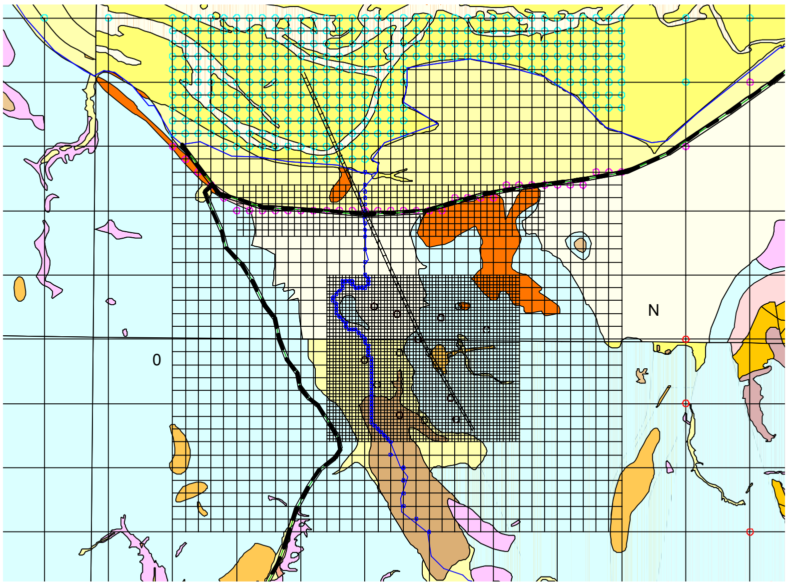
Business and scientific case for the development of an object-oriented groundwater model

Groundwater Systems and Water Quality

Commissioned Report CR/03/065N

National Groundwater and Contaminated Land Centre

Technical Report NC/01/38/3



BRITISH GEOLOGICAL SURVEY
Commissioned Report CR/03/065N

ENVIRONMENT AGENCY
National Groundwater & Contaminated Land Centre
Technical Report NC/01/38/3

Business and scientific case for the development of an object-oriented groundwater model

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Environment Agency Dissemination status
Internal: Release to Regions
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Project No. NC/01/38

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This document presents the business and scientific case for the development of an object-oriented groundwater model.

Cover illustration
Example prototype object-oriented groundwater model grid

Bibliographic Reference
Jackson, C.R., Hulme, P.J. & Spink, A.E.F. 2003. Business and scientific case for the development of an object-oriented groundwater model British Geological Survey Commissioned Report No. CR/03/065N

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Groundwater Systems & Water Quality Programme

National Groundwater & Contaminated Land Centre, Solihull 2003
British Geological Survey, Keyworth, Nottingham 2003

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Acknowledgements

This business and scientific case has been written as part of a continuing tripartite collaboration between Dr A. Spink of The University of Birmingham, the Environment Agency, represented by S. Fletcher and P. Hulme of the National Groundwater and Contaminated Land Centre and The British Geological Survey. The project has been co-funded by the Environment Agency's National Groundwater and Contaminated Land Centre and The British Geological Survey.

Summary

A new technology is set to transform the development and capabilities of models used for hydrological simulation. The approach is rapidly becoming popular because it enables applications to be developed that incorporate a high degree of complexity but which are accurate, easily modifiable, and easy to use, in addition to having a clear structure. The approach is that of the *object-oriented paradigm*.

Object-orientation offers the potential to solve many of the problems associated with existing modelling tools, which are used for the assessment and management of the water environment. The major benefit of the approach is that it enables applications to be developed which focus on physical processes and mechanisms. That is, it is now realistic to envisage the development of models that are constructed around hydrological or hydrogeological features. It should no longer be considered acceptable to 'fit' engineering problems into the fixed frameworks of current models. Tools can now be developed that enable user's to investigate processes rather than just being able to define parameter values.

The core principle of object-oriented model development is the reproduction of real-world features as computational equivalents. For example, considering a number of scales, aquifers, river catchments, wetlands or pumped wells could be defined as objects, each containing a complex but well defined behaviour. In particular, wetlands are generally simulated inadequately in existing models. Compared to current techniques it would be relatively straightforward to incorporate a number of different conceptual models of wetlands and detailed wetland processes in an object-oriented model.

Whilst object-orientation is a method for developing models, the approach offers major benefits to hydrogeological and hydrological simulation and management. This document presents a business and scientific case for the development of an object-oriented groundwater model. The objective of the work is to develop a high quality, publicly available piece of modelling software which simulates regional groundwater systems but which provides a platform for the eventual development of an integrated model of the *hydrological cycle*. The central principle of the development is to focus on physical processes. That is, to identify hydrogeological features or mechanisms which are represented inadequately, or not at all, in current models and then to construct computational equivalents. These will be incorporated into the overall object-oriented hydrogeological/hydrological model framework.

The development of the model incorporates three important objectives. First, the resulting model must be as good as existing groundwater models. Second, central to the model development is the goal of developing a tool that enables the simulation of hydrogeological features that are dealt with inadequately in existing groundwater models. Finally, the resulting model must be widely applicable to the management of UK groundwater and surface-water resources considering the prominent environmental management issues of the next twenty years. The model development will address:

- The accurate numerical representation of conceptual hydrogeological models with the objective of developing models that closely resemble hydrogeological systems instead of adopting the current approach of fitting hydrogeological understanding to the restricted structure of groundwater models.
- The detailed representation of wetlands with regard to the accurate simulation of aquifer-wetland interaction and the impact of groundwater abstraction of surface water flows.
- The accurate simulation of groundwater abstraction and rivers at the local scale within a regional context. The need to develop tools to accurately analyse the impact of abstraction on rivers, for example within Catchment Abstraction Management Strategies, to improve

the evaluation of abstraction licence applications and source protection zones, to accurately simulate pumped wells, well fields and artificial recharge schemes and to model river-aquifer interaction at the channel scale is central to the philosophy of the model development.

- The development of a user-friendly GIS based recharge model, which is fully integrated with the groundwater model.
- The development of an integrated object-oriented solute transport model for the simulation of contaminant transport in UK aquifers, for example, with regard to transport in dual porosity media such as the Chalk.
- The utilisation of the benefits of novel computing technology for the development of user-friendly hydrogeological modelling and management tools.

A prototype groundwater model has been developed which represents a first attempt at designing and implementing a framework of objects, which accurately represents the structure of common hydrogeological features within a regional groundwater model. The development of the model has been achieved through the collaboration of The Environment Agency, The British Geological Survey and The University of Birmingham. This has brought about the opportunity to steer the progress of modelling both within the UK and internationally. The recognition of the benefits of object-orientation by the project group is timely. The approach offers the potential to integrate tools for the simulation and management of water resources, water quality and ecology with the framework of the hydrological cycle. This project represents the beginning of that process but will significantly advance our ability to model, understand and manage the water environment.

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Document Structure

The document is split into two parts. In Part One the need for a new modelling approach with regard to water resource management is defined. The benefits of the object-oriented approach for the simulation of hydrological and hydrogeological systems are put in the context of prominent scientific issues, such as the Water Framework Directive, the CAMS process, the Habitats Directive and the management of wetlands. The project is split into a number of subtasks. The drivers for each task are described in addition to the resulting benefits and deliverables.

In Part Two more comprehensive information is presented regarding, the philosophy and advantages of object-oriented modelling, the current deficiencies of existing models and a vision of the future.

PART ONE

1 Water Resources Management

In the Environment Agency Framework for Groundwater Resources Conceptual and Numerical Modelling (Environment Agency, 2001) the following groundwater and surface water flow mechanisms are listed as critical in determining the effect groundwater abstraction has on the environment:

River/aquifer interactions. This area is the subject of current research programmes (e.g. CHASM and LOCAR).

Wetlands. There is considerable uncertainty concerning how groundwater interacts with the variety of wetland types that exist in England and Wales. Because of the potential complexity of the relationship it may be that this interaction can only be modelled with detailed local models. However, regional time-variant models must take into account the inflows and outflows of local wetland models if resources are to be assessed accurately.

Drift. Drift deposits significantly complicate the modelling of groundwater systems due to the variability of the sediments within them. These sediments may act to delay recharge to the aquifer or they can act to route precipitation away to recharge the aquifer elsewhere.

Recharge. This is the subject of an ongoing research project that is aimed at developing a consistent methodology for estimating recharge. Recharge is the largest part of the water balance and the input to which groundwater models are often most sensitive. It is therefore critical that the mechanisms of recharge in a catchment are recognised and quantities accurately estimated.

In the report referred to above, the potential to develop new codes based on the latest software development techniques (e.g. object-oriented code) is noted and it is recommended that the Environment Agency should take an interest in such developments on the condition that these new codes will be in the public domain, rather than proprietary. The advantage of the code being in the public domain is that it can be investigated, tested and improved by a large number of experts. This increases confidence in the code since all its features are public knowledge which is important when such models are used to back up regulatory decisions.

There are several pieces of legislation which will prompt the Environment Agency to look for methods of representing the above flow mechanisms with more confidence. These are:

Water Framework Directive. This will require integrated management of surface water and groundwater both in terms of resources and quality and their impact on ecology. The object-oriented approach allows surface water flow mechanisms, such as recharge through drift and unsaturated zone flow to be incorporated within the groundwater model. Simple objects can be used initially and further refined as understanding develops.

The ultimate aim of the Water Framework Directive is to return all bodies of groundwater to good status where practical. A programme of measures is required to achieve this. It is likely that that this programme will evolve alongside existing abstraction and discharge regimes with consequent financial implications for water companies and industrialists. Hence it is vital that both the regulator and the regulated have confidence in the understanding and simulation of the system if confrontation is to be avoided. This confidence is best built up via a stepwise approach; firstly, identifying where there is a risk of failing to meet good status and then establishing the possible causes, testing them and finally designing a solution. An object-oriented approach allows us to do this stepwise testing of conceptual models more readily than do existing procedural codes.

Habitats Directive. Mechanisms operating in wetland sites need to be studied using relatively dense monitoring networks to establish groundwater and surface water flows. Existing regional scale groundwater models cannot represent the local flow mechanisms operating within for example a wetland without setting up a sub-model with approximate boundary conditions. The object-oriented code allows grid refinement of the regional model itself in the areas of local interest only so that only one model needs to be run and boundary conditions are exact.

Catchment Abstraction Management Strategies (CAMS). The capability to confidently predict the impacts of groundwater abstractions on river reaches is an essential component of the Resources Assessment and Management (RAM) framework which the CAMS process uses to produce its water resources assessments. The current methods utilise analytical solutions which involve significant approximations (such as an infinite aquifer) and cannot predict the impact on more than one river reach. Object-oriented methods would allow an investigative tool to be developed for sensitive situations where the analytical methods are inadequate.

Abstraction Licensing. Current regional groundwater models developed by the Environment Agency, often in collaboration with Water Companies, cannot accurately represent the local effects of abstraction around the pumping wells themselves. The grid refinement capability and the potential to include a radial grid into the object-oriented code would mean that water companies could use the same regional model for management of its sources that the Environment Agency is using for its water resources and impact assessments.

The use of models as investigative tools within studies driven by such legislation will highlight further the deficiencies of our current modelling tools. Current simulation models of environmental systems are generally difficult to maintain, modify and integrate. However, advances in computing technology have resulted in the capability to develop numerical simulation models that can closely resemble the conceptual models of environmental systems. Object-orientation now enables hydrologists, hydrogeologists and modellers to address the failings of current simulation and management tools. The use of object-oriented methods presents the opportunity to develop the tools that will be required to find solutions to the problems of water resource management that are likely to be encountered during the implementation of new legislation.

The object-oriented approach can be used to develop models that address the failings of current tools and which can be formulated to incorporate management goals because it focuses on physical processes and mechanisms. For example, it is now possible to develop models that are constructed around hydrological or hydrogeological features. By representing real world features as separate entities, complex models can be developed which are clear, easily modifiable, flexible and efficient. Because complex behaviour can be hidden in discrete objects, the opportunity exists to develop models of hydrogeological features that are represented poorly in existing models.

2 Project Programme

2.1 OBJECTIVES

As described in the previous section the object-oriented approach provides a framework for the development of a model that closely resembles the hydrological cycle. It enables a vision to be formulated in which disparate and unrelated models of individual elements of the hydrological cycle are brought together within a consistent methodology. That is, object-orientation allows the development of a model with a structure that is similar to the hydrological cycle. In addition to this, the method allows the development of components that both describe and undertake the management of the hydrological cycle.

By decomposing complex hydrological and hydrogeological systems into discrete components or *objects*, a model can be developed which is accurate, efficient, flexible and easily modifiable. Complex processes and functionality can be incorporated in objects without damaging the clear representation of the hydrological cycle within the model. Considering this vision, the aim of this work is to develop a framework of objects that represent the groundwater component of the hydrological cycle. The work will focus on the development of modelling tools that advance our capability to simulate and manage components of groundwater systems. The structure of the groundwater model will enable other objects to be added easily when the need arises. For example, it is envisaged that objects can be developed later that define a strategy for the management of an aquifer, such as information relating to catchment abstraction management schemes. These objects could be given the ability to run the model and examine the effect of different management decisions.

An object-oriented regional groundwater model code has already been developed by the project partners. This has a number of benefits over other regional groundwater modelling codes but presents the opportunity to significantly advance our groundwater modelling capabilities. This project aims to develop this model code to progress UK groundwater modelling significantly. The project addresses issues relating to the accurate simulation of wetlands, abstraction boreholes and their influence on rivers and the irregular geometry of hydrogeological entities such as sinuous river valley gravels. With regard to the wider hydrological cycle, an object based recharge model will be developed using GIS technology. This could be a component of the broader object framework. Each of the proposed developments is described in detail in the following subsections. The benefits arising from each task are defined in addition to costs. Each sub-project will contribute to the overall goal of the work, which is to produce a model for the UK and international modelling communities that:

- can be used to further our understanding of hydrogeological processes
- more accurately represents hydrogeology
- is clear, easily modifiable, flexible. That is changes can be made easily and rapidly without the affecting the integrity of the rest of the model code
- is efficient
- forms the basis of the future development of hydrogeological modelling in the UK
- is a valuable tool for hydrogeological research and groundwater management

2.2 BENEFITS

There are many benefits associated with the development of the object-oriented modelling tools proposed in this Business and Scientific Case. These relate to both the advancement of the capabilities of models and to the development of tools to address current prominent scientific issues that are set to effect the management of the United Kingdom's water environment. A major benefit of the work outlined here is the co-operation between the three participating organisations. The collaboration of The Environment Agency, The British Geological Survey and The University of Birmingham presents the opportunity to develop tools that form an integrated approach to water resource and quality management and that address the UK's needs.

This proposal addresses issues relating to the management of the water environment, the improved conceptualisation of hydrological and hydrogeological features and the development of better simulation and management tools. The benefits of the project are discussed next in relation to these themes.

Benefits to water resource management
A major objective of the work is to develop tools that address prominent issues relating to the management of the UK's water resources, for example, the role of models in the implementation of the Water Framework Directive. Considering this theme of improving the management of the water environment, the project will produce the following benefits.

- The opportunity for the collaborating partners to develop tools, which address their operational needs with regard to the management of surface-water and groundwater systems within the context of the Water Framework Directive, Catchment Abstraction Management Strategies and the Habitat's Directive, for example.
- The potential to integrate tools for the simulation and management of water resources, water quality and ecology within a consistent framework by combining detailed component models of individual elements of the hydrological cycle, for example, wetlands.
- The opportunity to direct the progress of groundwater modelling both in the UK and internationally.
- The creation of a platform for the continued development of simulation and management models as requirements change.
- The development of models that focus on physical processes and mechanisms.
- The production of a globally available piece of modelling software focusing on the needs of the UK hydrological and hydrogeological modelling community but which also advances international modelling capabilities.

The accurate representation of conceptual models
The object-oriented approach can be used to circumvent problems associated with poor representation of conceptual hydrological and hydrogeological models in numerical models. The capability now exists to develop numerical simulation models that can closely resemble the conceptual models of environmental systems. The benefits of the accurate representation of conceptual models in a numerical framework are:

- The ease of transfer of conceptual models into numerical models. The removal of the need to 'fit' conceptual models of groundwater systems to the limited structure of numerical models. It should no longer be considered acceptable to fit engineering problems into the fixed frameworks of current models.
- The opportunity for the collaborating organisations to review the approach to the simulation of hydrogeological features. Where these methods are found to provide an

unsatisfactory understanding of a physical process, detailed conceptualisations of these features can be developed and incorporated easily into the object-oriented model framework.

- The reproduction of real-world features as computational equivalents simplifies the investigation of physical processes. The equivalence between computational and hydrological/ hydrogeological objects will enhance the interaction between model and developers and between hydrogeologists and groundwater modellers.
- The approach enables applications to be developed that incorporate a high degree of complexity but which are accurate, easily modifiable, and easy to use, in addition to having a clear structure.
- The approach increases the potential of users to investigate aquifer behaviour by examining different mechanisms instead of just modifying parameters.
- Complex processes and functionality can be incorporated in objects without damaging the clear representation of the hydrological cycle within the model.
- The opportunity to improve the representation of irregular hydrogeological features, such as sinuous valley alluvial deposits, sedimentary layers which thin out, faults and their adjacent hydrogeological units or clay lenses. These are very difficult to simulate using existing groundwater models. The approach will produce flexible, efficient and easily modifiable methods by which complex hydrogeological systems can be modelled numerically without restriction.

Accurate representation of individual hydrogeological mechanisms

Because objects can be developed to encapsulate complex behaviour or functionality they can be used to formulate detailed representations of hydrological/hydrogeological features. The approach presents the opportunity to:

- Simulate wetlands in detail within a regional context. This could entail the incorporation of multiple wetland conceptual models in a numerical model and enable the accurate simulation of aquifer-wetland interaction and the impact of groundwater abstraction on surface-water flows.
- Accurately simulate groundwater abstraction and rivers at the local scale within a regional context. This would be beneficial for the evaluation of the impact of groundwater abstraction on surface-water features, for example within the CAMS process, for the evaluation of abstraction licence applications and source protection zones and for the detailed simulation pumped wells, well fields and artificial recharge schemes.
- Develop a user-friendly object-oriented recharge model, which is fully integrated with the groundwater model.
- Develop an integrated object-oriented solute transport model for the simulation of contaminant transport in UK aquifers, for example, with particular regard to transport in dual porosity media such as the Chalk.

Accurate representation of pumping wells

Again because of the capabilities of objects, pumping wells could be represented in detail within a regional context. This would enable:

- The accurate simulation of pumped wells at the borehole scale in regional systems.
- The accurate representation of the impact of groundwater abstraction on wetlands, river and springs.
- The development of improved tools for the evaluation of abstraction licence applications.

- The improved definition of borehole catchments and source protection zones.
- The accurate and rapid analysis of pumping tests in complex systems.
- The accurate simulation of the operation of well fields and their impact on regional flows.
- The development of better tools for the identification of the benefits and impacts of artificial recharge schemes.

Simulation of aquifer features at the local scale
Local grid refinement has been implemented in a prototype groundwater model that has been developed by the project partners. This enables the simulation of some aquifer features at the local scale within a regional system. The further development of these techniques is proposed in order to:

- Accurately simulate rivers at the channel scale within a regional system.
- Simulate pumped wells at the borehole scale within a regional system.
- Simulate wetlands at the local scale within a regional system.

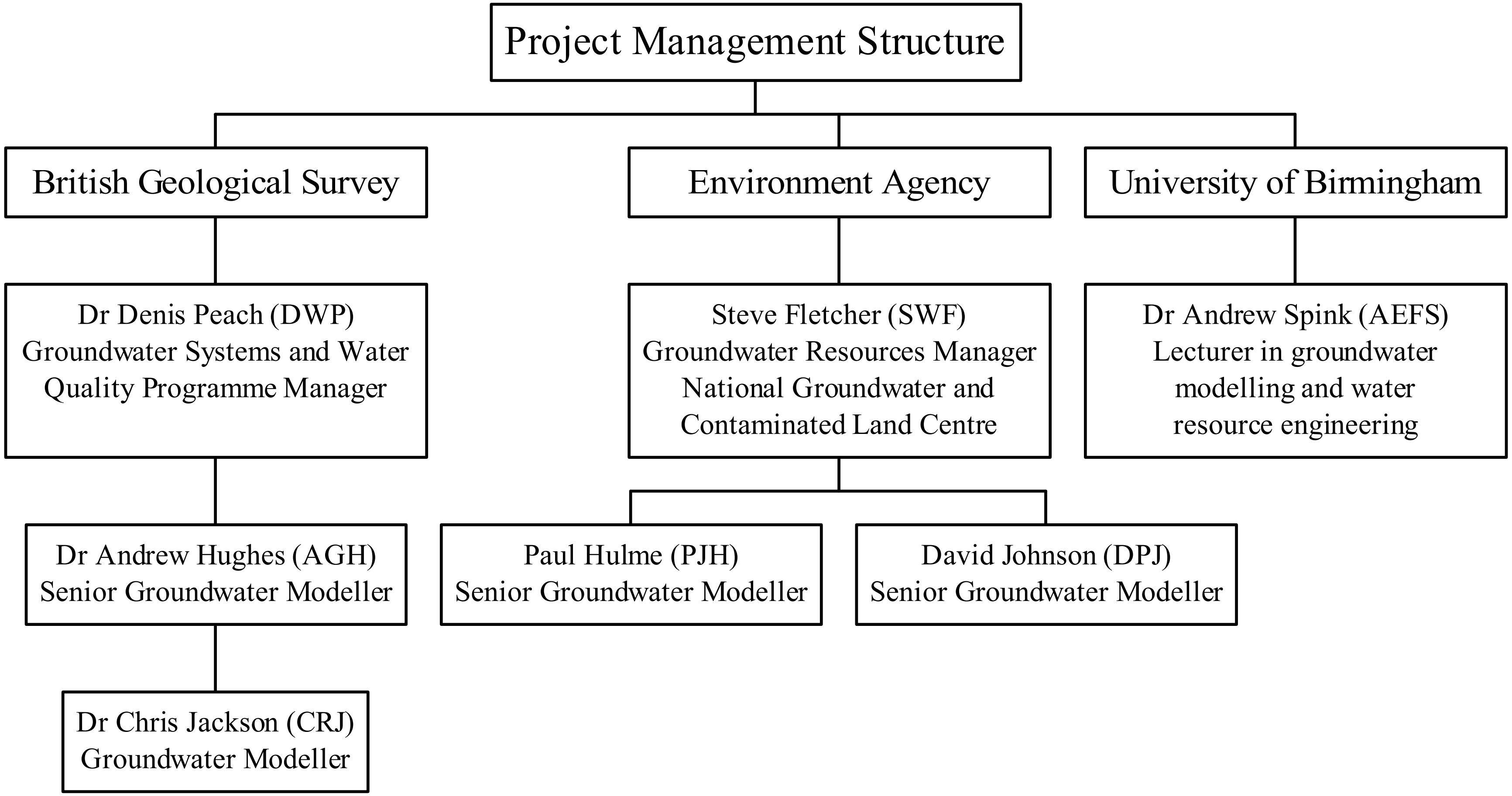
Separation of real and model data
It is proposed that techniques should be investigated to separate the storage of real data and model data. This would:

- Facilitate rapid model construction and modification. Graphical information systems (GIS) are powerful tools for the storage, management and visualisation of spatial data and these are in common use. GIS packages have only been used recently in conjunction with groundwater models but could significantly simplify the process of model development and application.

Benefits of the model code
In addition to the benefits that the object-oriented approach offers to environmental modelling and management the approach has many intrinsic benefits when considering the development of software:

- The object-oriented framework will form a platform for continued model development. A benefit of the use of object-orientation is its flexibility. Because, the system being modelled is broken into well-defined components, the model framework will be relatively easy to modify and develop over time.
- The code will be more easily modified than current models and the subsequent need for extensive model testing will be reduced.
- The incorporation of change will not be a major task because of component nature of code.
- The encapsulation of the functionality in objects means that it is easy to modify the behaviour of a hydrological/hydrogeological entity without creating errors elsewhere in the program. That is, because there are fewer dependencies between different parts of the model code it is easier to modify.
- The approach facilitates the application of novel computing technology to reduce run times and enable more detailed models of hydrogeological systems within a given computational budget
- The approach will prolong the life of the model code.

2.3 PROJECT MANAGEMENT ORGANOGRAM



2.4 PROJECT TASKS

2.4.1 Task 1: Accurate representation of hydrogeological features and processes

This task is central to the development of the object-oriented groundwater model. The work relates to the objective of producing a model that accurately represents conceptual groundwater models and which stops modellers fitting hydrogeological problems to the structure of groundwater models. In contrast the philosophy is to develop a model that can be tailored to complex aquifer systems. With respect to the aim of producing a model that better represents hydrogeology, it is conceivable that more than one model framework could be produced. Considering UK hydrogeology, it may be beneficial to develop different frameworks for different aquifers, for example for chalk, limestone or sandstone aquifers. The need for different frameworks will depend on the conceptualisation of groundwater flow within the different geological units because hydrogeology must determine the structure of the model. This is in contrast to most current approaches in which the structure of the system being modelled is fitted to the structure of the programming language used. The task of developing the object framework(s) will employ the expertise of both hydrogeologists and groundwater modellers.

In addition to investigating the benefits of the object-oriented approach to more accurately represent conceptual groundwater models, its potential for better representing the irregular geometries of hydrogeological units will be examined. The current approach of using horizontally continuous layers to model aquifer units is limiting. Different methods of model discretisation will be investigated with the objective of developing more flexible schemes, which better fit irregularly shaped hydrogeological entities. For example, the use of objects to represent sinuous valley alluvial deposits, sedimentary layers which thin out, faults and their adjacent hydrogeological units, clay lenses, and perhaps even individual fractures will be investigated. The implementation of such model features will be investigated through the development a two dimensional vertical slice model. This slice model will provide a tool for the accurate simulation of complex aquifer systems but will more importantly provide insights in the incorporation of hydrogeological complexity in a fully three dimensional groundwater model (see Section 5.4.1). A possible approach by which heterogeneity could be described more simply within a model could be the definition of objects that represent *hydrogeologically uniform entities*. Such entities could be constructed as discrete components and 'plugged' together to form a model of a groundwater system. Such an approach would circumvent the problems associated with the unrealistic description of aquifers as continuous layers. The layered approach often produces severely distorted vertical grids for which it is necessary to adjust the hydraulic parameters to represent the aquifer adequately.

Benefits

- Flexible, efficient and easily modifiable methods by which complex hydrogeological systems can be modelled numerically without restriction.

Deliverables

- 2D vertical slice model capable of representing complex aquifer geometries and processes.
- Report on the methods by which complex aquifer systems should be represented in a fully three-dimensional groundwater model, incorporating the findings from the development of the slice model.

Staffing

		Allocation Days	Cost £	
UoB	AEFS	30	12000	**12000**
EA	SF	5	2900	**6500**
	PJH	5	1800	
	DPJ	5	1800	
	Modeller			
BGS	DWP	5	2905	**6160**
	AGH	5	1815	
	CRJ	5	1440	
	SSO			
	HSO			
	SO			
	Total	**52**	**20016**	

2.4.2 Task 2: Representation of the conceptual models of wetlands as objects

The effect of natural and anthropogenic influences on wetlands is an issue of concern. Wetlands are complex systems incorporating a number of physical processes, such as, wetting and drying, evapotranspiration, vertical and horizontal seepage flows, surface channel flows and wetland-aquifer interaction. Furthermore, the conceptualisation of wetlands can vary significantly between sites. Because of the inherent complexity of wetlands, they are generally represented poorly in numerical models. For example, wetlands are often simulated using simple head dependent outflows. However, the use of object-oriented techniques now enables the detailed but straightforward representation of multiple conceptualisations of wetlands in a numerical model.

The objective of this sub-project is to examine the way in which wetlands are conceptualised and to define how these can be incorporated into the groundwater model. A wetland simulation component will be added to the existing regional groundwater model, ZOOMQ3D. The work will start with a detailed review of the current approaches to wetland simulation and an examination of the relevant information held by the collaborating partners. This will result in the definition of a series of wetland conceptual models. A suite of objects will then be developed to simulate the detailed structure and processes operating in wetlands. These will be integrated into the groundwater model and will enable wetlands to be simulated at the local scale within a regional system. The expertise of The Environment Agency will be crucial to the development of the wetland conceptual models. It is expected that a number of different conceptual models will be identified, though these may contain common components, such as surface channels or sedimentary layers.

The most important wetland conceptual model will be transferred into the numerical groundwater model. However, the object framework will be developed so that additional wetland conceptual models or components can be added easily and efficiently.

Deliverables

- The incorporation of an object-oriented wetland simulation component in the regional groundwater model, ZOOMQ3D.
- Documentation of the development of the conceptual wetland models and their representation as objects.
- User's guide for the simulation of wetlands using the modified ZOOMQ3D model.
- Recommendations for the future development of the object-oriented wetland components.

Staffing

		Allocation	Cost	
		Days	**£**	
UoB	AEFS	5	2000	**2000**
EA	SF	2	1160	**17060**
	PJH	10	3600	
	DPJ	10	3600	
	Modeller	30	8700	
BGS	DWP	2	1162	**11617**
	AGH	5	1815	
	CRJ	30	8640	
	SSO			
	HSO			
	SO			
	Total	**94**	**30677**	

2.4.3 Task 3: Accurate representation of pumping wells in regional models

Pumping boreholes are poorly represented in regional groundwater models. However, large-scale models are often used to examine, for example, the impact of abstraction on rivers or wetlands. The conflict between the need to model processes accurately whilst modelling large systems will be addressed by the development of a specially embedded pumping well object. This will have realistic pumped well characteristics as part of its structure. R-theta-z co-ordinates have many advantages over Cartesian co-ordinates when simulating pumped wells. Research will be undertaken to identify a method by which a detailed radial flow model can be embedded into a regional model which uses a Cartesian system. The present situation is that reliable and detailed work relating to wells can be conducted using a radial approach but great difficulty is faced when behaviour relating to regional influences, such as recharge or rivers, needs to be addressed. Such developments have not been made previously and would address a serious failing of current models.

Benefits

A number of benefits would result from the realistic representation of pumped wells in regional models. These would include:

- The accurate representation of the impact of groundwater abstraction on wetlands, river and springs.
- The improved definition of borehole catchments and source protection zones.
- The ability to accurately and rapidly analyse pumping tests in complex systems.
- The accurate simulation of the operation of well fields and their impact on regional flows.
- Improved tools for the evaluation of abstraction licence applications.
- Better tools for the identification of the benefits and impacts of artificial recharge schemes.

Deliverables

- The incorporation of the pumping well object in the regional groundwater model, ZOOMQ3D.
- Documentation of the development of the pumping well object.
- User's guide for the simulation of abstraction boreholes using the modified model.
- Updated particle tracking code for use with mixed radial-Cartesian grid models.

Staffing

		Allocation Days	Cost £	
UoB	AEFS	20	8000	**8000**
EA	SF	1	580	**2380**
	PJH	5	1800	
	DPJ			
	Modeller			
BGS	DWP	1	581	**31196**
	AGH	5	1815	
	CRJ	100	28800	
	SSO			
	HSO			
	SO			
	Total	**132**	**41576**	

2.4.4 Task 4: Development of a GIS and object based recharge model

Powerful tools for the storage, management and visualisation of spatial data are graphical information systems (GIS) and these are in common use. GIS packages have only been used recently in conjunction with groundwater models but offer major benefits to groundwater modelling. In addition to the storage of data, some GIS packages can be customised to perform user-defined tasks. For example, ArcView, the most commonly used GIS package, allows new functionality to be added using an object-oriented technology (COM). This is compatible with the object-oriented language used to develop the groundwater model, ZOOMQ3D. COM technology allows the construction of separate objects that can be 'plugged' together to form applications. The use of COM by ArcView8.1 and its ability to be customized using object-oriented programming languages means that it is well suited for combination with the object-oriented groundwater model.

The objective of this sub-project is to use a GIS package for construction of a time-variant distributed recharge model. The approach will be to use GIS software to store, manage and calculate areally distributed recharge whilst employing object-oriented technology to link the recharge and groundwater models. In summary, the aim is to develop a tool that will facilitate the easy transfer of information between the recharge model and the groundwater model. The medium term vision of the use of GIS for recharge calculation is to formulate rainfall, evapotranspiration, surface run-off and soil-moisture balance processes as objects within the GIS code if possible. Recharge can be calculated using a number of methods and these could be written as objects within ArcView, for example. The initial task will be to assess the ease with which recharge processes can be represented in a GIS. This may lead to the development of a recharge model, which closely resembles the physical structures through which recharge occurs. However, if this is identified as being a major task, a recharge model will be developed that calculates distributed recharge using more standard techniques. This will still be compatible with the groundwater model but employ the capabilities of a GIS to store and manage spatially variable data.

Benefits

- The construction of a grid independent, generally applicable recharge model, which incorporates the conceptual understanding of groundwater recharge in UK aquifers.
- A platform for the future development of recharge models within The Environment Agency and The British Geological Survey.

Deliverables

- A GIS based recharge model that is fully compatible with the object-oriented groundwater model.
- Documentation on the application and use of the recharge model.

Staffing

		Allocation	Cost	
		Days	£	
UoB	AEFS	2	800	**800**
EA	SF	1	580	**18630**
	PJH	5	1800	
	DPJ	25	9000	
	Modeller	25	7250	
BGS	DWP	1	581	**18296**
	AGH	25	9075	
	CRJ	5	1440	
	SSO			
	HSO	25	7200	
	SO			
	Total	**114**	**37726**	

2.4.5 Task 5: Channel scale representation of rivers in regional models

As with abstraction wells, rivers are often represented in models at scales, which are very different from that of their real dimensions. For example, in conventional models, due to the inflexibility of mesh refinement, rivers are frequently represented as features, which are hundreds of metres wide. This problem is a result of the conflict between model accuracy and efficiency. To solve this problem, methods will be investigated to represent rivers at the channel scale within regional groundwater models. This will involve the development of numerical schemes that can refine the model grid along irregular one-dimensional river channels from the regional to local scale. The development will use object-oriented techniques to construct a more accurate representation of the groundwater-surface water model interface.

The approach to the development of the current object-oriented groundwater model has been to separate models of parts of the hydrological cycle within objects. This philosophy will be maintained. The objective is to develop a surface water model object and a groundwater model object. Though these will be distinct components they will interact dynamically. For example, it may be the case that the surface water and groundwater models can be run simultaneously and interact but that they use different time-scales.

Benefits

- The ability to simulate river-aquifer interaction at the channel scale within regional models.
- Improved representation of the impact of abstraction on river flows

Deliverables

- Updated river model object with the capability to model river-aquifer interaction at the channel scale within a regional context.
- Documentation on the simulation of rivers using the modified ZOOMQ3D model.

Staffing

		Allocation	Cost	
		Days	£	
UoB	AEFS	10	4000	**4000**
EA	SF	2	1160	**10560**
	PJH	5	1800	
	DPJ	5	1800	
	Modeller	20	5800	
BGS	DWP	2	1162	**22072**
	AGH	10	3630	
	CRJ	60	17280	
	SSO			
	HSO			
	SO			
	Total	**114**	**36632**	

2.4.6 Task 6: Investigation of the benefits of parallel and distributed computing and COM technology in environmental modelling

With regard to the long-term aim to develop a comprehensive model of the hydrological cycle, the use of advanced computing techniques is highly desirable. Consider the vision of the future development of the model in which separate models of parts of the hydrological cycle are run simultaneously but which interact. The application of techniques for the efficient simulation of such a distributed system would be highly beneficial, however, most existing models do not take advantage of current computing technology. In effect, the opportunity to simulate complex system in detail is hindered by the limited use of novel computing technology.

Two areas of investigation will be undertaken within this task. The first area of investigation will be the examination of distributed computing technology and the application of COM. COM and distributed computing technologies have two potential benefits. First, COM facilitates the development of simulation components, which can be 'plugged' together to construct hydrological models. It is conceivable that the user could pick a series of self-contained COM components from a list in order to construct a model. This would enable rapid model development and promote the reuse of code between different simulation models. Furthermore, as many commercial software packages are COM compliant, for example ArcView, the technique allows the use of such tools for improved hydrological modelling and management. As previously stated, the use of COM could enable the development of a distributed object-oriented, time-variant recharge model within a GIS. The second benefit of distributed computing is that it can enable significant gains in computational efficiency to be made by sharing computational effort between networked computers. The second area of investigation will focus on the possible application of parallel and multithreaded computing in simulation. Again, these are techniques which produce significant gains in computational efficiency. Multi-threading allows the division of computational effort between processors. This would assist in the efficient simulation of detailed regional groundwater models.

Benefits

- Significant gains in computational efficiency allowing more detailed models of hydrogeological systems to be run within a given time-scale.
- The application of COM compliant software tools, such as ArcView, in conjunction with the object-oriented groundwater model for improved hydrological modelling.

Deliverables

- Document describing the benefits of parallel and distributed computing, especially COM and recommendations for the use of such technology by the object-oriented model.
- Document describing the implementation of COM within ArcView and the potential for its application to the object-oriented groundwater model.
- A computational efficient multi-threaded numerical solver object for use by the regional groundwater model ZOOMQ3D.

Staffing

		Allocation	Cost	
		Days	£	
UoB	AEFS	10	4000	**4000**
EA	SF			**360**
	PJH	1	0	
	DPJ			
	Modeller			
BGS	DWP			**6123**
	AGH	1	363	
	CRJ	20	5760	
	SSO			
	HSO			
	SO			
	Total	**32**	**10483**	

2.4.7 Task 7: Development of a solute transport model

Steady-state particle tracking has recently been incorporated in the regional groundwater model, ZOOMQ3D. The implementation of both forward and back-tracking allows the identification of flow paths, recharge and discharge areas and borehole catchments, for example. This particle tracking code could easily form the basis of a solute transport model. Therefore, the objective of this task is to develop a solute transport model to simulate the processes of advection, mechanical dispersion and mass transfer diffusion. This is likely to take the form of a Random-Walk transport model. However, a review of solute transport modelling will be undertaken at the start of the task, to identify the advantages and disadvantages of different modelling techniques.

The Random-Walk method is a robust and reliable technique for the study of solute transport. With this technique, the Advection-Dispersion Equation is not solved directly, rather dispersion is modelled as a stochastic variable and is added to the advective component. This approach circumvents some of the problems associated with numerical solution of solute transport equations, such as numerical dispersion and grid orientation limitations. Farahmand-Razavi (1995) developed a Random-Walk solute transport model for the simulation of advection, dispersion and mass transfer diffusion in a Chalk aquifer of the UK. The author states that the Random-Walk technique simplifies the process of modelling these processes and illustrates this through its application to the simulation of saline intrusion in a coastal aquifer.

Benefits

- In combination with the local-grid refinement technique incorporated in current object-oriented model and the development of mixed radial-Cartesian mesh models for the accurate representation of pumping wells, the developments will improve the simulation of contaminant transport, in UK aquifers.
- Simple representation of diffusion mass transfer in Chalk aquifers.
- Improved methods for the identification of source protection zones.

Deliverables

- Solute transport model capable of simulating, advection, dispersion and mass transfer diffusion.
- User guide for the use of the object-oriented solute transport model.
- Summary review of methods for the simulation of solute transport.

Staffing

		Allocation Days	Cost £	
UoB	AEFS	5	2000	**2000**
EA	SF	1	580	**2750**
	PJH	2	720	
	DPJ			
	Modeller	5	1450	
BGS	DWP	1	581	**11036**
	AGH	5	1815	
	CRJ	30	8640	
	SSO			
	HSO			
	SO			
	Total	**49**	**15786**	

2.4.8 Task 8: Model validation – application to real aquifers

The application of the model to real aquifers is an important part of the validation process. This will take place in parallel to the model development. A core aim of the project programme is to develop the existing regional groundwater model, ZOOMQ3D, for the solution of current problems in parallel to the development of the framework. Applications will be selected by the project partners and will contain sufficient complexity to evaluate all aspects of the object-oriented model. The Environment Agency will undertake a significant role in the identification and application of the model to appropriate aquifers.

Each individual component or mechanism of the object-oriented model will be tested rigorously. This will include testing against analytical solutions, if applicable, and benchmarking against existing groundwater models. A document containing the details of all model tests will be produced to allow end users to reproduce the model validation tests. Through the collaboration of the core group of project partners, it is anticipated that the models will also be used in live research programmes. The British Geological Survey has a number of research activities within which testing can be undertaken. The National Groundwater and Contaminated Land Centre (NGWCLC) has conducted a review with The Environment Agency regions to determine a national modelling strategy that will provide opportunity for testing. Specifically, the role of these organisations will be to test and apply the model in the following steps:

- Familiarisation and testing
- Application of the model to two regional aquifers and its comparison with existing regional groundwater models developed by The Environment Agency

This will ensure that the code is tested against a range of aquifer conditions that are relevant to UK hydrogeology and important environmental issues. Experience gained during the testing of the model will result in modifications to the model framework or code where appropriate. Because of the object-oriented structure of the code, individual components of the model will be added in sequence. Consequently, testing will be an iterative process and will run parallel to the development of the model.

Benefits

- Rigorous testing of model developments.
- Familiarisation of code by modelling groups within collaborating organisations.
- Close link between model development and review by user's to focus attention on their needs.

Deliverables

- Document containing full description of model testing and CD of all validation models.

Staffing

		Allocation	Cost	
		Days	£	
UoB	AEFS	2	800	**800**
EA	SF	2	1160	**22860**
	PJH	10	3600	
	DPJ	10	3600	
	Modeller	50	14500	
BGS	DWP	2	1162	**7672**
	AGH	10	3630	
	CRJ	10	2880	
	SSO			
	HSO			
	SO			
	Total	**96**	**31332**	

2.4.9 Task 9: Development of the model framework

The development of the model framework will occur within an iterative process of review and modification. The deliverables from each project task will advance the model framework. However, the process of incorporating the findings from each sub-project into the overall model framework will require careful evaluation and management. Consequently, this task focuses on the evaluation of the sub-project findings, their effect on the development on the model framework and the direction of the further work. The task will entail the review of the progress of the work and the resulting benefits at regular intervals during the project. The principal aim of the sub-project is to provide a forum for the development of solutions to current problems associated with groundwater modelling within the project programme. This will focus on the needs of the collaborating partners and of the UK and international modelling communities.

This forum will take the form of regular meetings during the project with the specific aim of discussing important hydrogeological, groundwater modelling and water management issues associated with the project programme. The issues identified during these meetings of the core group of hydrogeologists and groundwater modellers will inform the direction of the project tasks. In addition to these meeting, the core group will investigate other related work in the field of object-oriented environmental modelling in order to inform the development of the model framework. For example, tools for the simulation of other physical processes, such as surface-water flows, or applications for the management of environmental systems, shall be examined, with regard to improving the flexibility and applicability of the model.

Benefits

- Development of the model within a process of regular review to ensure that the work fulfils the objectives of the project.
- Development of the model in parallel to the review of other related work to inform its development and promote its compatibility with other modelling or management applications.

Deliverables

- Final model framework that fulfils the objectives of the project.

Staffing

		Allocation	Cost	
		Days	£	
UoB	AEFS	10	4000	**4000**
EA	SF	10	5800	**13000**
	PJH	10	3600	
	DPJ	10	3600	
	Modeller			
BGS	DWP	10	5810	**12320**
	AGH	10	3630	
	CRJ	10	2880	
	SSO			
	HSO			
	SO			
	Total	**70**	**29320**	

2.4.10 Task 10: Management of the model development

There are a number of issues relating to the development of a freely available piece of groundwater modelling software. This sub-project will formally identify the steps required to manage the development of the model with the aim of producing a globally available piece of high quality modelling software. Up to this stage, the development of the object-oriented groundwater model, ZOOMQ3D, has been undertaken and managed by the *core group* of project partners: Andrew Spink of The University of Birmingham, Steve Fletcher and Paul Hulme of The Environment Agency and Denis Peach, Andrew Hughes and Chris Jackson of The British Geological Survey. This core group will continue to lead of the project. However, it is envisaged that collaboration with other interested parties may occur where beneficial to the project.

The core group will continue undertake the management of the model development. Within this sub-project they will address issues relating to the objective of producing a globally available software framework. The following points will be addressed by the core group:

- Conception of an external project review panel.
- Public dissemination of information during the project
- Method of dissemination of the model and related documentation at the end of the project
- Identification and need for a code guardian and their duties on project completion
- IPR of the collaborating partners and its relation to the global dissemination of the final model

Some proposals have been formulated with regard to the above issues. For example, it is envisaged that the dissemination of information relating to the development of the model, will occur through seminar presentations and scheduling of public meetings for interested parties. This will be a useful form of consultation for the project's core group and will provide valuable input to the development of the model. The nature and frequency of these meetings will be defined this task.

With regard to IPR, many of the scientific developments contained in the current object-oriented model, ZOOMQ3D, were developed by The University of Birmingham, prior to the involvement of The British Geological Survey and The Environment Agency. The British Geological Survey and The Environment Agency were granted a licence "in perpetuity" to use the earlier version of the model, ZOOM2D. Consequently, The University of Birmingham are the owners of the intellectual property right to many of the scientific developments incorporated in the model. However, The British Geological Survey and The Environment Agency have funded the further development of the model and therefore have intellectual property rights to the components of the model developed during this subsequent work. The issues surrounding IPR and the development of the model will be addressed at an early stage of the project.

Deliverables

- Document defining the steps requires by the project partners to produce a globally available piece of commonly applied, high quality modelling software.

Staffing

		Allocation Days	Cost £	
UoB	AEFS	5	2000	**2000**
EA	SF	5	2900	**4700**
	PJH	5	1800	
	DPJ		0	
	Modeller			
BGS	DWP	5	2905	**6160**
	AGH	5	1815	
	CRJ	5	1440	
	SSO		0	
	HSO		0	
	SO		0	
Seminars and meeting of review panel			10000	
	Total	**30**	**22860**	

2.5 COST SUMMARY

	Project Cost Summary	NUMBER OF DAYS				COST				
		Total	EA	BGS	UoB	Total	Unit Cost	EA	BGS	UoB
1	Accurate representation of hydrogeological features and mechanisms	60	15	15	30	24660	411.0	6500	6160	12000
2	Accurate simulation of wetlands through the development of wetland objects	94	52	37	5	30677	326.4	17060	11617	2000
3	Accurate representation of pumping wells in a regional groundwater model	132	6	106	20	41576	315.0	2380	31196	8000
4	Development of a GIS based recharge model	114	56	56	2	37726	330.9	18630	18296	800
5	Channel scale representation of rivers in a regional groundwater model	114	32	72	10	36632	321.3	10560	22072	4000
6	Investigation of the benefits of parallel and distributed computing in groundwater modelling	32	1	21	10	10483	327.6	360	6123	4000
7	Development of a solute transport model	49	8	36	5	15786	322.2	2750	11036	2000
8	Model testing and validation - application to real aquifers	96	72	22	2	31332	326.4	22860	7672	800
9	Development of the model framework	70	30	30	10	29320	418.9	13000	12320	4000
10	Management of the model development	30	10	15	5	22860	762.0	4700	6160	2000
		791	282	410	99	281052	355.3	98800	132652	39600

2.6 PROJECT SCHEDULE

	Number Days	Year 1												Year 2												Year 3											
		1	2	3	4	5	6	7	8	9	10	11	12	1	2	3	4	5	6	7	8	9	10	11	12	1	2	3	4	5	6	7	8	9	10	11	12
1 Accurate representation of hydrogeological features and mechanisms	52						S						R																								
2 Accurate simulation of wetlands through the development of wetland objects	94												R																								
3 Accurate representation of pumping wells in a regional groundwater model	132																	S				R															
4 Development of a GIS based recharge model	114										S				R																						
5 Channel scale representation of rivers in a regional groundwater model	114																									S				R							
6 Investigation of the benefits of parallel and distributed computing in groundwater modelling	32															R																					
7 Development of a solute transport model	49																																		R		
8 Model testing and validation - application to real aquifers	96														R							R								R					R		
9 Development of the model framework	70													R												R											F
10 Management of the model development	30												R																								
Project Meetings																																					

S Summary report

R Annual or end of sub-project report

R Final project report

2.7 PROJECT STEERING

The project core group will meet every six months to review the progress of the project and discuss the outcome of the work to date. In addition, to these meetings, it is expected that the external review panel will meet at regular intervals during the project after its inception. The nature of the review panel will be defined shortly after the beginning of the project as part of Task 10. In addition to these meetings, feedback from scheduled seminars will assist the core management group to assess the progress of the programme.

2.8 REPORTING

Reports will be written at the end of each of the Tasks 1 to 8, describing the work undertaken and the relevant outputs. For the tasks of longer duration, a summary report will be written at the halfway point. A report describing the procedure for the management of the project (Task 10), with the aim of producing a globally available piece of modelling software, will be completed by the end of the first year of the programme. This will define the strategy for the management of the model development for the final two years of the programme. As part of Task 9 a detailed report will be produced at the end of each year of the programme describing the development of the overall model framework. A final project report will be produced at the end of year three.

PART TWO

3 Requirements for Groundwater Models

Sustainability of a groundwater resource is linked to both the quantitative development of that resource and the protection of its quality. The consideration of the long-term is central to the principle of sustainability. However, the management of a resource is a dynamic and continually changing process. This is because the quality of a groundwater resource is affected by human activity though the hydrogeological setting and the climate determine the extent to which an action affects the quality of groundwater.

Management schemes have to change as a resource is developed due to the fact that groundwater systems are complex and their behaviour is non-linear. However, the development of a scheme assumes that the factors influencing such impacts are understood. In order to manage the exploitation of a groundwater resource knowledge of these processes and their controls is essential. Without this, water resource engineers cannot make informed judgements about what action should be taken to manage the system for the benefit of both water consumers and the environment. One method by which a better understanding of the behaviour of a groundwater system can be gained is through the use of models. Models are powerful and widely used tools to investigate the behaviour of water resources systems in general and groundwater in particular. A systems analysis approach and the use of models are invaluable in the assessment of a sustainable management policy for a groundwater resource.

Digital models have allowed the numerical simulation of complex real world aquifers and are of fundamental importance in testing our understanding of aquifer systems. They provide a framework within which improved understanding of physical processes takes place, they allow practical problems, such as resource allocation, to be addressed and they are an expression of what is currently known or assumed about an aquifer. Furthermore, models provide the only means by which novel mechanisms can be examined quantitatively and confirmed or rejected on the basis of field evidence. Consequently, it is important that the model's design allows new processes to be formulated and added to existing models. Within the constraints imposed by the design of the base model, *object-oriented* methods allow this to take place without wholesale re-writing of the model code.

As models move from development and use in research, they become the day-to-day tools of hydrogeologists engaged in the operation and management of aquifer systems. This process has highlighted the deficiencies in some modelling approaches and heightened awareness of the need for further development. In order to evaluate, which, if any, areas of a modelling methodology should be improved the following list of objectives might be considered. These are predominantly related to the development of a better regional groundwater model, with which this business and scientific case is concerned.

1. Does the model represent the hydrogeological mechanisms accurately and at the correct scale?
2. Does the model provide a framework that is adequate to improve the understanding of physical processes?
3. Does the model incorporate the required mechanisms/processes?
4. Does the model provide an adequate basis for the development of tools for aquifer management?

5. Does the model facilitate the evaluation of practical problems satisfactorily, for example resource assessment and groundwater quality assessment?
6. Can new mechanisms be incorporated easily as advances in the understanding of the physics of groundwater flow and solute transport are made? Is it extensible?
7. Does the model facilitate investigative modelling in order to test conceptual models?
8. Does the model provide a satisfactory framework for research?
9. Is the model a sustainable platform for the future development of groundwater modelling over the medium to long term?
10. Does the approach make modelling more accessible to numerate hydrogeologists?
11. Can a model be modified rapidly and easily without changing the basic code?
12. Can areas of interest be added and removed dynamically? Is it flexible?
13. Is the model user and developer friendly?
14. Are data stored and managed satisfactorily by the model?
15. Is it easy to interrogate, manipulate and visualise the results?
16. Is the model efficient? Could advances in software development enable more detailed simulations to be run within a given time or cost budget?
17. Can new software development methods improve the representation of the hydrogeology within a model and improve its efficiency, flexibility and maintainability?

When considering the current state of groundwater modelling, the answers to many of these questions illustrate that major advances could be made to existing regional groundwater models. This is highlighted in the next section where a number of the deficiencies of current models are described.

4 Current Deficiencies

4.1 COMPUTATIONAL PROBLEMS OF CURRENT APPROACHES

Whilst the power of desktop computing has increased enormously in the last decade, with the exception of user interfaces, groundwater modelling technology has shown no significant advances. As described in more detail in the Section 5, currently most groundwater models are written in structured procedural programming languages, such as Fortran. In this approach the design of the model is based on the identification of the *algorithm*. The algorithm specifies the sequential steps that must be taken to achieve some result. In procedural programming, the algorithm, or the models functionality is assigned significantly more importance than the *data* on which it acts. Consequently, many data are made common, which means that they are accessible to all parts of the model's code. This means that great care must be taken when modifying the code, for example to implement a new process or mechanism.

The fact that data can permeate through much of a procedural program has serious consequences for the extensibility, modifiability and life expectancy of the code. For example, when a better description of a physical process is obtained, it is important to correct its representation in the model. Changes can also be required to test hypotheses about the operation of a particular physical mechanism itself. Unfortunately, it is often difficult to do this in existing groundwater models because data commonality means that alterations can propagate errors along a number of paths through the code. Consequently significant periods of testing are required to revalidate the model. Furthermore, because of the sequential nature of the majority of groundwater models a number of operations are performed at different locations within the code, which relate to a single mechanism, for example river-aquifer interaction. This repetition of similar tasks at different places within the program again complicates its modification when a new mechanism has to be incorporated in the model. A report describing the implementation of the representation of the variation of hydraulic conductivity with saturated thickness in MODFLOW (Taylor et al., 2001) illustrates these problems. The following three short extracts are taken from this report.

- *"Mechanisms are more important than parameters and it is therefore necessary to be able to change the model code to include new mechanisms when required."*
- *"Overall the work has suggested that it is more effective to adapt a code to include mechanisms observed in the field than to constrain the conceptual model to include only the mechanisms available in the code."*
- *"MODFLOW has a modular structure and the code is generally well laid out and documented. New packages can be added easily, but changes to the code require care. This is mainly due to the widespread use of conditional statements in conjunction with GOTO statements."*

The new approach for the development of a regional groundwater model, *object-orientation*, will eliminate many of these problems. By minimising the dependencies between parts of the code, it is envisaged that a model framework can be developed which focuses on mechanisms. By localising effects within discrete areas of the code it will be significantly easier to modify or incorporate new hydrogeological mechanisms without causing errors in other parts of the program. Modelling practitioners will then be able to investigate mechanisms more easily instead of just modifying parameter values.

4.2 HYDROGEOLOGICAL COMPLEXITY

In addition to the lack of emphasis on mechanisms in current groundwater models, the representation of the geometry of hydrogeological units is difficult within the framework of a layered finite difference model, which is represented as a continuous three-dimensional array. Because layers have to be continuous across the model domain it is difficult to represent spatially discontinuous features. For example, the vertical shift in hydrogeological units across a fault, sinuous alluvial deposits in river valleys, spatially variable glacial drift cover and the thinning out of sedimentary layers are all example of spatially discontinuous hydrogeological features that are difficult to simulate.

The problems associated with the incorporation of the complex geometry of hydrogeological features in groundwater models is related to the numerical structures which can be used to represent them. Whilst current computing technology enables the investigation of methods to improve the representation of such complex features, this has not been a significant area of research. In addition to the requirement to improve the geometrical representation of aquifers in models, there is also a need to improve the representation of mechanisms. For example, consider the conceptualisation and simulation of wetlands. Wetlands are complex and generally small-scale features, which incorporate a number of physical processes and which are often conceptualised in a number of different ways. It is for these reasons that they have often been represented by the most basic of functions within numerical models. This issue should now be addressed and research into improved methods for the representation and simulation of such features is timely.

4.3 ISSUES OF SCALE

An essential feature of a groundwater flow model is an ability to represent aquifer features at different spatial scales. This is necessary both to focus on regions where there is particular interest and to maintain accuracy where the solution is highly variable. Because the behaviour of a numerical solution depends on the physical properties of the aquifer the hydrogeology must determine the discretisation of space and not the numerical technique. Unfortunately conventional finite difference methods have difficulty in fitting the mesh to the hydrogeology. Consequently, models generally contain additional nodes in regions where there is little interest and where they are not required for accuracy.

Telescopic mesh refinement is used to simulate aquifers more efficiently. However, this method has a number of drawbacks and is not always applicable. Whilst the method reduces the number of nodes involved in simulating an aquifer, the gains in computational efficiency are moderated by the need to determine boundary conditions for embedded models. It is often stated that the rapid gains in computing power and its reducing cost negate the requirement to improve the efficiency of numerical techniques. However, the demand to model more complex problems increases in parallel with improvements in computing. Consequently, novel methods to more accurately and efficiently simulate aquifers remain of benefit. An example of this is the need to be able to simulate the effect of groundwater abstraction on river flows. Currently, it is difficult to simulate in detail groundwater flow to wells and their influence on rivers or wetlands. It is envisaged that the approach proposed here can address these issues.

4.4 DATA STORAGE AND MANAGEMENT

An important development in the field of geosciences is the application of database technology and graphical information systems for the storage, management and processing of data. These techniques offer significant benefits to groundwater modelling but it is only recently that they have been applied. The major benefit they offer is the capability to separate real data from models. Currently, this is not the case and significant amounts of information are bound up in individual models. For example, consider the spatial variation of hydraulic conductivity within an aquifer system. Information on this parameter can be obtained from a number of sources, for example from pumping test analyses, laboratory experiments or previous modelling investigations. These data are generally gathered by the hydrogeologist and transferred directly into a groundwater model. Parameter values are assigned on the model grid, which then acts as the store of this information. Consider then, that another modeller either wishes to construct a model which covers part of the area of the first or wants to modify the structure of the previous model. Because the model contains no information relating to the source of the data on which it is based, the user cannot be sure of its quality. Consequently, it is usually the case that the primary data must be collected again and re-examined. If the first model is to be modified, for example by refining the grid in the region of an abstraction borehole or river, new parameters values will have to be assigned manually. The drawback is that data is grid dependent but the grid is a feature of the model only and not reality. A better approach would be store data separately from the model and then allow the model to interrogate the data during its construction or modification.

4.5 MODEL OUTPUT

In addition to data input, there are problems associated with the processing of model output. This has in part lead to the development of graphical user interfaces (GUIs), which facilitate post processing. In part the problem is due to the complexity with which model results are output during a simulation. For example, considering MODFLOW, the most commonly applied regional groundwater model, much of the output data is written in a binary format. The development of a suite of graphical user interfaces by commercial companies has simplified the post processing of this data. However, many of these still do not allow the rapid and simple interrogation of the raw data, which is a requirement. Consequently, individual modellers commonly spend time writing bespoke pieces of code to extract information from binary output files. The need for such interfaces could be questioned given the abundance of more generally applicable very high quality data processing software that is routinely used by hydrological modellers. These software packages, such a spreadsheets, GIS packages and visualisation software are generally superior to those contained within an individual GUI. Their use could be facilitated by presenting model output in a clear, transparent and format independent way.

5 The Object-Oriented Approach

5.1 OBJECT-ORIENTED PHILOSOPHY

The vast majority of groundwater models are written using procedural programming languages, such as Fortran. However, developing efficient and clear programs that are easily modifiable is difficult using this approach. A more recent and radically different approach to developing software is the *object-oriented method*. A central concept is the use of *abstraction* (see glossary) to deal with complexity. This has a number of advantages over procedural programming for the construction of complex models because it enables the direct representation of real world objects. Whilst the method is commonly used to develop commercial software, it has not been extensively used to develop groundwater models.

In particular object-orientation offers significant benefits to the accurate representation of physical mechanisms in models. It can also greatly simplify the maintenance and development of a model as the understanding of the physics of groundwater flow improves. This is because real world objects are modelled by computational equivalents. Because objects are discrete and hide their data and functionality it is easy to alter their behaviour without affecting other parts of the model. Furthermore, because object-oriented models contain a high degree of modularity, programs can be developed that are more easily modified and which have a longer life. After specifying the methods by which objects interact internal changes to an object are straightforward to perform. This also means that new programs are also more easily developed since they can be based on previously constructed, high quality, discrete components. These concepts and the further benefits of the object-oriented approach are discussed in more detail in Appendix 1.

A prototype groundwater model has been developed which represents a first attempt at designing and implementing a framework of objects, which accurately represents the structure of common hydrogeological features within a regional groundwater model. The decomposition of real world entities, such as rivers and wells and model entities such as grids and numerical solvers produces a cleaner and more transparent code. This model forms the basis for the future development of the approach and in particular a means by which the ideas behind object-oriented groundwater modelling can be disseminated to the wider hydrogeological community.

5.2 CURRENT MODEL STATUS

A regional groundwater model, ZOOMQ3D, has been in development since September 2000 by The University of Birmingham, The British Geological Survey and The Environment Agency, National Groundwater and Contaminated Land Centre. The model represents the first attempt by the project partners to identify a framework of objects that can be used to advance UK groundwater modelling.

ZOOMQ3D is a quasi three-dimensional regional groundwater model that incorporates the functionality required by any such proprietary piece of groundwater modelling software. Its development has two main purposes. The first objective has been to allow the investigation of the use of objects in groundwater modelling. The second has been to illustrate the benefits of the approach to the wider hydrogeological community. This is an ongoing process but has started with the presentation of the work at seminars and meetings of modellers and water resource engineers. The model code has also been used by The British Geological Survey on commercial projects, in part with the purpose to illustrate the benefits of the object-oriented approach. Whilst the current model has a number of benefits over other existing regional groundwater models, it is only viewed by the project partners as step towards the development of the final object-oriented regional groundwater model that better represents UK hydrogeology.

The development of the current regional groundwater flow model ZOOMQ3D has enabled the investigation of the use of objects for the simulation of groundwater systems. The experience gained in the development of the model has led to an appreciation of the potential benefits of the approach. It is the aim that this model will be used by other groups within The British Geological Survey and The Environment Agency other than the small number of individuals within the core group. Through its dissemination to modellers in The Environment Agency regions and other modellers in The British Geological Survey, feedback will be generated regarding the advantages and disadvantages of the methodology and its implementation in the model. This information will assist in the development of the new frameworks on which the final model will be based.

The current framework of objects used within ZOOMQ3D is shown in Figure 1. Towards the top of the figure and top of the *class* (the template for an object) hierarchy are classes representing individual *models* of the hydrological system. For example, there are classes defined to represent models of surface water channels, recharge through the soil zone and the groundwater system. Consequently, an attempt has been made to separate *simulators* within the framework. Classes have also been defined to represent individual components of each of these systems. For example, real world hydrogeological entities such as observation wells, abstraction wells and springs are declared as classes. Finally numerical operations have been simplified by decomposing elements of the solution method into classes. By separating components of the grid discretisation method and numerical solution method into classes, the representation of complex models has been simplified significantly.

Whilst the use of the object-oriented approach to develop ZOOMQ3D has resulted in a regional groundwater modelling code that is more flexible, more easily extensible and clearer than comparable simulation models that are presently available, it is apparent that further research is required to develop an object-oriented model code that better represents UK hydrogeology and which forms the basis for the future advancement of groundwater modelling both in the UK and internationally.

In summary, the objective of the research is to design a framework of objects that can closely represent conceptual models of hydrological/hydrogeological systems. The framework must be flexible, easily modifiable and extensible and define an architecture for the accurate simulation of UK hydrogeology. The philosophy is to mimic real world entities in a computational environment in order to avoid many of the problems associated with existing modelling approaches.

Currently, MODFLOW (McDonald and Harbaugh, 1988) is the most commonly used model for the simulation of groundwater flow. With the aim of familiarising modellers to object-oriented groundwater modelling, one of the objectives of the development of ZOOMQ3D has been to ensure that the model contains all the functionality of this earlier code. This has been achieved and ZOOMQ3D contains all of the following features:

- Representation of confined and unconfined conditions,
- Spatially varying aquifer properties (hydraulic conductivity, specific storage, specific yield, vertical leakance),
- Spatially and temporally varying recharge,
- Horizontal anisotropy,
- Head dependent transmissivity,
- Vertical discretisation (layering),
- Horizontal and vertical moving boundaries i.e. dewatering and rewetting of model nodes,
- Abstraction wells,

- Head dependent leakages
- River-aquifer interaction, including the simulation of ephemeral rivers and baseflow accounting,
- Steady state particle tracking.

A complete description of these mechanisms and the validation is given in three reports by The British Geological Survey (Jackson, 2001, Jackson 2002a and Jackson 2002b). In addition to these mechanisms, ZOOMQ3D incorporates:

- Local grid refinement
- Variation of hydraulic conductivity with depth
- A new spring mechanism

These are not incorporated in the USGS MODFLOW model. The benefits of local grid refinement are described next.

5.2.1 Local Grid Refinement

The areal extent of an aquifer is large compared to the discharge/recharge mechanisms such as wells, springs and rivers that typically operate in the aquifer. A modelling technique that easily allows for extensive aquifer bodies, but represents small-scale features correctly is a more appropriate approach. The technique of local grid refinement has been implemented in ZOOMQ3D which gives it a significant advantage over existing groundwater models. The technique enables interest to be focussed on small areas of a model domain and allows local hydrogeological features to be simulated accurately and efficiently within a regional context. Local grid refinement techniques have been and continue to be developed at the School of Civil Engineering, University of Birmingham (Hayes, 1999; Jackson, 2000). The potential for the future development of local grid refinement and its associated benefits are discussed in Section 2.4.3 with regard to pumping wells.

An example of the use of local grid refinement to simulate local features within a regional system is presented by Jackson (2000). The investigation compares the performance between a MODFLOW model and ZOOM2D, an earlier model incorporating local grid refinement, which are used to simulate a group of abstraction wells. Both models (Figures 2a and 2b) refine the coarse 1km square base mesh to a mesh of 50 m square cells in the region of the local well field. An additional ZOOM2D model is run in which the grid is refined to 10 m around each borehole in the well field. The models are compared by determining the length of time the each takes to converge to a steady state solution from an initially flat groundwater head profile. This is shown in Figure 3 and Table 1, which illustrates the change in drawdown at one of the abstraction wells as the solution converges to the steady state groundwater head profile. The 50 m grid ZOOM2D model, which resolves to the same spatial scale as the MODFLOW model, is twenty six times faster because it does not have to perform calculations at the many distant and essentially redundant nodes. The 10 m grid ZOOM2D model, which increases mesh density one hundred times is still twenty one times faster.

In addition to this application of the local grid refinement technique, The British Geological Survey has used ZOOMQ3D to simulate a pumping test in a group of wells contained within a regional model. The model has proved to be successful in simulating the response of a number of observation boreholes within a relatively complex area of a Chalk aquifer.

To simulate groundwater flow in the Chalk aquifers of the UK, a number of researchers have included the variation of hydraulic conductivity with saturated depth in regional groundwater models (Taylor et al., 1999). This has been included in ZOOMQ3D, which because of its object-oriented nature has been a straightforward task.

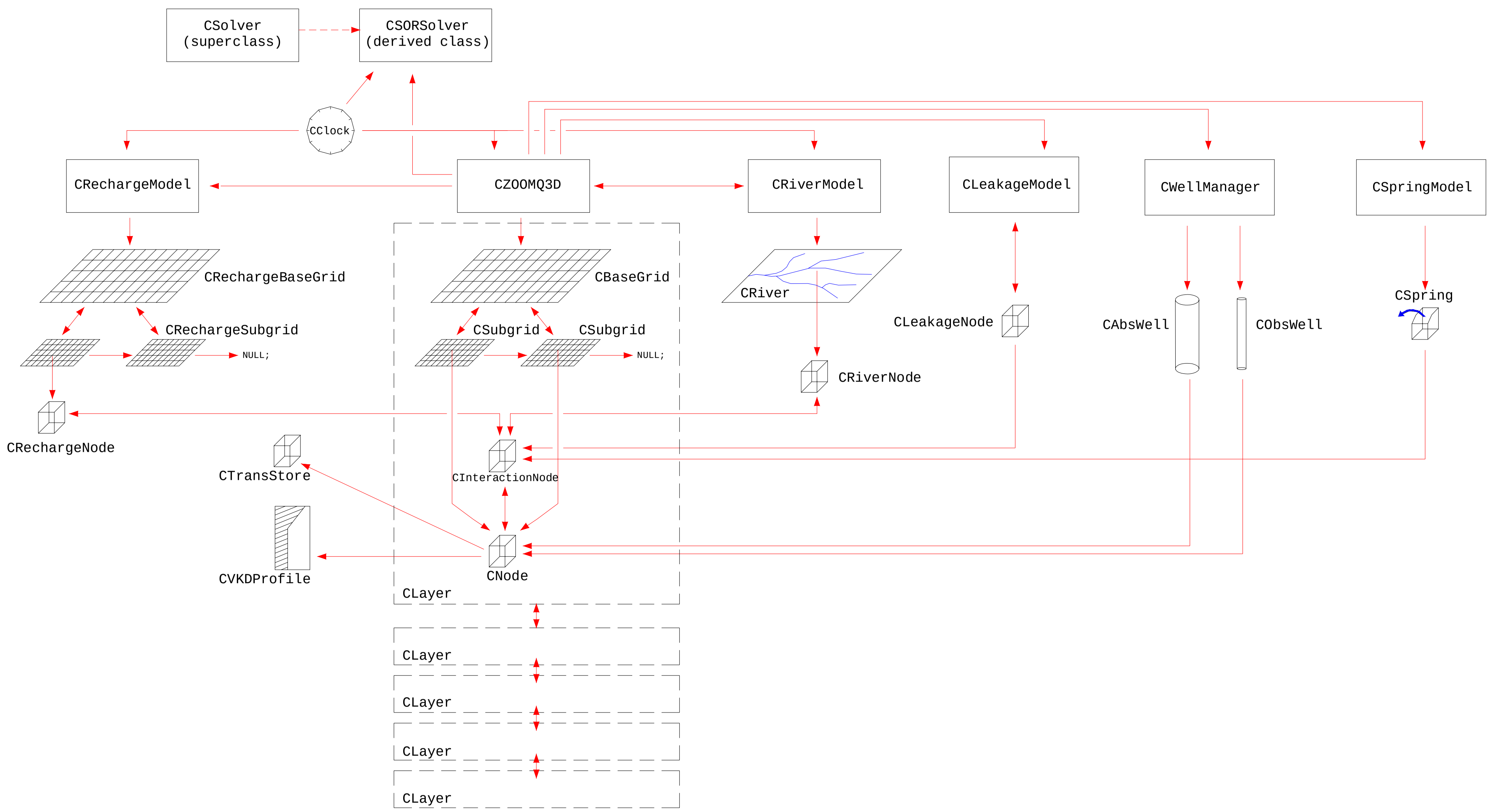


Figure 1 ZOOMQ3D object framework

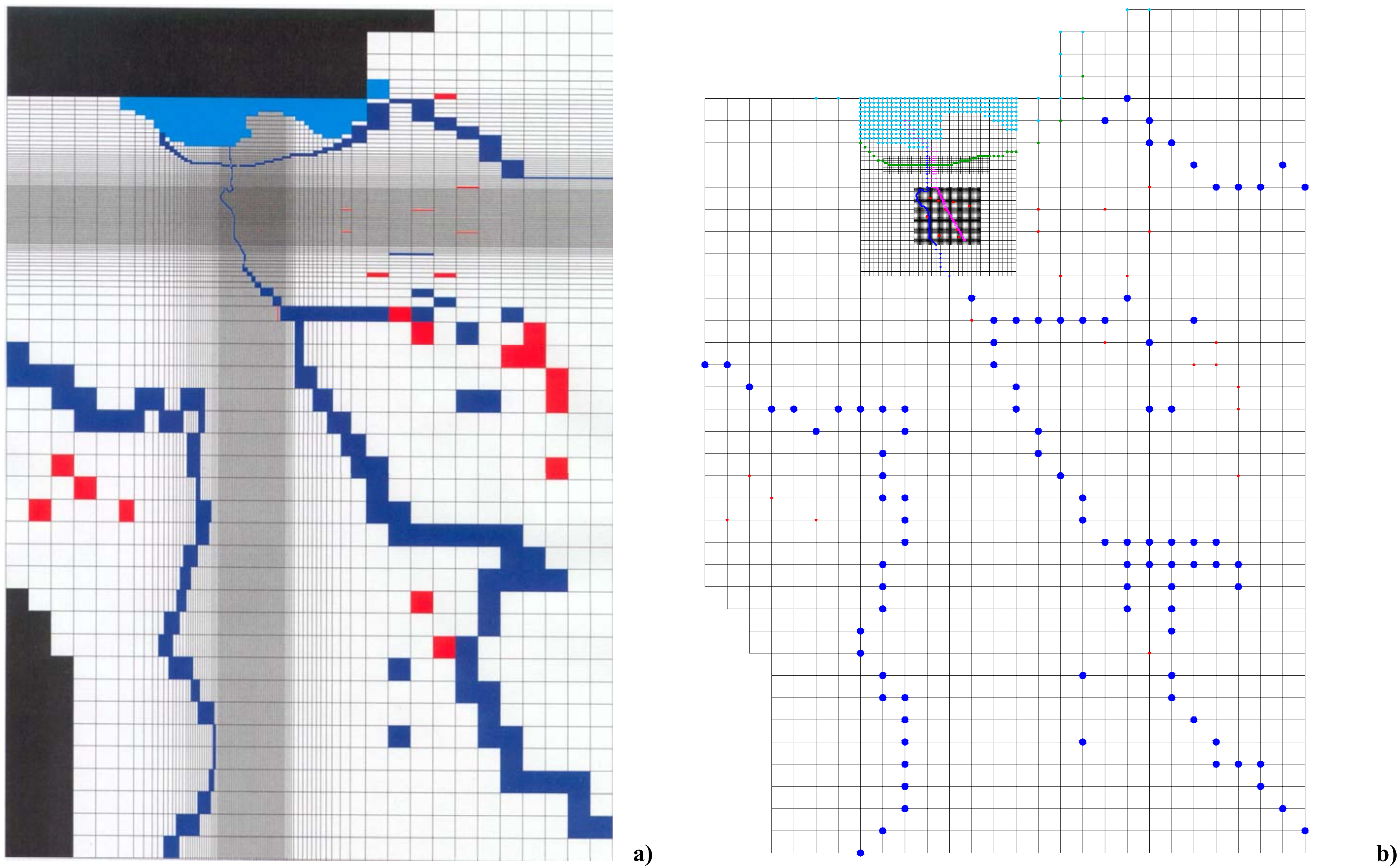


Figure 2 Example of a) a conventionally refined MODFLOW model grid and b) a locally refined ZOOMQ3D grid

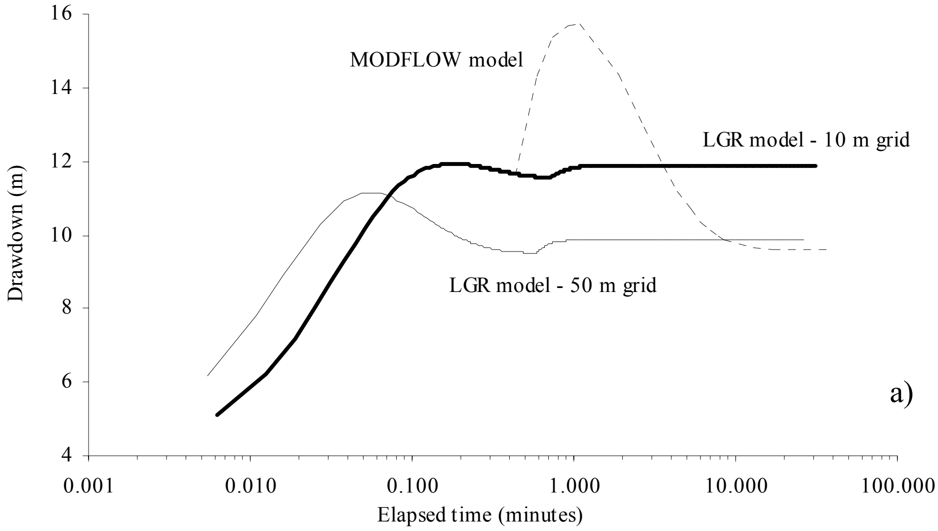


Figure 3 Comparison of the MODFLOW and ZOOM2D models (Drawdown greater on 10 m grid due to smaller scale representation of well)

Table 1 Comparison of the MODFLOW and ZOOM2D models

Model	Finest mesh size	Time required for model to converge to within one ten thousandth of a millimetre of the final head value at the pumping well
MODFLOW	50 m	58 minutes
ZOOM2D	50 m	2.2 minutes
ZOOM2D	10 m	2.8 minutes

5.3 OBJECT-ORIENTED MODELLING RESEARCH

Object-oriented methods are becoming more widely adopted by investigators in the field of geosciences for the development and implementation of modelling software. The method is being used to develop models which more clearly represent physical processes and to improve the implementation of numerical simulation methods. A greater number of investigators is also using the approach to couple data assimilation, simulation and visualisation software that have often previously been defined as separate components. A literature review of recent research related to object-oriented groundwater modelling is presented in Appendix 2. This serves to illustrate many of the benefits of the approach and outlines some of the areas of study in which object-oriented techniques are being applied.

5.4 THE POTENTIAL OF OBJECT-ORIENTED MODELLING

5.4.1 Accurate representation of hydrogeological features and mechanisms

Object-orientation presents the opportunity to represent both the geometry of hydrogeological entities and physical mechanisms operating within aquifers accurately. The numerous restrictions associated with current groundwater models causes modellers to fit hydrogeological problems to the structure of groundwater models. In contrast an object-oriented model could be developed to accurately represent aquifers using computational equivalents of hydrogeological entities. For example, the current approach of using horizontally continuous layers to model aquifer units is limiting and often requires hydraulic parameters to be adjusted to produce satisfactory models. Novel methods of model discretisation, which can be elegantly implemented as objects, could be developed to resemble irregularly shaped hydrogeological entities. For example, the use of objects to represent sinuous valley alluvial deposits, sedimentary layers which thin out, faults and their adjacent hydrogeological units, clay lenses, and perhaps even individual fractures would be significantly simplified using object-oriented techniques. A possible approach by which heterogeneity could be described more simply within a model could be the definition of objects that represent hydrogeologically uniform entities. Such entities could be constructed as discrete components and 'plugged' together to form a model of a groundwater system. Such an approach would circumvent the problems associated with the unrealistic description of aquifers as continuous layers if objects could be made to have the same shape as hydrogeological units.

Development work on a typical cross section, such as that shown in Figure 4, would allow a number of problems to be examined. Some of the work would be of assistance in setting the framework of objects that will form the basis for three-dimensional modelling. In other cases the section will provide a valuable test-bed for exploring flow mechanisms and their representation.

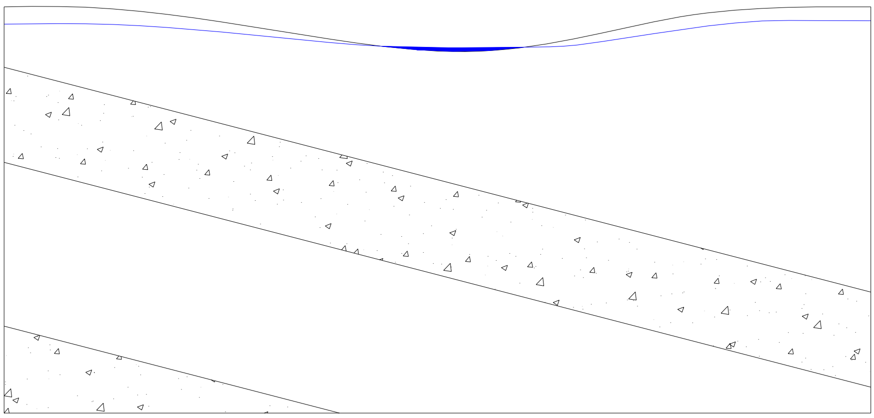


Figure 4 A typical cross-section through an aquifer system

The typical section, shown in Figure 4, demonstrates some of the features and the problems that need to be solved. Amongst them are:

- *The accurate representation of geological structure*. Basic elements might be thought of as bands of material which similar hydraulic properties.
- *The representation of the free (phreatic) surface*. This provides a dynamic boundary to the system with the consequence that objects associated with the free surface must themselves transform.
- *The representation of seepage faces*. Intersections between the free surface and ground level provide both dynamic features and distinct boundary conditions.
- *River-aquifer interaction*. There are many possible combinations of processes that require investigation.
- *Unsaturated zone behaviour*. This could be explored on a section.
- *Scarp slope behaviour*. A combination of different hydraulic properties, springs and seepage faces leads to a common but demanding set of processes.

- *Variable hydraulic conductivity with depth*. Current models based on so-called variable hydraulic conductivity with depth calculation do not in fact simulate variable hydraulic conductivity with depth.
- *The presence of fissures*. This is an extreme case of variable hydraulic conductivity.

In addition to the potential to develop models, which can accurately represent the structure of conceptual models of groundwater systems, object-orientation could significantly simplify the incorporation of complex physical processes within model. For example, considering wetlands, which are complex local scale features, a suite of objects could be developed to represent their different components. These could each be given complex behaviour, however, because functions, or processes, can be hidden within objects, the structure of the model can be made to remain clear and explicit. Furthermore, because of this compartmentalisation of the behaviour of hydrogeological entities it is easily to modify the functionality of an object without causing problems elsewhere in the program. That is, it is easy to modify and investigate mechanisms.

5.4.2 Data storage and management

A further concept that has started to be investigated is the storage of data in groundwater models. A problem with many conventional models is that information relating to aquifer parameters is stored on the model grid. Consequently if the mesh is modified the model's aquifer parameters also have to be re-assigned. A better approach would be to store and manage groundwater information outside of the model and allow it to interrogate the data store. Data storage and management could be performed using, for example a graphical information system. One aspect of the storage and management of data has been addressed in the current object-oriented regional groundwater model ZOOMQ3D. This relates to the definition of rivers within models.

Conventionally groundwater models store the attributes of rivers on the model mesh. Consequently, if the mesh is altered new parameter values, such as channel width, bed thickness and river stage, have to be redefined. In ZOOMQ3D a technique has been developed to store the geometry and hydraulic parameter of rivers outside of the simulation model. First, arbitrary points are chosen along the real river. At these points data is stored describing the geometry of the channel its hydraulic properties (Figure 5a). A mathematical curve is then constructed through these points using *cubic splines* (Figure 5b). These splines and their associated data are stored outside the model. The splines are interrogated by the model's grid objects when the mesh is created. Model river objects are then constructed, which on their creation extract data from the splines and spline points to assign their parameters values (Figure 6a). When the model mesh is modified through local grid refinement the splines are re-interrogated by the new grid objects and the model river nodes are reconstructed (Figure 6b).

Using this approach the model grid can be redesigned quickly because new parameter values do not have to assigned to the modified model manually. Other methods of storing, managing and transferring information between simulation models and data stores can be envisaged. For example, a worthwhile area of research is the investigation of the coupling of the capabilities of GIS software with simulation models. A number of investigators are already examining techniques for interfacing GIS packages with Groundwater models (Rindahl, 1996; Sebhat and Heinzer, 2000; Raterman et al., 2001). The ease with which modellers can simulate hydrogeological systems will be greatly enhanced if these investigations result in the decoupling of data and models.

The simplicity with which data can be entered into a model and its output analysed is an important issue when designing a groundwater model. To simplify these operations a number of graphical user interfaces (GUIs) have been developed, often by commercial software houses, for existing groundwater models, for example for MODFLOW. With regard to MODFLOW it can be argued that these GUIs have become popular because of the complexity of the input and output files that are used by the model. First, considering the input to MODFLOW, which consists of a number of fixed format ASCII files. Whilst these can be opened in a text editor and modified they are relatively complicated and time consuming to construct because of the use of fixed format input. ASCII is considered an excellent file format for groundwater models because it is important that users are able to examine the input parameter values directly. However, many models do not use a simple and clear structure within each input file. The philosophy behind the structure of the input files designed for ZOOMQ3D is that the data they contain should be almost obvious to the user without a manual and that they are easily modified. This philosophy will be maintained in the model proposed for development here.

Accepting the fact that ASCII data files should be used for model input is actually a minor matter. A much more significant question is how data should be stored on hydrogeological parameters and then transferred to a model (or to its ASCII input data files). In most modelling applications hydrogeological data is collated from a number of sources and input into the model through a GUI. Consequently, hydrogeological data are stored on the model mesh and become grid dependent. If another model of the same area is developed later it can be difficult to know which model data are real and which have been adjusted through calibration. Consequently, it is generally necessary to re-collate the original information. A better approach would be to store real data separately from the model and then allow numerical models access to this data when they are constructed.

5.4.3 GIS

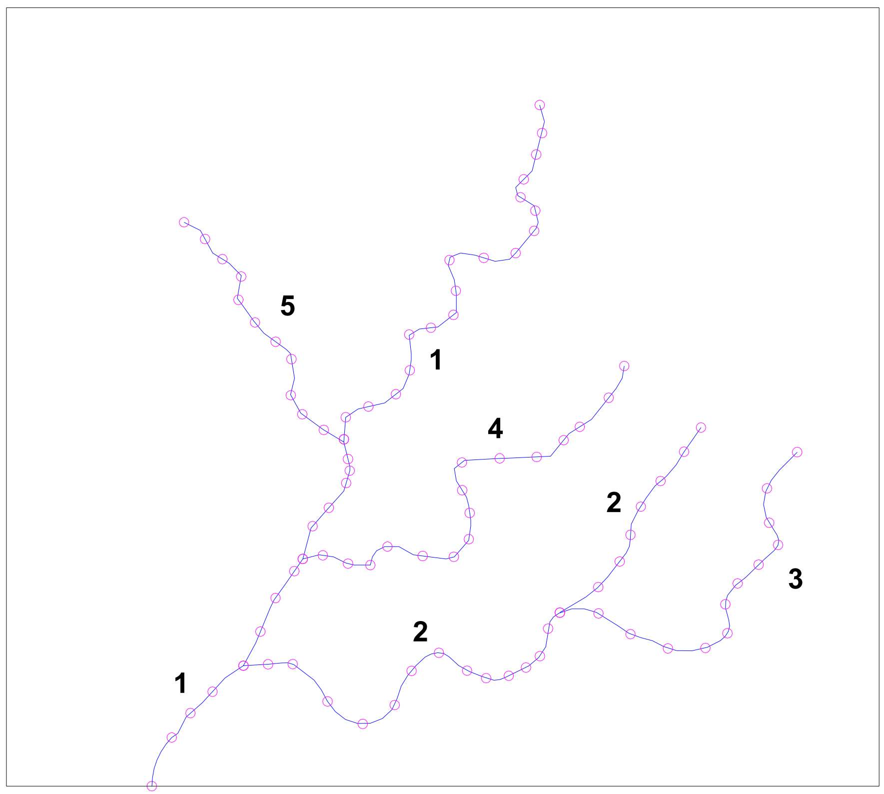
Powerful tools for the storage, management and visualisation of spatial data are graphical information systems (GIS) and these are in common use. GIS packages have only been used only recently in conjunction with groundwater models but offer significant benefits to groundwater modelling. In addition to the storage of data, some GIS packages can be customised to perform user-defined tasks. For example, ArcView8.1 allows new functionality to be added using any COM (Component Object Model) compliant programming language, such as Visual C++. COM technology allows separate objects to be created that can be 'plugged' together to form applications. It may be advantageous to construct the framework of objects for the groundwater model using COM objects. Even if this is not the case, the use of COM by ArcView8.1 and its ability to be customized using object-oriented programming languages means that it is well suited to be combined with an object-oriented groundwater model.

5.4.4 The Need for GUIs

The proliferation of the use of graphical user interfaces has also become common because of the complexity and format of the output files which many groundwater models produce. Again, considering MODFLOW, GUIs have become popular because much of its output is written to *binary* files. Consequently, additional software is required to read data from these files and then visualise it. That is unless the user writes bespoke pieces of software to convert the files to a format that can be imported into other general visualisation software. The philosophy of ZOOMQ3D has been to write simple ASCII output files, which contain one type of data, for example the variation of groundwater head over time at observation wells. In this case a large number of high quality data manipulation and visualisation software applications can be used to examine the model output. For example, Microsoft Excel can be used to draw hydrographs of groundwater head over time at observation wells. The major benefit of this approach is that commonly used software such as this can generally be used to produce visual output which is far superior to that generated by GUIs.

5.4.5 Code and computing issues

The selection of the programming language with which to write the object-oriented groundwater model will be decided by the project partners after the project has commenced. There are a number of issues to be addressed and these are concerned with the balance between the complexity of the adopted approach and the capabilities of the model code. One of the most commonly used and powerful object-oriented programming languages is C++; the language used to develop the prototype regional groundwater model, ZOOMQ3D. In addition to encapsulation of data and functionality in objects, re-use has been one of the classic motivations for object-orientation. That is the ability to reuse previously constructed high quality components to build applications (Box, 1998). However, being strict this is actually a difficult task in C++ because of *binary incompatibility* of compiled objects. The binary incompatibility of C++ objects means that the issuing of updated model classes to users requires them to recompile and link the model code. It may be the case that this is not envisaged to be a concern in the development of a regional groundwater model which is a relatively specialist piece of software. However, if binary incompatibility is considered to be important then the COM (Component Object Model) programming language could be used to circumvent these problems. The use of COM enables applications to be developed from truly separate components. A benefit of COM is that it allows the rapid reuse of the objects by other environmental software modelling applications based on the same technology. Furthermore, the use of COM would be beneficial in the development of applications which could distribute their workload between processors and over networks; a significant potential benefit for large applications. Also ArcView8.1 is built using COM and consequently it use could have significant advantages for the coupling of a regional groundwater model with a GIS package.



a)

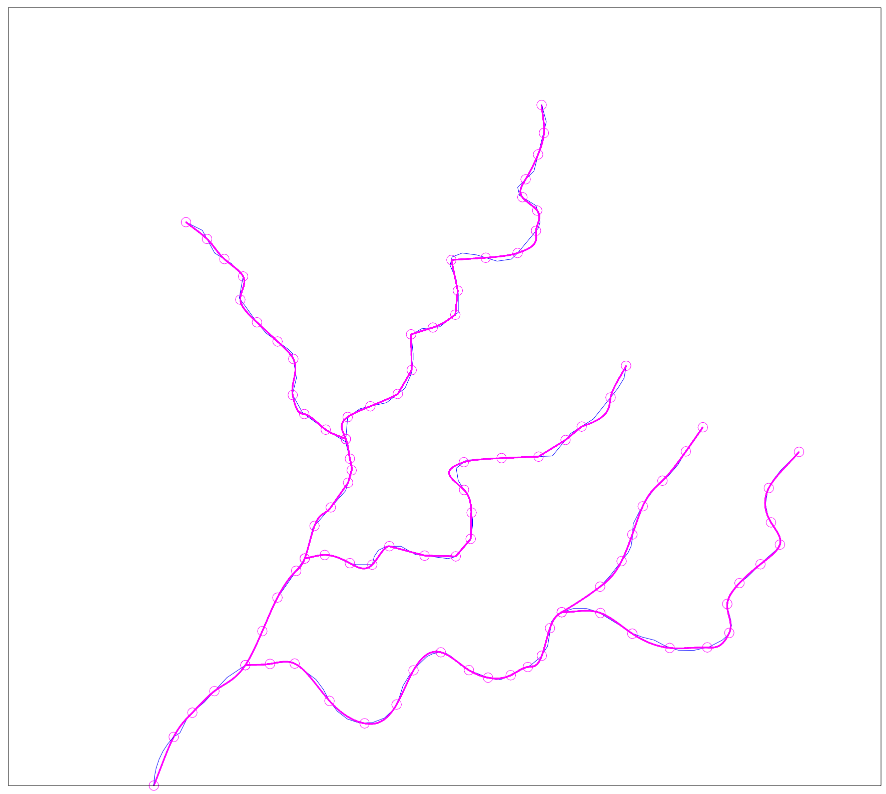
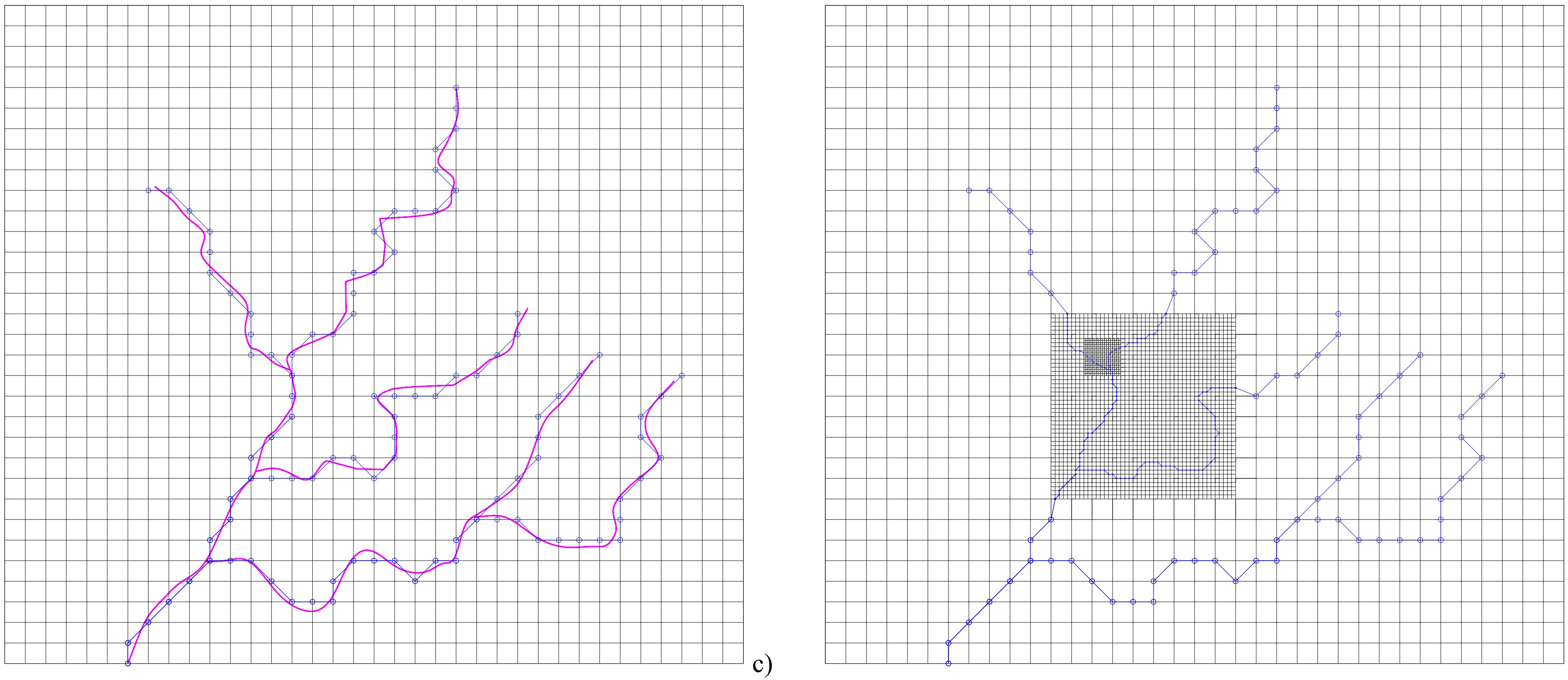

b)

Figure 5 a) Spline data points along the river channel. b) Mathematical description of the real river as cubic splines through spline points



c) d)

Figure 6 **a) Construction of model rivers nodes by interrogation of the cubic splines by the base grid object and b) Regeneration of the model river nodes after local mesh refinement by re-interrogation of the cubic splines by each of the model grid objects.**

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7 Glossary of Object-Oriented Terms

Abstraction	A mental facility that permits one to view problems with varying degrees of detail depending on the current context of the problem.
Architecture	The logical and physical structure of a system, forged by all the strategic and tactical design decisions applied during development.
Class	The definition or blueprint for an object.
Encapsulation	The property of being a self-contained unit. Coding an object so that it contains, manages, and controls access to its own data.
Framework	A set of interrelated reusable classes that form the basis for an application.
Inheritance	i) The ability to build objects that are derived from existing objects. ii) A relationship among classes, wherein one class shares the structure or behaviour defined in one (single inheritance) or more (multiple inheritance) other (parent) classes. Inheritance defines an "is-a" hierarchy among classes in which a subclass inherits from one or more generalized superclasses; a subclass typically specializes a superclass by augmenting or redefining its existing structure and behaviour.
Object	Something you can do things to. An object has both data and functionality that define its behaviour. The structure and behaviour of similar objects are defined in their common class.
Object-Oriented Programming	*i) Object-oriented programming is a programming technique that speeds the development of programs and makes them easier to maintain through the re-use of "objects" that have behaviours, characteristics, and relationships associated with them. The objects are organized into collections, which are then available for building and maintaining applications. Each object is part of a class of objects, which are united via "inheritance" and share certain characteristics and relationships.* ii) A method of implementation in which programs are organized as cooperative collections of objects, each of which represents an instance of some class, and whose classes are all members of a hierarchy of classes united via inheritance relationships.
Polymorphism	The idea that different objects do the "right thing". Poly means many, and morph means form. Polymorphism refers to the same name taking many forms (Liberty and Hord, 1996). That is, polymorphism is the attribute that allows one interface to control access to a general class of actions. The specific action selected is determined by the exact nature of the situation. A real world example of polymorphism is a thermostat. No matter what type of heating system (gas, oil, electric etc) a house has, the thermostat works in the same way. This same principle applies in OO programming. A function can be developed to act on a number of different objects. The code determines which procedure to run depending on which object is being operated on by the function. Polymorphism helps reduce complexity by allowing the same interface to be used to access a general class of actions.
Subclass	A class that inherits from one of more classes (which are called its immediate superclasses).
Superclass	The class from which another class inherits (which is called its immediate subclass).

Appendix 1 Further discussion of the benefits of the object-oriented approach

Most groundwater models are written using procedural programming languages. Procedural programming is the forerunner to object-oriented programming. In this earlier method the system is decomposed into a series of operations that act on data, the most fundamental of which is the program statement. Consequently, the development of a procedural program involves the identification of the steps that are required to achieve some result; that is, the identification of the algorithm. In this approach, the data is separate from the procedures that act upon them and the important programming task is to ensure that the operation of the procedures is well understood. This means that the data should not be altered unexpectedly.

As procedural programming was applied to more complex problems it became difficult to understand the code and monitor the effect that procedures had on the data (Ponnambalam and Alguindigue, 1997). This drawback spawned the development of structured programming based on the concept of functions. In this case the program is simplified by breaking it down into smaller subprograms, each of which performs a subtask of the overall algorithm. The principle is one of divide and conquer. Any task that is too complex is decomposed into a set of functions, each of which is sufficiently small that it is easily understood. Structured procedural programming has been and still is a commonly used and successful approach for dealing with complex problems. This is particularly true for numerical computation applications. However, as Liberty and Hord (1996) state:

> *"... some of its deficiencies became all too clear. First, the separation of data from the tasks that manipulate the data became harder and harder. It is natural to think of your data and what you can do with your data as related ideas.*
>
> *Second, programmers often had difficulty structuring a program to solve a problem while solving the problem at the same time. It was a classic inability to see the forest for the trees. Instead of solving problems, they often spent their time reinventing new ways to fit the problem to the structure."*

The problem of the creation of a maze of algorithms when modelling complex systems spawned the development of the object-model. This is based on the principle that it is natural to think of data and the tasks that can be performed on that data as related ideas. Object-orientation is described by Khoshafian and Abnous (1995) as:

> *"... the software modelling and development disciplines that make it easy to construct complex systems from individual components.*
>
> *The intuitive appeal of object-orientation is that it provides better concepts and tools with which to model and represent the real world as closely as possible. The advantages in programming in data modelling are many."*

Conceptually object-orientation is based on the principle of abstraction to deal with complexity. Through the use of objects, which contain both data and the functions that operate on it, complex systems are decomposed into separate, discrete units. The maze of algorithms all acting on the same data that arises in procedural programs is transformed into a system of objects each with its own well-defined behaviour. Through the use of abstraction computational objects are designed to represent objects in the real world; a major advantage of the programming paradigm. Not only can classes, the templates for objects, be defined to have a similar structure to features in reality but they can also be designed to be manipulated in the same way.

The correspondence between user defined classes and real world objects also simplifies the translation of a problem from the design stage into a program. This is because a more consistent language can be used over the development life cycle of a program. Collaboration between the eventual users and the model developers is made easier because both can consider the same objects. Even though each group visualises the mechanics of an object differently, the use of a common language allows the parties to consider its behaviour jointly. This results in the development of programs that better fulfil the requirements of users, be they groundwater models or not. As Khoshafian and Abnous (1995) state:

> *"Object-orientation provides better paradigms and tools for interacting easily with a computational environment, using familiar metaphors."*

Appendix 2 Literature review of object-oriented groundwater research

A number of investigators have used object-orientation to improve the implementation of numerical methods for solving groundwater flow problems. Desitter et al. (2000) examine the use of object-oriented techniques to overcome the problems associated with procedural programming methods. They state:

> *"Object-oriented programming and modern code development now enable the construction of a new generation of environmental modelling systems that offer the possibility of an open, easily maintained and easily extensible framework for code development. The speed at which new models can be developed or upgraded can be significantly increased by object-oriented programming and the confidence that can be placed in such codes is also higher as the basic building blocks are subjected to a greater degree of scrutiny."*

They illustrate this by developing a generalised framework of finite element objects, which can be adapted easily to solve different systems of partial differential equations. They apply the model to solve Richard's Equations for unsaturated flow in one and two dimensions and use it to show the complexity of the code which can be developed in a short period of time.

Krabbe and Matheja (1997) develop an object-oriented framework for the development of a distributed transport model using the random walk method. To overcome some of the problems associated with the random walk technique the investigators propose the use of a significantly increased number of particles. For example, they state that meaningless concentrations may appear in parts of the models area with low particle numbers. To facilitate the management of a large number of particles they develop an object-oriented framework to manage the random walk process using multi-threading; a method by which computational effort can be split between multiple processors.

Tucker et al. (2001) also present an object-oriented framework for the simulation of hydrologic and geomorphic systems. They describe the representation of elements of a triangulated irregular network and their associated polygonal cells as objects. These are used to solve partial differential mass balance equations to simulate, for example groundwater flow. They state that the object-oriented approach provides an efficient means of both storing and interrogating the triangulation network. It is also concluded that the strategy enhances modularity and portability and has the potential to reduce software development time.

An organisation that has started to develop object-oriented models for the simulation of large regional surface-groundwater systems is the South Florida Water Management District, US. Larrondo-Petrie and France (1995) describe the application of object-oriented analysis in the development of a framework for the incorporation into the South Florida Water Management Model. This analysis is performed to describe the mechanisms, terminology and interactions contained in the current suite of models that are used to simulate surface water and groundwater water flow and quality and ecological processes in the area.

The motivation for the work is described by the investigators and is relevant to the development of the generic regional groundwater model proposed here. They state:

> *"The current simulation models [for the South Florida Water Management District] are difficult to manage and maintain. New developments in technology and methodology, such as object-orientation, distributed processing, Graphical Information Systems (GIS), visualisation techniques, graphical user interfaces (GUI), electronic information sharing through the Internet and increases in*

storage and processing power, warrant the efforts to develop a comprehensive hydrologic regional simulation model. In doing so, the integration of other District and external models will be investigated to eliminate duplication of effort, increase usability and usage and make results more consistent and accurate."

Haitjema (1999) discusses the inception of a group of groundwater model developers who are investigating object-oriented methods. The group are examining the adoption of a set of standards for the construction of analytical elements objects, for example line sinks, used in the analytical element method (AEM) for groundwater flow simulation. One of the advantages of the approach is the ability to allow individual developers to more quickly implement a new model design through the use of the resulting well tested low level components: the analytical element objects.

In addition to the development of object-oriented models to improve the implementation of numerical methods, a number of investigators have used object-oriented techniques to develop frameworks for the coupling of software components, for example, the coupling of a river basin model with decision support system (Reitsma and Carron, 1997) and the construction of tools for data management, visualisation and modelling of environmental systems (Bethers et al., 1998; Jacob, 1999; Sydelko et al., 2000).