R&D Project 0295
Geochemical process modelling

Progress Report for Period
January - March 1992

British Geological Survey
Hydrogeology Group
March 1992

Progress Report 0295/4/A

Geochemical process modelling

J A BARKER

Progress Report 0925/4/A

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

British Geological Survey
Hydrogeology Group
Crowmarsh Gifford
Wallingford
Oxfordshire
OX10 8BB

1. INTRODUCTION

This is the third progress report on an R&D project concerned with the modelling of geochemical processes that are important in determining the quality of groundwater. The project began on 1 March 1991 and is due to run until the end of December 1993.

The initial phase of the project is concerned with reviewing the literature and available codes for groundwater pollution modelling. Three previous reports have been produced: The first Progress Report (R&D 0295/1/A) in July 1991, the first Interim Report (R&D 0295/2/A) in September 1991, and the second Progress Report (R&D 0295/3/A) in December 1991. The Interim Report gave a draft outline of the final review document.

2. SUMMARY OF PROGRESS

2.1 Reviewing

The process of collecting and reviewing literature relevant to the project has continued and has remained the major activity. Six BGS scientists have been involved in collecting information on: geochemical and biochemical processes, models of those processes, and applications of such models.

A number of books and reports of particular relevance to the project have been purchased and more are on order.

A review of microbiological processes (excluding modelling) has been completed and a draft report has been produced. That information will appear in the final review report. Since the work was only partly funded by the NRA, consideration is being given to turning the draft report into a BGS Technical Report in the near future. The main headings of the draft report are:-

1. Introduction
2. Microbial presence in geological formations and groundwaters
3. Controls on the growth of microbes in the subsurface
4. Microbiology and groundwater quality, pollution and contaminant movement
5. Microbiological effects on oxidation of pollutants
6. The significance of microbial activity to contaminant transport modelling
7. Conclusions

Denitrification is a problem of particular interest and has been the topic of a separate NRA/BGS project. It has not been specifically considered during the review just outlined.

2.2 Software

About 400 codes of potential use to the NRA have now been identified and included in a database. Information on those models is continually being added, but for some models little information has yet been obtained. There are currently about 50 fields in the database to characterize the models. These cover a wide range of information including: basic details

(cost, supplier, etc), transport processes (convection, dispersion, diffusion, etc), aquifer condition (confined, unconfined, isotropic, etc), computer requirements, and user-friendliness (pre-processors, post-processors, etc).

One important field is that referring to publications where the use of the models is described. It has been found convenient to create a separate reference database in the form of structured word processor (WordPerfect) files, so that the data input work can be delegated to non-scientific staff. Those files will probably be converted to a crude flat-file database which can be imported into a database such as dBase IV or a reference database.

We currently possess, have ordered, or have requested about 15% of the codes listed in the database. These have been obtained in a number of ways, both in response to this project and other work of the hydrogeology group.

3. WORK PROGRAMME TO END OF JUNE 1992

The work programme will be very much a continuation of the work over the last three months. However the emphasis will move from the collection of information to the critical assessment of material obtained.

(a) Continued reviewing of all topics relevant to the project.

(b) Completion of the review of processes and modelling. (Although the collection of information on computer models will continue beyond this phase of the project.)

(c) Continued input of information into the model database, identification of codes of potential value to the NRA.

(d) Writing of dBase IV applications programmes to sort and extract data from the database of groundwater models.

(e) Evaluation of some computer codes already available or obtained. Determine details of data needs, user-friendliness, computer hardware requirements and so on.

(f) Ordering further codes of particular merit for detailed evaluation.

(g) Preparation of a tentative list of models for NRA use. This list should attempt to provide tools to cover the important scenarios of interest to the NRA. The models will probably fall into three categories: (i) off-the-shelf models, (ii) off-the-shelf models that require some modification, and (iii) simple models that BGS can develop to fill identified gaps.

(h) Critical re-assessment of the problems of providing databases of hydrogeological and geochemical parameters (see below).

(i) Completion of the report reviewing biochemical processes (outlined earlier in this report).

The preparation of databases of parameters needed for groundwater quality models has proved to be far more tricky than originally envisaged. The main problems are: the vastness of the quantity of data of interest, copyright considerations for existing databases, and availability (including the cost of obtaining) certain types of information. The whole issue needs to be re-assessed and discussed with the NRA.

Risk assessment and quality assurance are two topics that were originally considered as part of a miscellaneous modelling review. It now seems more logical to consider these topics alongside related ones such as decision support systems within the context of the methodology development.

4. FINANCES

The financial situation will be conveyed separately - as agreed between BGS and NRA.

John A Barker
Project Manager
BGS Hydrogeology Group
Wallingford

31 March 1992