Client:
Environment Agency, UK

National Groundwater Modelling System

Phase 2 – Detailed architectural design (Change Control Note 2005/03)

Software Requirements Document

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Preface

Groundwater Models have been in use by the Agency and its predecessors for many years and these have been initiated and implemented at Regional level. These models were not linked in a national context. Groundwater models are also costly and have not been easily linked to the needs of operational customers. The fragmented approach to modelling was highlighted by the development of source protection zones in the early 1990's. It was recognised that a centrally co-ordinated, strategic approach was required to avoid duplication and reduce the risk of challenge.

To address this situation, a Strategic Review of Groundwater Modelling (R&D Project W6-034, R&D Technical Report W214; Brown and Hulme, 2001) was undertaken. The main output of the Strategic Review was the *Environment Agency Framework for Groundwater Resources Conceptual and Numerical Modelling* (R&D Technical Report W214) which contained a nationally consistent technical approach and programme for regional groundwater resources assessment and modelling.

The Head Office Hydrogeology Team presented a summary *Implementation Plan* for this work jointly with the Science Group which was accepted by the national Water Resource Management Team (WRMT) in October 2004. Regional modelling strategies were also recognised by WRMT as strategic Water Resources capital programmes. This work therefore supports the Streamlining Abstraction Processes (SAP) and Restoring Sustainable Abstraction (RSA) programmes managed by the national Water Resources Regulation team.

The Head Office Hydrogeology team is now developing a more detailed *Implementation Strategy* comprising a series of measures to support groundwater modelling, ensuring appropriate national consistency, improving efficiency and accessibility by customers. The Implementation Strategy will address concerns like national planning of model development, benefit realisation, succession planning, business efficiency, IS performance, and customer accessibility to models.
An *IT Strategy for Groundwater Resource Assessment and Modelling* is being prepared to address the infrastructure and IS performance issues.

The National Flood Forecasting Projects (NFFS) is currently implementing an IT architecture for a centrally hosted flood forecasting system for the Environment Agency (EA). It is recognised that there are strong links between the proposed IT Strategy for Groundwater Modelling and the NFFS. A feasibility study has been conducted which concluded that the IT-backbone, named National Groundwater Modelling System (NGMS), can be based on the NFFS architecture (and software components) if some minor modifications and extensions are implemented. This outcome was the starting point of phase 2, the detailed architectural design. In this phase the required modifications and extensions need to be made explicit.

Phase 2 of the NGMS will produce the following documents…
1. Update of phase 1 User Requirements Document (URD)
2. Update of phase 1 Software Requirements Document (SRD)
3. Architecture Design Document (ADD)
4. User Interface Specification Document (UISD)

5. Interface Definition Document (IDD)
6. Hardware and Infrastructure Design document (HID)
7. Update of Project Implementation Plan (PIP)

This document is presents the Software Requirements based on the discussions of 20 May 2005, 20-21 June 2005 and the written feedback provided by EA.

Guide to the reader

The document lying before you provides the high level functional software requirements for the *National Groundwater Modelling System (NGMS)*. This design document is intended to provide an answer to the following question: *"What will the NGMS do for me?"*

The level of detail that is contained within this document is limited to providing the reader an overall picture of the software functionality.

New in this document

The following updates have been made in this version:

- The name of the system is now National Groundwater Modelling System (NGMS)
- The role Administrator is now called Custodian
- The data storage requirement has been updated

Contents

1 Introduction

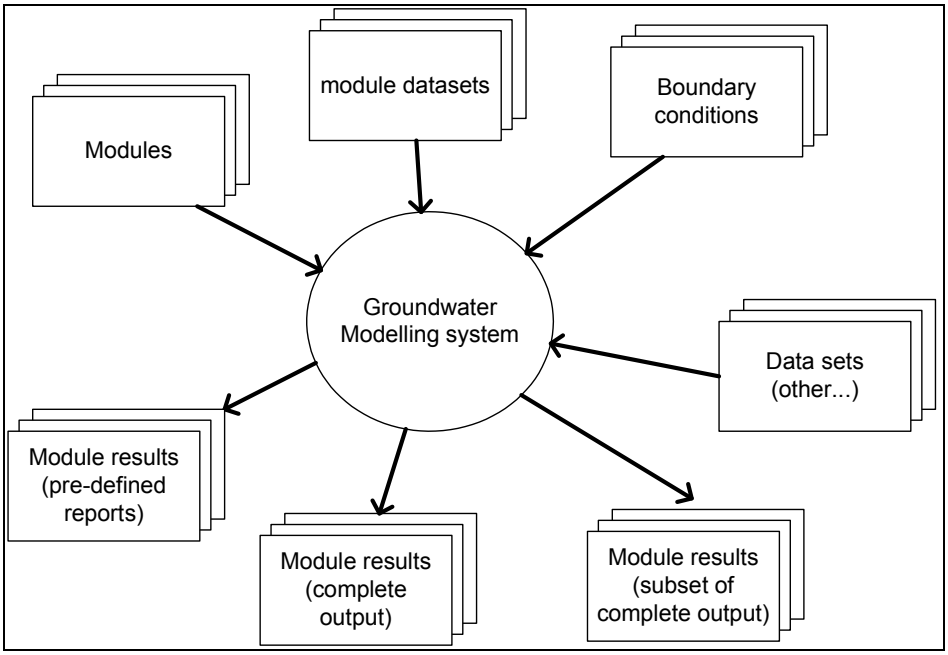
Current Groundwater Modelling systems used with the Environment Agency (EA) are operated and maintained on a number of standalone servers. This means that models (and the associated data, both input and output) are hard to access and that the effort required performing a module run is excessive.

A centralised system has a number of key benefits:

- Ability to execute model runs efficiently and with minimal system knowledge.
- Change Management controls on modules, module data sets, output etc.
- Wider access to module data (input and output)
- Increased knowledge sharing

System Context

The diagram below shows the Groundwater Modelling system in the centre and all the information and control flows across the system boundary. It illustrates external systems or components that are likely to have an interaction with a Groundwater Modelling system and need to be considered when proposing a solution.



The external entities are described below:

- **Module**
  These are executable(s) that encapsulate the underlying physics of Groundwater modelling (for example Modflow96).

- **Module datasets**
  Module datasets are the parameterisation of the physical aspects of the groundwater system (aquifers etc.) and the system parameters. These parameters are derived from, among other data, geological maps etc.

- **Boundary conditions**
  The criteria that describe the situation being modelled. These include, for example, precipitation and evaporation for the recharge modules, and recharge and abstractions for the groundwater models.

- **Module results (complete output)**
  The output file created when executing the Module (e.g. Modflow). These files consist of a number of data values per model cell and per time step. The size of these output files can be quite considerable, in some cases reaching several GBs.

- **Module results (subset of complete output)**
  A subset of the data contained within the Module output file. These subsets are typically created via bespoke applications, which extract the appropriate data from the complete results data file.

- **Module results (pre-defined reports)**
  A report (graphs and tables) in a pre-defined format. These will be generated using the output from a Module run.

General constraints and assumptions

In assessing the user requirements for a Groundwater Modelling system, a number of constraints and assumptions have been noted. These have an impact on the type of functionality that can be provided by a system and the suitability for potential system architectures.

The assumptions and constraints identified at this stage are listed below:

- The module input and output files can be large.
  They can range from ~Mb's up to over 10 GB's. Initial analysis has shown that they do compress (using Winzip) quite considerably but the resulting files are still of the order 10-100MBs.

- Only subsets of the module output files are ever used in analysis and reporting.
  The full output from a Module run is rarely analysed in its entirety, usually slices are taken on a spatial or temporal basis for further investigation.

- Module run times can exceed 12 hours.
  This is not expected to be an issue as this is the expected duration for most large scale models.

- The scope of the system is to provide an environment to execute pre-configure Groundwater modules, not to provide a complete module development environment.

- As well as a centralised system, there is considerable benefit in having a version of the system that can operate in "stand-alone" mode. This could prove useful in enabling model development, demonstrations of models and output to third parties etc.

2 General requirements

The following general software requirements are identified.

Nr.	Requirement
1	IT solution must conform to the Agency's published Enterprise Architecture principles:- "Hosting Principles", "Information Layer principles" and "Overarching Principles" (2 11/2004).
2	IT solution must conform to the Agency's published Technical Standards.
3	IT solution must not adversely impact existing services or applications in respect of its use of shared Agency infrastructure. More specifically, the IT solution should offer functionality to restrict the network load for example by limiting the maximum file size sent and the data flow.

3 User Interface

The interface provides the user with the main link to the system. The key functionality is described in the table below. Note that the possible types of interfaces (and the functionality they provide) could be quite varied, for example, the interface could range from:

- A client application that just allows the downloading of the results (raw output files) and saving to the local disk. The data can then be analysed using existing tools, or
- A client application that includes the tools to display and manipulate the data.

The actual development of the interface would likely follow an evolutionary path, i.e. start out with the basic NFFS functionality extended with a basic "download-only" and then progress to a more fully featured client application.

Nr.	Functionality	Who	Description	Ref[1]
1	Configure boundary condition datasets	Custodian	Define the datasets associated with the boundary conditions. These datasets should be located in the central datastore and should be available for selection (to be used as part of a module run or for update and review).	UC 5.7
2	Configure report types	Custodian NSU	Define the format and contents of the report templates. The reports should be generated automatically by the system and be ready for displayed via the Web Server.	UC 5.7
3	Configure what-if scenarios	Custodian	Configure the set of options that are allowed when making alternative module runs.	UC 5.7
4	Configuration of other utilities	Custodian NSU	Configure other parts of the system • Workflows (batches) • Post processing profiles • Graph & map displays • Etc.	UC 5.7
5	View module input data sets		Enable viewing of module data sets (input) e.g. by providing meta data details and map displays on a OS base map	UC 4.11
6	Select module & module dataset and scenario (package) to execute.	User	Select the module, the appropriate dataset and the scenario to be used in a model run. The datasets should be maintained within the central datastore.	UC 4.3, 4.4
7	Submit package to be executed	User	Submit a request to execute a particular module run with an associated dataset.	UC 4.3 4.4

Nr.	Functionality	Who	Description	Ref[1]
9	Configure spatial slicing profile	User	The user should be able to select, on a static map layer, an area or location(set) which provides the 'cookie cutter' how to extract a susbset of data from the raw output set.	UC 4.12
10	Configure standard post-processing profile	User	Combine variable selection, time frame, spatial slice with a default graphic layout option	UC 4.13
11	Configure custom post-processing profile		Combine variable selection, time frame, spatial slice with a user defined set of data manipulation functions	4.1.9
12	Select subsets of module results (includes selecting previous output runs)	User	Select data subsets of a module run output file (this subset may be created during the workflow by specification a post-processing profile)	UC 4.13
13	View subsets of model results in pre-defined and user defined selections	User	View data subsets in tables, graphs and maps. This also includes comparison of runs and presentations of differences (e.g. with base case).	UC 4.5, 4.6
14	Export subsets of module results	User	Download selected data subsets to a client in PI, shape or xls format (supported data format depends on data set type).	UC 4.7
15	Selection of (subsets) of output data to be viewed or downloaded via a map based interface		The user should be able to select (subsets of) output datasets via a map based interface. The map layer can be static and serve as background only for geographical reference.	UC 4.12
16	Modify boundary condition sets (limited; undefined)	User	Perform limited modification (subject to certain criteria) of the boundary condition sets. The modified boundary condition sets would be marked as a new version of the original dataset and would be maintained in the central datastore.	UC 4.1
17	Modify boundary condition datasets (pre-defined type of changes)	User	Perform limited modification (subject to certain criteria) of the boundary condition datasets. This modification should be carried via definition of what-if scenarios. If what-if scenarios are applied this should will be registered by the system.	UC 4.1
19	Modify boundary condition datasets	Custodian	Perform unlimited modification of the boundary condition datasets. The modified datasets would be marked as a new version of the original dataset and would be maintained in the central data-store and made accessible via the cobnfiguration.	UC 4.1
20	Selection of (subsets of)		The user should be able to select (subsets	UC

Nr.	Functionality	Who	Description	Ref[1]
	boundary condition datasets to modified via a map based interface.		of) boundary condition sets via a map based interface. The map layer can be static and serve as background only for geographical reference.	4.1
21	Export module datasets & boundary condition sets	Custodian	Download module datasets and boundary conditions sets from the Groundwater modelling system in raw, PI, shape or xls format (supported data format depends on data set type)	UC 5.3, 5.6
22	Upload module datasets & boundary condition sets	Custodian	Upload new or modified module datasets and boundary condition sets into the Groundwater modelling system.	UC 5.2, 5.5
23	Archive (and retrieve) critical module runs or sets of module runs	User	Archive (sets) of module runs with input and output data. Retrieve archived module runs. This is *no* generic backup functionality.	UC 4.8, 4.14
24	Publish model results to web server	User	Select subsets from module output (predefined tables, graphs, reports & user specific information) and export to disk where it can be handed over to webserver	UC 4.10
25	Access to system from outside EA network	User	Getting access to the EA network from outside the EA network.	UC 4 (all)
26	Setting user access levels	System	It is required that user access levels can be set for all types of users (roles) within and outside the EA.	UC 7.3
27	Restricting data flows over network	System	The required LAN and WAN capacity for communication between server and clients (flow and size of individual files) should be restricted. The maximum data flow and package size should be configurable.	UC 4, 5, 6
28	Manage module runs to prevent overflow of disk accounts		Enable deletion of module runs and data sets within a module run to keep conrol of the temporary data store	UC 7.3
29	Capture all relevant meta data on a module run in a logbook	User	Provide a logbook structure to capture meta data. Populate automatically where possible (e.g. file references). Check on empty fields	UC 4.8

[1] Refers to use cases in User Requirements Document

Future requirements

4 Running modules

All software requirements in this section related to the following Use Cases: 4.1.3, 4.1.4, 4.2.3, 4.2.4, 4.3.2, 4.3.3 and 6.2.

4.1 Task Controller/Dispatcher

Nr.	Functionality	Who	Description	Ref
1	Dispatch of tasks	System	Performs the dispatch of the tasks (e.g. a module run) to the appropriate module controller for subsequent execution. The tasks should be scheduled to be dispatched at a particular time or ASAP. It should be possible to specify the dispatch destination (in the scenario of having multiple module controllers and associated hardware).	
2	Monitoring of status of tasks	System	Monitor and report the status of tasks (via feedback from the modules and Module Controller), including, • when they have been dispatched by whom • progress on task execution • automated analysis of module check parameters (to be performed on a regular discrete basis), to be displayed on request • details of task completion	
3	Prioritisation of tasks	System	It should be possible to give priorities to tasks either pre-defined on the basis of the type of task or user defined.	
4	Interruption of tasks	System	Automatically interrupt the execution in case of unexpected run-time duration or unexpected output file size (both pre-defined by custodian as part of module data set)	

4.2 Module Controller

Nr.	Functionality	Who	Description	Ref
1	Module execution	System	Initiate execution of the task (via a batch or script file).	

Nr.	Functionality	Who	Description	Ref
2	Monitoring of status of task	System	Obtain status information and report back to task controller/dispatcher.	
3	Communication between system and module adapter via a standard XML format.	System	The communication between the system and module adapters runs via a standard XML exchange format (the NFFS Published Interface)	
4	Tracking of input, output and versions		Functionality is required for automatic tracking which input and output data relate to a module. Also version of modules, module datasets, boundary condition sets etc should be registered. This track record needs to be included in the model run's logbook (see UI-Req….)	

4.3 Module

Nr.	Functionality	Who	Description	Ref
1	Provide groundwater modelling capability	System	The following modules are assumed to be run from the system: • Groundwater modules… – Modflow (96, VKD) • Recharge module (custodians only) – 4R – EA recharge code • In a later stage of development this set of modules might be extended with – MODPATH – ICMM – ZOOMQ3D – MikeSHE Other module types are expected to be replaced in the near future by one of the above mentioned modules.	

4.4 Adapter

Nr.	Functionality	Who	Description	Ref
1	Provide a module interface between Groundwater Modelling system and third party	System	The NFFS Publsihed interface will be utilized for communication between the system and modules. Where required the PI-definition will be extended. The	

	modules.		system will be able to connect to modules that can communicate in the PI format. For each module type, a module adapter has to be developed that communicates in the PI format. Adapters are required for: • Groundwater modules… – Modflow (96, VKD) • Recharge module – 4R – EA recharge code • In a later stage of development this set of modules might be extended with – MODPATH – ICMM – ZOOMQ3D – MikeSHE	

5 Data Manipulation Utilities

Nr.	Functionality	Who	Description	Ref
1	Storage of data in standard format file	System	The raw output from all modules should be stored in a standard file format (time series, grids, parameters, diagnostics etc.). As far as possible and practical, existing standards should be adopted. All data manipulation tools will work on the standard files	4
2	Cookie cutter to slice output files and store resulting files.	System	Perform a pre-defined operation on the output file obtained from a module run. The available operations are defined by the spatial slicing profile in combination with the variable selection, the vertical layer selection and the time frame should include selections of subsets of the data (by cell location/area and/or time-step).	4.5
3	Processing output files on request of user (standard processing)	System	Processing of output files can be either done in workflows following the module run or triggered by a user. The following type of processing is required: • Stream accretion: XY-profile along river/streamline (cell 1,2,3…n) of flow accumulation, either at an instantaneous moment in time or as time averaged. Used to display the gain and loss of surface water along the open water body from and to the aquifer. X-axis = cell/node ID's, Y-axis = accumulated flow rate • stream outflow hydrograph: XY-time line of flow passing at cell x (i.e. accumulation of upstream outflows) X-axis = (absolute) time, Y-axis = flow through cell x • Splodge plots Map-view of locations where data set	4.5, 4.6

			values are represented with proportional circles • Winterbourne signature: Series of vertical lines, where each line represents a time step, and the vertical represents the river sections. For each time line is indicated when a certain threshold of the flow (e.g. zero flow) is passed. Colours may be used to indicate the flow value • Ground water unit budget – map overview for entire model area: Map-view of ground water units with cumulative horizontal flows between the units. This can be either averaged flows, accumulated flows (i.e. volumes) • Groundwater unit budget - Vertical view for selected groundwater unit Cross section of layers with inflows and outflows (both horizontal and vertical) • Duration curves • Frequency curves • Bar charts • Map view of isolines - Contour plots • Tables using format templates	
4	Processing output files on request of user (user-defined processing)	System	Processing of output files can be either done in workflows following the module run or triggered by a user. The following type of user defined processing is to be supported: basic statistics for each spatially defined unit: • temporal mean./min./max./standard deviation/accumulation • accumulation by distance (= accretion for streamlines) for each time step • spatial mean/min./max./standard deviation/accumulation for each averaged time span/each time	4.6

			span minimum/each time span maximum • spatial mean/min./max./standard deviation/accumulation (low priority) • temporal threshold exceedance • spatial threshold exceedance (contour lines) • frequency (temporal) • classification basic mathematics: • difference • proportion • change over time	

6 Publication of results

6.1 Report Publisher

Nr.	Functionality	Who	Description	Ref
1	Preparation of pre-defined reports	System	The system should be able to generate predefined reports. The reports are prepared in HTML format and web-compatible figure format (e.g. jpeg/gif/png)	UC 3.1, 3.2
2	Publish predefined reports	System	Transfer the reports from the central system to a network disk from where it can be taken manually for further processing and publication on the Web Server	UC 3.1, 3.2

6.2 Results Display

Nr.	Functionality	Who	Description	Ref
1	Select pre-defined reports	User	Select one of the published reports for display.	UC 3.1, 3.2
2	View predefined reports	Viewer	Display (or download) a selected report.	UC 3.1, 3.2
3	Printing of reports	Viewer	Print a selected report	UC 3.1, 3.2
4	Download of reports	Viewer	Download a selected report in a fixed format (e.g. PDF format).	UC 3.1, 3.2

7 Import and Export

Nr.	Functionality	Who	Description	Ref
1	Import datasets	System	Import the external datasets into the system for storage.	
2	Export datasets	System	Export data from the central system to a defined location in defined formats. These may be: • Standard EA formats for time series and grids (much preferred!) • ASCII, XLS, Shape	

8 Database and Archive

The Central Storage is meant to kept information for a defined period of time (rolling barrel). When this period expires, the information (data) is removed from the system.

In case data should be kept for later use, this data should be archived before it expires. Therefore an archive utility is required.

8.1 Central Storage

Nr.	Functionality	Who	Description	Ref
1	Provide a repository for the module datasets	System	This allows selection for use in other module runs.	
2	Provide a repository for the module boundary condition datasets	System	This allows selection for use in other module runs.	
3	Provide a repository for the module run output datasets (complete)	System	Allows access to the data manipulation utilities.	
4	Provide a repository for the module run output datasets (subsets)	System	These datasets result from the operation of the data manipulation utilities ("slicing").	
5	Provide a repository for what-if scenarios	System		
6	Provide a repository for pre-defined report templates.	System		
7	Provide a repository for report output files.	System		
8	Provide repository for archived runs	System		UC.4.8

The central storage is likely to take the form of an Oracle database (as with the NFFS architecture) together with storage of files on disk. The majority of the data will be the large input and output files. The database will store a reference to the location of the files; they will not be stored within the database itself.

8.2 Archiving

Nr.	Functionality	Who	Description	Ref
1	Archiving a selected module with all input and user selected parts of the output.	User	It is required to be able to make an archive of a selected module run with all relevant input and output data. Selection of parts of output that should be included in the archive is required. Archiving requires the system to automatically track all input and output data that relate to a module run. Also references to for example module versions are required.	UC 4.8
2	Restoring of archives	User	It should be possible to restore an archive into the system for rerunning.	UC 4.9
3	Export of archives	User	Allow the archiving of module run data (input and output) to a defined location or database.	UC 4.7, 4.9

9 Data volumes

This section attempts to detail the potential data volumes associated with the Groundwater Modelling system. The assumptions and sample data figures are those that have been obtained during the various workshops and site visits.

In the table below an overview is presented of the collected information.

Module dataset	**Input file sizes**	**Output file sizes**	**Nr of runs per year**
Midlands (3 GW module datasets)			
• West Midlands Worfe (Modflow)	150 Mb (17 Mb zipped)	Raw output: 1.9 GB (sample files showed 75% reduction when zipped) Post processed output: 45 Mb (13 Mb zipped)	0 to 20
• East Shropshire (Modflow)	201 Mb	2 Gb	0 to 20
• *New* Notts-Doncaster-Selby (Modflow)		4 Gb (estimate)	
Southern (7 GW module datasets) Examples:			
• Dour (ICMM)	8 Mb	Raw output: 223 Mb	20
• Itchen (4R)	631 Mb ?	100 Kb	?
• Itchen (Modflow VKD)	?	Raw output: 972 Mb	
Anglian (development of 8 GW module datasets planned) Examples:			

Module dataset	Input file sizes	Output file sizes	Nr of runs per year
• Yare & North Norfolk (Modflow VKD)	Recharge file (RCH)… 701 Mb (480 stress periods) (or 21 Gb for daily stress period for a 40 year period) Stream file (STR)… 1.9 Gb (480 stress periods) (or 58 Gb for daily stress period for a 40 year period) In total: input file size equals 5.5–7 Mb per stress period.	Full output: 14 Gb With recharge, abstraction & evaporation: 18 Gb (Yare & North Norfolk model has 6 layers, 315 rows, 395 columns)	6 critical runs to be stored 60-90 non-critical runs
<u>Thames</u> (4 GW module datasets)			
• Kennet (Modflow)	300 Mb	2Gb	0-20
• London Basin Model (ICMM)	100 Mb	1 Gb (?)	0-5
• Mimram (Upper Lee) (Modflow)	150 Mb	1 Gb	0-10
• Colne (Modflow)	300 Mb	2 Gb	0-10
<u>Northeast</u> (3 GW module datasets)			
• Chalk model	3 Mb	4.5 Mb	0-10
• Sandstone model	355 Mb	430 Mb	?
• Corallian model	31 Mb	42 Mb	not run for 3 yrs
<u>Northwest</u> (4 GW module datasets)			
• Wirral (Modflow)	200 Mb	300 Mb	0-5
• East Cheshire (Modflow)	70 Mb	200 Mb	0-5
• Sefton	240 Mb	880 Mb	0-4

Module dataset	Input file sizes	Output file sizes	Nr of runs per year
(Modflow) • Fylde (ICMM)	2 Mb	70 Mb	0-2
Southwest (5 GW module datasets) • Bourne & Nine Mile (Modflow)	529 Mb (zipped: 70 Mb)	1.6 Gb	10-20
• Avon (Modflow)	3 Gb (zipped: 300 Mb)	4.2 Gb (zipped 1.8 Gb)	> 30 (but not all need archiving)
• New Wylye (Modflow)	1.9 Gb	637 Mb	
• Future Stour Frome and Piddle (Modflow)	3 Gb (zipped: 300 Mb)	4.2 Gb (zipped: 1.8 Gb)	> 30 (but not all need archiving)
• River Allen	?	?	?
Wales (???)			
Science Group (no other module datasets than run by the regions) • Operational models (testing purposes)	500 Mb	1 Gb	10
• EA recharge code	1 Gb	1-2 Gb	50
• ZOOMQ3D	500 Mb	500 Mb	50

Please note that no data is obtained for Wales.

Based on the above mentioned table the following assumption are derived about data volumes:

Total data storage required to accommodate volume related module runs on an annual basis for the coming 2-3 years is…

- Number of module datasets operational in NGMS: 40
- Average data volume per run: 6 Gb
- Average number runs per year: 10
- Total annual storage requirement: 2400 Gb

The total annual storage requirement may be reduced by 50-75 % to 600-1200 Gb storing files in compressed formats.

When the NGMS becomes operational, especially the number of runs made with the system are expected to increase. It is assumed that in 3-5 years, the average number of runs made per year are doubled. This means that the total annual data storage requirement may also double.

Summarizing, it is noted that…

- Data storage requirements are large: > 1000 Gb annually
- Flexibility is required with respect to the capacity of the data storage facility
- A large part of the storage is rather static. The data storage capacity that should be directly available to the users is probably around 20 % of the total required capacity.

Overruling statement by EA regarding storage requirements

An additional analysis by the groundwater modelling team has determined that the initial disk capacity requirement will be around 300 Gb. Annually, the disk space requirement is expected to increase by 25 %. This means that in 5 years time the disk space requirement will be around 900 Gb.

The abovement mentioned reduced figures are to be applied in the technical options assessment and the business case.