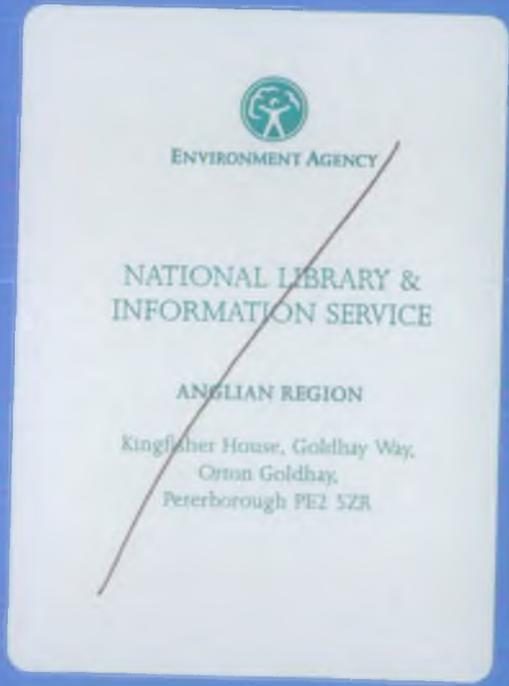R&D Project 0295
Geochemical process modelling

Progress Report for Period
~~October - December 1992~~
Jan — Mar 1993

British Geological Survey
Hydrogeology Group
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Progress Report 0295/10/A

NRA
National Rivers Authority

Geochemical process modelling

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Progress Report 0295/11/A

1. INTRODUCTION

This progress report is the eleventh report produced from the NRA R&D Project 0295 on *Geochemical Process Modelling*, which is concerned with the modelling of groundwater pollution.

A joint NRA/BGS seminar on the project was held on 10 December 1992. There were two purposes to the seminar: (i) to pass on to NRA staff concerned with groundwater model applications an outline of the results of the project thus far, and (ii) to elicit from NRA staff ideas on the most useful directions for the project to take within the flexibility allowed by the contract.

The previous progress report (0295/10/A) presented an agreed description of that seminar, concentrating on the needs of NRA that emerged from the discussions. On 3 March 1993 a follow-up meeting to the seminar was held between Mark Gout, John Barker and David Kinniburgh to discuss the outcome of the seminar; the previous progress report was used to guide those discussions. This report is mostly an agreed record of the conclusions from that meeting.

The most important consideration was to ensure that future work on the project should be well targeted on the real current needs of the NRA. The perception of those needs had changed significantly since the instigation of the project.

2. CODE DEVELOPMENT BY BGS

It was agreed that effort expended by BGS on the development of new computer code would be much better spent on advising the NRA on broader issues. This is the major change in direction of the project since its start.

The original intention was to identify 'gaps' in the range of modelling tools available and attempt to fill those gaps, taking account of specific NRA requirements. Model computer codes have proliferated at such a rate that there are now few significant gaps. Also, to prepare a robust code takes a very considerable effort (several man-years for larger codes), so it would only be possible to provide a very modest additional contribution to the available set of modelling tools within the limited project budget.

Equally important to the decision not to undertake code development was the recognition of more important current needs of the NRA with regard to modelling to which the project could make a useful contribution. These topics are outlined below.

3. MODELLING METHODOLOGY

It had always been intended that the project should be concerned in part with a critical discussion of the problems of and approach to model application. As the project has proceeded, continued discussions have revealed that it is in the broad area of how best to make use of models, whatever their state of development, that there is a great need within the NRA.

In the first technical report from the project (September 1991) the following topics were identified as warranting coverage under the methodology review:-

    a: Model selection

    b: Model validation

    c: Quality assurance

d: Risk analysis

e: Expert systems

f: Geostatistical techniques

g: Site-specific versus generic modelling

h: Distance and time scales in modelling

i: Models in data collection and analysis

That technical report provided a brief description of the relevance of each topic - which will not be repeated here.

The December 1992 modelling seminar helped to identify additional and more specific topics and sub-topics as being of concern to the NRA (see particularly Section 2.5.2 of report 0295/10/A). In particular guide-lines are required for:-

j: Deciding which combinations of pollution type, aquifer type and flow system would be of concern.

k: Estimating the influence of specific geological factors.

l: Deciding when modelling would have some net benefit.

m: Identifying which models would be appropriate in certain situations and at different stages.

n: Setting up of specific types of models (including data requirements).

o: Good modelling practice (e.g., the need to establish the flow pattern).

p: Planning and preparation of tender documents for modelling.

q: Training.

The importance of further topics came out of the discussion meeting on 3 March 1993.

r: The organisation of modelling (group size etc).

s: The relevance of models to the Groundwater Protection Policy.

t: Models and the concept of vulnerability (e.g. How do simple assessment systems such as DRASTIC relate to deterministic models?).

u: Legal aspects to modelling (e.g. What type of questions are put by lawyers in court to 'expert' witnesses using models?).

v: Models in the clean-up versus treatment debate.

BGS will aim to cover all of the above topics within the, now very broad, theme of modelling methodology. Some of them will appear as independent topics while other will more appropriately be dealt with as sub-topics. The expansion of this list is possible because of the time freed by the decision to drop the development of new modelling code from the project.

Arguably, some of the topics fall somewhat outside the modelling arena, however, BGS take the term modelling in a very broad sense and are happy to accommodate the real needs of the NRA.

4. TRAINING

Built into the project is the idea of BGS providing some training.

While BGS would be willing to provide instruction in the use of a number of modelling packages, some significant difficulties are recognized and were discussed at the follow-up meeting to the seminar:-

> 1. NRA regions are far from equally endowed with modelling staff: users of modelling results, experienced modellers, and junior modellers.
>
> 2. It would be of little value to attempt to teach groundwater modelling to complete beginners in just a day or two.
>
> 3. It would be unrealistic to expect non-chemists to appreciate the use of a geo-chemical model such as MINTEQA2.

With these in mind, it was decided that the best use of the project resources - and NRA staff time - would be to use the training time to work through a number of case studies. These cases could be either real or perhaps hypothetical cases based on one or more real cases.

The best way forward on this was seen to be for NRA to supply BGS with a set of cases of interest, well before the 'training' begins, so that BGS can work these up into instructive examples using various modelling codes.

5. DATABASING

The three fundamental ingredients of the project are: models, modelling methodology and databasing of parameters for use in models. The initial and continuing intention is that BGS would supply NRA with one or more PC-based databases of aquifer parameters and chemical parameters of value in pollution modelling. (The first technical report of the project (September 1991) discusses the various types of data of importance to modelling and the feasibility of providing databases of such information.)

The idea of what exactly those databases should contain has developed over the period of the project. In summary it is seen that:-

(1) Databasing of aquifer properties for the NRA by BGS is now being undertaking as a major independent project. (Such an effort was in fact one of the early recommendations from this project.) Within this project BGS would aim to provide summary information from that activity, as far as it had been developed by the end of this project.

(2) Geochemical parameters that can be of interest are so great in number that the best approach is:-

a.   To provide a guide to sources of parameter values (a database of databases, manuals etc.)

b.   To provide approximate values (or ranges of values) appropriate to classes of the more important pollutants.

(3)   The databasing activity should take account of the needs of the NRA decision makers who often have to make rough assessments of pollution, often in a period of a day or less.

6. NRA MODEL USE

At the discussion meeting on 3 March 1993, an important topic of discussion was who are the model users in the NRA and what are their main uses. This is not directly important to the work programme but very useful background information in that it would identify how the products of the project would be used.

It was concluded that the most important group of NRA staff who will make use of the project results are Groundwater Pollution Control Officers. And the typical problem such people are likely to use the work for would be in planning applications, especially in reviewing protection zones. More specific problems that must regularly be tackled are:-

Point sources of pollution - What is under threat and in what time?

Polluted sources - Where is pollution from? What is the forecast maximum concentration? Instructions to consultants may need to be devised quickly.

Concerns that are associated with these activities include:-

Are the assumptions inherent within the models properly understood and appreciated?

Is the problem being tackled at the appropriate scale (regional/local)?

Is adequate internal expertise available or is their a list of suitably qulified consultants?

7. REVISION OF TARGETS & TIMESCALES

It was agreed at the 3 March meeting that the original reporting timescales were inappropriate, especially given the change in programme. However, it is useful to have targets and deadlines, so a revision to the original schedule is given below. There may be additional products from the project and they will be provided along with the Draft and Final project reports.

Progress Report	1 July 1993	Summary of progress during previous 3 months.
Interim Technical Report	1 October 1993	Discussion report on methodology for application of transport models. Manual for BGS-developed databases.
Draft Project Report	1 January 1994	
Final Project Report, Database disks	1 April 1994	

8. WORK PROGRAMME TO END JUNE 1993

(a)   Review of modelling methodology (much expanded).

(b)   Begin a wider search for databases of geochemical parameters.

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

9. FINANCES

The financial situation at the end of the 1992/93 financial year will already have been conveyed to the NRA.

It is anticipated that approximately 20% of the remaining project budget will be spent during the quarter April-June 1993.