change in water supply (UV). This method is suitable for use when a number of possible solutions have been determined, and the optimal one must be selected. A water resource system stretched to capacity at peak demand could be relieved in a number of ways, including transporting water, building a reservoir or developing an ASR system.
SCA methodology would allow a subjective assessment of each solution, and help in the identification of an optimal solution.

**IX.IV.  Metagame and Hypergame analysis**

Game analysis views any situation as a game (a model of interactive decisions) which can include of actors who have: aims; strategies and preferences; a series of options and outcomes; promises and imposable sanctions. Metagame analysis is a method managers can use to determine the best course of action in a situation involving conflict. By visualising the problem from each person’s point of view, and determining all conceivably likely scenarios a solution can be arrived at. The approach is a Socratic system where leading questions are asked to determine all aspects and possible solutions to the problem. This method is best implemented with the help of computer software, such as CONAN, in order to allow rapid analysis and presentation of results in a meeting situation. Hypergame analysis takes this procedure further by viewing actors as being involved in their own game.

**Metagame Procedure**

The initial step in Metagame analysis is to describe a scenario, highlighting all actors and the various options they have. Through the interplay of these actors, their options and the imposition of sanctions or the offer of promises a series of scenarios can be generated, often using a computer to systematically work through all options. The feasible scenarios are then highlighted and classified according to desirability. Finally, once the optimum feasible scenario is highlighted, plausible approaches to achieving this outcome can be outlined.

**Hypergame procedure**

Hypergame analysis recognises the fact that actors have their individual ideas. Not only do they each have their own preferences, but they may also believe differently about the preferences and strategies of other actors. Initially the model is laid out, either as a matrix or, if the sequence of decisions is important, on a tree diagram. This model can become very complex so simplification of all but the most essential facets of the examination can be required. Once described, all the options are worked through systematically, generating a series of scenarios. These can then be analysed, each in turn, to identify the optimal solution.

**Application**
Metagame and Hypergame analysis are useful in a confrontational scenario where a manager really needs to see the whole picture to determine not only his ideal solution, but also how to act to achieve that goal, game analyses are a way of structuring a problem in a clear manner. Ideally suited to dealing with personnel, this approach is limited in its use within a technical scenario.

IX.V. Robustness Analysis
Every decision limits the number of possible future outcomes available to the decision-maker, therefore when choosing it is important to ensure that any decision made does not overly limit future possibilities and so is robust. Robustness analysis provides an approach to the structuring of problem situations in which uncertainty is high, and where decisions can or must be staged sequentially. It identifies the options in decisions early in the sequence that, relative to other choices, will keep open a wide range of options for the future.

Procedure
The procedure of robustness analysis is very simple. After identifying the resources that are available prior to the decision making process (e.g. an inventory) and the impending commitments (i.e. urgent decisions) a brief summary is made of all possible outcomes that are satisfactory, taking account of the effect of alternate futures resulting from events beyond the decision makers control. This summary may be simplified if the problem becomes too extensive. The possible outcomes are then rated as to their desirability and then listed against the decision options. The robustness of each decision option is the ratio of the number of attainable outcomes if the decision option is taken to the number included in the total set of possible outcomes. From this it is possible to compare the various decisions and their outcomes in a number of situations. The decision-maker can then balance the probabilities of the positive outcomes of varying desirabilities to the negative outcomes and base their decision on this.
Figure IX-3 Procedure of robustness analysis (After Rosenhead, 1989).
The robustness of decision-set $d_i$ in future $F_j$ can be defined as

$$r_{ij} = \frac{n(S_{ij})}{n(S_j)}$$

where $r$ is the robustness, $S_{ij}$ is the full set of solutions incorporating $d_i$ which are acceptable under $F_j$, $S_j$ is the set of all full solutions acceptable under $F_j$ and $n(S)$ is the number of elements in set $S$. Values of robustness are relative. It is therefore meaningless to determine an optimal solution and verify this by determining a value for the robustness of that solution.

More complex forms of analysis place emphasis on the differing import of future outcomes. If complex analyses are performed, different forms of analysis are be useful in different scenarios. Four cases are distinguished:

1. **UE and UR both low.** Robustness analysis may be inappropriate. Other approaches such as sensitivity or risk analysis may be more suitable;
2. **UE high, UR low.** Single future robustness analysis may be sufficient, if coupled with sensitivity analysis;
3. **UE low, UR high.** The preservation of options that are acceptable across futures may be more important than the preservation of options within futures;
4. **UE and UR both high.** The full matrix of robustness scores ($r_{ij}$) is relevant.

It is very important in any field of work to try not to limit oneself through a bad choice of action. Frequently events do not pan out as predicted, and in this scenario it is essential that we can cope with the unexpected. By using robustness analysis in our choice of options we are attempting to insure ourselves against the unpredictability of the future so that whatever happens we still have positive choices leading to a successful if not necessarily optimal conclusion.

Within the field of hydrogeology robustness could be used to provide essential aid in the development of almost all projects, for example wellfield design, where options including later expansion and flexibility of use are important and must be taken into account.
Appendix X. Attachment: Compact Disk containing water chemistry data and the code for DP-Pulse (Version 1)