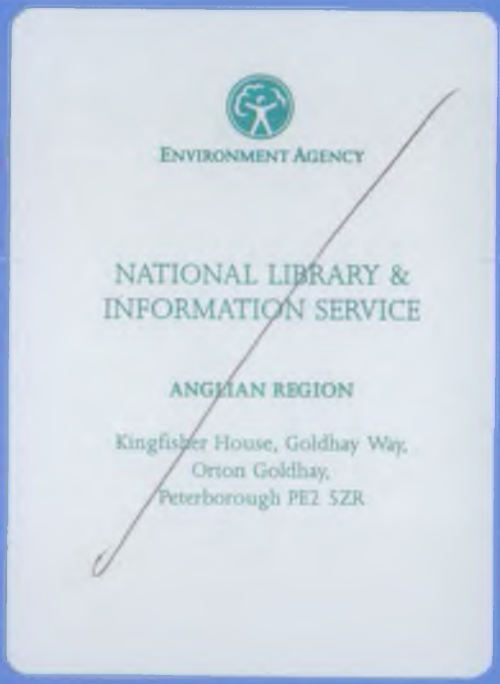
R&D Project 0295
Geochemical process modelling

Progress Report for Period
March - June 1991



British Geological Survey
Hydrogeology Group
July 1991

Progress Report 0295/1/A

NRA
National Rivers Authority

Geochemical process modelling

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Progress Report 0925/1/A

This report has been produced
under contract to the
National Rivers Authority by the

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1. INTRODUCTION

This is the first progress report on an R&D project concerned with the modelling of geochemical processes that are important in determining the quality of groundwater.

The inception of the project started with a draft Project Investment Appraisal (PIA) for from (the late) M Morgan-Jones in April 1990. After a series of written exchanges and meetings the final PIA form was completed by M W Grout in February 1991 and the project began on 1 March 1991. The project is to run for three years, finishing at the end of December 1993.

The work is to be mainly carried out within the Hydrogeology Group of the British Geological Survey (BGS), but two staff from the Fluid Processes Group have minor involvement because of their specialist knowledge.

No progress report was required at the end of the 1990/91 financial year as the project had then only been running for one month.

The following names appear in this progress report:-

NAME		ROLE IN PROJECT
M Morgan-Jones	NRA	Former Project Leader
M W Grout	NRA	Project Leader
G C Brighty	NRA	R & D Co-ordinator
J A Barker	BGS	Project Manager
P Cottis	BGS	Finance Officer (has taken over from A Cox)

2. SUMMARY OF PROGRESS

2.1 Reviewing

Six BGS scientists have individually begun collecting relevant references, each in their own area of specialisation. Several previously-conducted on-line literature searches that are relevant to this project have been identified; some further searches have been requested and others planned.

A large amount of reference material will be collected over the period of the project, it has been decided that it will be necessary to use a computer database to store that information. Literature describing a number of (reference) database packages has been obtained and the BGS library have been asked to provide a recommendation of the choice. It is intended that information collected during on-line searches can be pulled directly into the chosen database.

2.2 Software

After a brief review of database packages for personal computers, the DBase IV database package was purchased. This is already in use in the Hydrogeology Group; in particular, by the aquifer properties section who will be aiming to provide a database of aquifer properties for this project. It is intended that DBase IV will also be used for storing geochemical parameters and lists of models. Initially, it had been hoped that the DBase IV database package would also be suitable for collecting references, but after some investigation it was decided that a specialist package would be required.

A Fortran compiler for Personal Computers has been purchased in anticipation of modelling work later in the project.

2.3 Books

Three books have been purchased. Two of these are specifically concerned with recent work on modelling of the unsaturated zone (an area where particular problems were anticipated with regard to producing practical models): *Field-Scale Water and Solute Flux in Soils*, eds. K Roth et al; *Transfer Functions and Solute Movement through Soil*, W A Jury & K Roth. The other book is a reference manual of physicochemical data for groundwater.

3. RELATED WORK

An important aspect of the design of this project was that the BGS staff involved could feed in experience from related NRA projects. Four of the BGS scientists involved in this project have been carrying out R&D work for the NRA in the areas of:-

Aquifer protection specifications. [111]

Bacterial denitrification in aquifers. [129]

Groundwater storage in British Aquifers. [128]

Impact of broadleaf plantations on groundwater. [102]

Groundwater Pollution by synthetic organic solvents. [130]

Because of this involvement and the comparative urgency of the work, particularly on protection zones, staff time spent specifically on the geochemical process modelling project during the first three months of 1991/92 financial year has been very limited.

Other relevant NRA R&D projects within the Hydrogeology Group of BGS are:-

Aquifer protection studies using packer systems. [108]

Diffuse pollution from agricultural practices - nitrates. [113]

4. WORK PROGRAMME TO END OF SEPTEMBER 1991

(a) Continued collection and reviewing of information on modelling and processes.

(b) Preparation of a brief initial review of biochemical processes.

(c) Databasing of information on relevant models and selection of codes to purchase and evaluate. Tentative identification of needs for code development.

(d) Consideration on whether and to what extent data collected and databased by the aquifer properties section of the Hydrogeology Group, might be of value in groundwater quality prediction.

(e) Reporting on: First phase of modelling and process review; and database development, including general recommendations on databasing.

5. FINANCES

During the last financial year (1990/91) the work was invoiced at £8,000.

In a letter dated 8 May 1991, G C Brighty conveyed the following figures to J A Barker, and they have been passed on to P Cottis (BGS Finance).

PERIOD	OLD BUDGET £K	INFLATED BUDGET £K
1991/92	27.7	30.3
1992/93	23.4	25.6
1993/94	21.8	23.8

Estimates of quarterly invoicing for 1991/92 are:

April to June	£0.7K
July to September	£12.0K
October to December	£9.0K
January to March	£8.0K

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Project Manager
BGS Hydrogeology Group
Wallingford

11 July 1991