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Comparative evaluation of the usage of models for groundwater flow and pollution studies
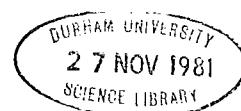
Bell, John Francis

ABSTRACT

This thesis is concerned with the usage of models for prediction of groundwater flow and quality in aquifers.

A critical review of current practical applications of groundwater models and modelling trends has been undertaken. On the basis of this study and taking into account the recent increase in the availability of relatively cheap microcomputers, several potential lines of alternative modelling techniques have been examined.

The uncertainty inherent in the collection of any groundwater data from the field and the identification of boundary conditions suggest that the commonly employed large complex distributed-parameter models are no more valuable as predictive tools than less complex alternatives, which have been largely neglected.

The recent rapid developments in microcomputer technology and availability provide an opportunity for much wider use of groundwater models in planning and management as well as the more traditional scientific and engineering applications.

Three prototype models, utilising new or neglected techniques and taking advantage of the wide availability of microcomputers, are presented. These models seem to offer new possibilities in modelling to a broad range of those involved in practical groundwater management and resource planning.

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COMPARATIVE EVALUATION OF THE USAGE

OF MODELS FOR GROUNDWATER FLOW AND POLLUTION STUDIES

by

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A thesis submitted to the Faculty of Science

at the University of Durham for the degree of

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Department of Geological Sciences, November 1981

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DECLARATION

The content of this thesis is the original work of the author (any joint research, where included, is acknowledged by reference). It has not been previously submitted for a degree at this or any other University.

John Bell

J.F.Bell
Durham, November 1981

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ACKNOWLEDGMENTS
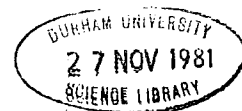
PART ONE

CRITICAL PACTICAL REVIEW

CHAPTER ONE

INTRODUCTION TO GROUNDWATER MODELS

1.1 PREAMBLE

Originally, the purpose of this research was to investigate groundwater pollution arising from the leaching of coal mining wastes. Initial attempts at making use of complex distributed-parameter numerical models such as those by Guymon (1970) and Amend (1975), were abandoned because the quality of data available did not justify the model complexity and consequent extensive computing resource requirements. As a direct result of this, a critical examination of modelling techniques and their results was undertaken as a research project, with a view to determining practical limits for their application and developing new techniques to exploit the capabilities of the desktop microcomputer.

1.2 METHODS OF MODELLING

The flow of water and the description of the movement of chemical species through a porous medium involves a very complex series of processes. Any attempt to model such phenomena must be accompanied by a clear understanding of the governing physics and chemistry.

A broad summary of the major approaches to groundwater modelling is given below :

```
                          METHODS
                             |
                             |
          ------------------------------------------
          |                                        |
    MATHEMATICAL-----HYBRIDS----------ANALOGUE
          |                                        |
    -------------------------         --------------------
    |         |        |             |                  |
ANALYTICAL    |    NUMERICAL    ELECTRICAL           PHYSICAL
         STATISTICAL    |                                |
                        |                                |
          ------------------------            -----------
          |                    |              |         |
        LUMPED           DISTRIBUTED         SAND       HELE
       PARAMETER          PARAMETER          TANK       SHAW
                              |
                 ------------------------
                 |          |          |
                FDM        FEM        BEM
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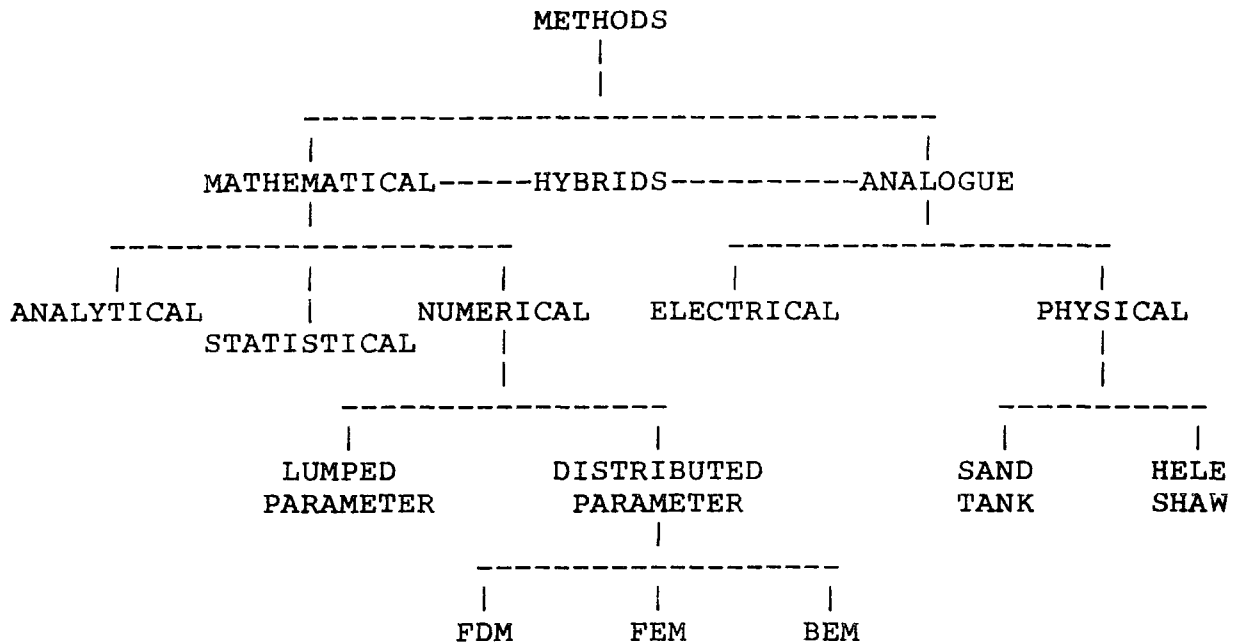
Analytical solutions of the equations governing fluid flow and the transport of chemical species are confined to a few idealised cases with simple boundary conditions and as such are of relatively limited practical value. Complex groundwater flow and groundwater quality problems are therefore often tackled by employing a wide range of physical, analogue and mathematical modelling techniques. Such models are limited by the facts that the physical and chemical characteristics of the porous medium and transported fluids are known in little detail and that the physics and chemistry of flow and solute transport are by no means perfectly understood.

Examples of the principal model types are discussed in varying degrees of detail subsequently and their comparative evaluation in the solution of practical problems forms the basis of this study. Each method is briefly described,

examples are given and a comprehensive review of recent applications is presented. Some original models are developed and their applications illustrated. The vast number of individual models in each category could not possibly be fully discussed but the main features of the different approaches to modelling are considered and their relative merits critically evaluated.

1.3 APPLICATIONS OF MODELS

When considering which type of model to employ in a groundwater study, it is imperative to realise the assumptions and limitations of the chosen model. The validity of a particular model will depend on :

(1) the extent and reliability of data available;

(2) the approximations introduced by the scale of the model;

(3) the representation and knowledge of boundary conditions; and

(4) the assumptions made about physical processes.

This last point is particularly important in the relatively poorly understood aspects of unsaturated flow and solute transport.

Different hydrological and hydrogeological problems require different solutions; indeed the number of models almost equals the number of investigations. However, the fundamental principles and equations from which the wide variety of models arise are relatively few; varying assumptions, degrees of simplification, refinement and size account for the diversity of approaches available. To understand the applicability of the various approaches, it is necessary to understand both the limitations of the modelling techniques as well as the behaviour and characteristics of the particular porous medium and mobile fluid.

Models can be subdivided on the basis of their objectives and data requirements into three categories :

(1) Prediction models : where specific predictions of flow, and/or water quality is required and large amounts of field data are available. The general problem is the definition of a number of variables in both space and time. The variables may be of a purely physical nature (head or pressure or flow) or may involve chemical aspects (concentration or concentration gradient). The space is in general 3-dimensional and the time scale may vary from seconds through minutes, hours, days and weeks to years, decades or even millions of years. The temporal and spatial values of the physical and chemical variables depend on the temporal and spatial variation of the physical and chemical properties of both the porous medium and mobile fluid phases, together with the variation of sources and boundary conditions. This type of modelling relies on the availability of extensive field data collected over an extended

time period.

(2) Inverse models : where the characteristic properties of the porous medium are deduced from observations of spatial and temporal variables. Here the problem is given the way in which certain variables behave, deduce the likely properties of the porous medium and mobile fluid. Temporal and spatial observations of physical and chemical variables are required as data. Knowledge of sources and boundary conditions through time is also essential. Such models are often used to generate data for the more normal prediction models, for example Emsellem and De Marsily (1971), Nutbrown (1976) and Darr (1979).

(3) System analysis models : where the model is used to predict the sensitivity of a system to proposed changes in policy. Such models may be used to aid the understanding of interactions between processes, Gilham and Farvolden (1977); to identify and assign data collection priorities, Gilham and Farvolden (1977); to assist in resource management decision making and policy making, Maddaus and Aaronson (1972), Gorelick et al (1979), Mido (1980b); and to make upper and lower bound predictions, Aguado et al (1977). Sensitivity analyses may be carried out by employing either of the parameter or component perturbation strategies described by McCuen (1973) for the groundwater context.

In all cases the aim is to reduce a system consisting of a large number of inter-reacting variables to a manageable mathematical or physical analogue. A comprehensive 3-dimensional model presents several major difficulties

recognised by Frind and Verge (1978). Firstly, the computing and physical resource costs are very high; secondly, the labour involved in laying out the model and acquiring and preparing the data is very considerable; and finally, the satisfactory representation of boundary conditions is problematical. For these and other reasons a variety of simplifying assumptions are frequently made in modelling.

Most groundwater models comprise regions of large areal extent compared to the saturated thickness of the porous medium and the 3-D problem is simplified to 2-D by assuming sub-horizontal flow and transport. Where vertical flow is more important, for example in many waste disposal models, the problem is represented as a 2-D section in the vertical plane. Even greater simplifications to 1-D models are sometimes used in solute transport models by considering movement along a predetermined streamline. The amount of detail in which a 3-D, 2-D, or 1-D approximation is considered is also the subject of much variation. Analytical models provide continuous representation as do some physical analogues, but most models are discretized to varying degrees in both space and time.

The size, complexity and speed with which results are generated for any model depends not only on the purpose of the model but also on the magnitude of the allocation of physical and computational resources to the modelling project. This resource allocation is in practical terms a financial one and the modeller's task is to provide the most suitable model within the budget available.

The primary danger when using groundwater models as tools to solve problems is lack of thought. When used indisciminantly and thoughtlessly models can waste considerable time, effort and resources. A little time spent in pre-planning and selecting the model appropriate to the problem is repayed by relevant and meaningful modelling results.

1.4 SCALE OF MODELS

Scale in tackling a problem in groundwater behaviour is a very important consideration discussed by Mercer and Faust (1980b). The modelling of groundwater flow and transport can be approached on a number of different physical scales : molecular, microscopic, mesoscopic and macroscopic.

(1) Molecular scale : flow and transport mechanisms are considered at molecular level and the concepts of kinetic theory and statistical mechanics are employed. Chemical reactions are best modelled at this level.

(2) Microscopic scale : pore space is treated as a fluid continuum with the porous medium forming a rigid or semi-rigid boundary and the concepts of classical fluid mechanics are used. In rare cases a pipeflow analogue of this kind may be applied on a macroscopic scale to represent flow through karstic formations - see Thrailkill (1974).

(3) Mesoscopic scale : the geometry of fracture networks is modelled and flow is considered by a combination of

classical fluid mechanics and statistical mechanics. This level of modelling is rare but is employed in the simulation of laboratory experiments and some research into the precise nature of rock permeability.

(4) Macroscopic scale : where most practical regional groundwater flow models are founded and the resistance to flow is represented by an estimate of bulk rock-mass permeability. The details of the flow and transport process are "averaged" into a few measurable field response characteristics and only an approximate representation of behaviour is attempted.

The problem of scale is a vital one and consideration of a natural rock as a porous medium illustrates its importance. At the molecular level a sub-unit will consist of molecules of water, a transported material or the rock skeleton. At the microscopic level a sub-unit will be either part of the fluid phase or the rigid rock skeleton. At the mesoscopic level sub-units will comprise porous rock containing relatively static fluid or joint and fissure openings containing relatively mobile fluid. At the macroscopic level, sub-units are represented by a porous medium with a specific resistance to flow and dispersive and absorptive capability.

All the models to be discussed fall into the macroscopic scale category and the physical and chemical processes and equations considered are those appropriate to the macroscopic scale.

1.5 LIMITATIONS OF MODELS

There are a number of potential areas of error and misuse in the application of modelling techniques to groundwater problems. These are discussed to varying degrees by Evenson et al (1974), Baski (1979), Darr (1979), Mercer and Faust (1980a,b,c) and Faust and Mercer (1980). The principal mistakes and abuses are :

(1) Use of the most complex model available (Mercer and Faust, (1980a)). Even if little or no data is available a very complex and extensive distributed-parameter model is adopted. In most cases a simple analytical or lumped-parameter model would suffice. The aim should be to employ the simplest model adequate to the task.

(2) Use of the largest model available (Baski (1979); Mercer and Faust, (1980a)). Large models are often used to give a detailed solution to a problem where the available data is very limited. Such models are wasteful of resources since costs for distributed-parameter models tend to rise as the square of the number of nodes. Large models are often used to imply a spurious accuracy unsupported by data.

(3) Use of models designed for other problems (Mercer and Faust, (1980a,c)). Problems are adapted to suit the available model rather than the model tailored to the problem. All models have implicit assumptions and limitations which should guide and restrict their fields of application.

(4) Misunderstanding of basic physics and chemistry
(Evenson et al (1974); Mercer and Faust (1980b); Faust and
Mercer (1980)). Models based on erroneous physical and chemical
concepts are applied. For example, flow models based on
intergranular, homogeneous porous sediments are applied when a
pipeflow analogy is appropriate.

(5) Misunderstanding of data reliability (Evenson et al
(1974); Mercer and Faust (1980a)). Many of the larger, more
complex models have been designed and operated by specialist
modellers rather than those who collect and interpret the data.
As a consequence, the credibility and reliabily of data may
remain unquestioned by the modeller and lead to bizarre errors
and predictions.

(6) Inadequate model calibration and validation (Evenson
et al (1974); Baski (1979);). Models may be calibrated on data
available at one time and henceforth assumed to be correct and
checks with newly aquired data are not made. There is also a
tendency for models to be validated by their ability to
regenerate the calibration data rather than subjecting them to
independent test.

(7) Inadequate data reliability (Evenson et al (1974);
Darr (1979); Mercer and Faust (1980a,c)). Boundary conditions
may be improperly understood or interpreted and data errors
introduced at the model calibration stage. "Garbage in /
garbage out" is a wholly appropriate phrase in such
circumstances. A poorly formulated model may waste good data
but no model can overcome the problems created by absent or

erroneous data.

(8) Inflexibility. Where models are developed in conjunction with a particular field project or management problem, insufficient flexibility in the early formulation of the model may lead to difficulties at a later date. Assumptions and limitations may be forgotten and errors introduced as a result.

(9) Discretization errors (Mercer and Faust (1980a)). Discretization errors occur in both analogue and computational models where a continuous porous medium is represented by a discrete number of points or nodes. These errors are apparent when analytical solutions are used to validate such models.

(10) Numerical and measurement errors (Mercer and Faust (1980a)). Errors occur in computational models due to the finite precision of the arithmetic employed. Normally such errors are small but the modeller must be alert to situations where such errors become cummulative. Similarly in various types of analogue models, instrument precision may limit accuracy and cummulative or systematic errors may be present.

1.6 TRENDS IN MODELLING

In the past decade or so, the models used in groundwater investigations have been largely numerical; superseding earlier analogues because of their much greater flexibility and development speed. Various analogue models and

hybrid models remain in use but are largely confined to qualitative and demonstration uses.

Dominating the field of groundwater modelling since the mid-1960's and still maintaining their importance are the finite difference methods (FDM); though finite element formulations (FEM) have gained in popularity since the early-1970's. As groundwater quality models developed in the early 1970's, the method of characteristics (MOC) describer by Gardner et al (1964) was widely adopted to overcome numerical dispersion problems inherent in the application of FDM and FEM. A further class of numerical solutions based on the boundary integral equations and known as boundary element methods (BEM) have developed in the 1970's but have yet to find major acceptance in practical groundwater modelling.

Prickett (1979) recently reviewed the extent to which various models are in use. The breakdown of a survey of 68 currently active models was as follows :

Numerical		Analytical	Statistical	Analogue	
FDM	FEM			Elec	Phys
32	17	2	1	10	6
49		2	1	16	

The type of model finding most favour at any particular time depends on two factors : the current level of understanding of the physical and chemical processes and the current modelling technologies available. Large distributed-parameter computational models came into use with the expansion in the availability and power of large mainframe computers in the mid-

1960's. However, the sophistication of such models has rapidly overtaken the availability of data and many models cannot be justified as practical predictors and find their main application as research tools.

During the late 1970's and early 1980's a great deal of attention has been payed to the treatment of aquifer characteristics as random stochastic variables in distributed parameter models. This work was led by Freeze (1975) and extensive additions have been made by Gelhar et al (1979), Smith and Freeze (1979) and Smith and Schwartz (1980).

The recent rapid rise of the desktop microcomputer is likely to have a profound effect on the use of models since increasingly complex models can be applied in situations where the use of a mainframe computer would have been either too costly or too time consuming. Mido (1980) has pointed out the value of microcomputers and their application to groundwater modelling forms a significant part of this thesis. Many of the original models presented take advantage of the interactive and graphical capabilities of low-cost desktop microcomputers. The models are devised for the non-expert computer user and employ rigorous error checking and input prompting routines.

DATA RELIABILITY FOR GROUNDWATER MODELS

2.1 GOVERNING EQUATIONS

Groundwater flow and quality models are based upon a small number of governing equations which are solved by various analytical and numerical methods.

The general form of the equation for flow through a porous medium may be written :

$$div(\{T\}.grad(h)) + \{q\} = \{S\}.dh/dt \qquad (2.1)$$

where h   is the head potential,

   $\{T\}$ is the transmissivity,

   $\{S\}$ is the storage coefficient,

and $\{q\}$ is a generalised source term.

The equivalent form of the convection-dispersion equation for water quality models may be written :

$$div(\{D\}.grad(c)) - div(\{u\}.c) + \{q\} = dc/dt \qquad (2.2)$$

where c   is the concentration,

   $\{D\}$ is the dispersion coefficient,

and $\{q\}$ is a generalised source term.

The vector {u} is a velocity term given by ({T}/{n}.h).grad(h) and provides the coupling between equations (2.1) and (2.2). The parameter {n} represents the flow porosity of the porous medium.

In order to solve equations (2.1) and (2.2) over a spatial region it is necessary to know {T},{S},{D} and {q} over that region. The precision with which any model can predict the dependent variable h and c is controlled by the precision with which {T},{S},{D} and {q} are determined. For steady-state models when the right hand side of both equations is zero, {S} is not required.

2.2 ESTIMATION OF {T} AND {S} THE AQUIFER CHARACTERISTICS

The values of {T} and {S} for a porous medium as previously discussed in section 1.4 depend on scale. In some cases the permeabilities {k} and saturated thicknesses {b} are measured to estimate {T} = {k}.{b}. Laboratory measurements on small samples are very unlikely to give a representative estimate of the bulk property on a field scale. Thus the only reliable source of regional {T} and {S} values come from large scale field pumping tests.

The detailed procedure for field pumping tests are discussed by Ineson (1963) and Monkhouse (1975). Available test data falls into three broad categories :

(1) Completion tests : normally short duration tests, often carried out by drilling contractors to give a rough idea of the likely yield of a new well. Only very approximate estimates of {T} can usually be derived from such tests. {S} cannot usually be estimated.

(2) Step tests : normally carried out to determine the yield-drawdown characteristics of water wells and involving pumping to pseudo-equilibrium drawdown for a series of increasing abstraction rates. It may be possible to infer an approximate {T} value from yield-drawdown characteristics using the curves presented by Walton (1970). {S} cannot normally be calculated but must be guessed in order to estimate {T}.

(3) Aquifer tests : carried out to determine {T} and {S} and involving abstraction at a constant rate for an extended period and observation of drawdown in a number of surrounding wells and boreholes. Such tests are very expensive and are relatively rare. They provide the best available estimates of {T} and {S}.

Analysis of pumping test data to give {T} and {S} is a complicated procedure involving the application of various analytical models for two-dimensional radial flow. A comprehensive guide to the methodology is given by Kruseman and DeRidder (1979). Subjective curve matching procedures are generally used and different answers are often obtained by different analysts using the same data. Under certain circumstances, the analysis can be rendered very imprecise because of the precision of the test data and the limitations

of the analytical models.

The principal problems arising with the application of analytical models to estimate {T} and {S} from pumping tests are :

(1) Selection of model : solutions are available for aquifers of infinite extent, for confined or unconfined conditions, with isotropic or anisotropic aquifer characteristics, with recharge and barrier boundaries, with or without an infiltration source, for fully or partially penetrating wells, with delayed yield from confined storage and many more. But the model required can only be inferred from the test data and the hydrogeology of the area around the well is not normally known in sufficient detail for this to be predetermined.

(2) Design of test : in order to drill observation wells at optimum locations to the correct depth it is necessary to know the detailed hydrogeology of the site. But the test must be designed without such knowledge and is therefore always a compromise to anticipate as many eventualities as possible.

(3) Conduct of test : the duration of the test and frequencies of readings can normally be amended during the test period. The abstraction rate is usually decided on the basis of a completion test or step test and is also limited by the pump capacity. Even under ideal conditions, a constant pumping rate is difficult to maintain and slight deviations always occur. Water level measurements, particularly early in the test when

rapid changes occur, are subject to errors both in the level and time of observation.

Uncertainties in the values of {T} and {S} obtained arise from a number of sources. An attempt has been made to quantify these uncertainties so that a realistic estimate of the reliability of pumping test data for incorporation in models can be made. The sources of uncertainty include :

(1) Representative uncertainty : any estimates of aquifer characteristics used in modelling are taken to be representative of a certain sub-unit of the formation. Pumping test data is normally so sparse that several tests on wells in a small area almost never take place and the 'local' variation of {T} and {S} is not well known. Reeves et al (1975) present data for 7 sites where tests were carried out on pairs of wells from 25 to 100m apart. Ratios of {T} values from pairs of tests vary from 1.2 up to 5. {S} values are not quoted but re-examination of the data by Reeves (pers. comm.) suggests ratios between 1.4 and 8.5. This implies that field properties are very variable and even if data analysis were perfect, uncertainties amounting to a factor of 2 in {T} and as much as 4 in {S} are to be expected.

(2) Model selection uncertainty : estimates of aquifer characteristics are made by comparing observed data with analytical models. Uncertainty can arise in the choice of the appropriate model. To discover the likely magnitude of such variations a series of synthetic datasets were generated to perfectly fit 6 different analytical models. Random errors were

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introduced in the data to allow for water level errors of up to 10mm and time errors of 5 seconds. These errors are similar to those suggested by Monkhouse (1975). The abstraction rate was assumed to be subject to a 2% random error suggested by Backshall et al (1972). Estimates of {T} and {S} were made by fitting all datasets to all models. Where fits were very bad the results were discarded. The results were as follows :

Set		1 {T}	2 {T}	3 {T}	4 {T}	5 {T}	6 {T}
Set	Model	(All values in m2/day)					
1	Infinite aq	111	–	–	397	[596]	95
2	Vert leak	–	95	190	127	143	–
3	Del yield	–	278	88	223	374	–
4	Partial pen	80	96	88	119	119	–
5	Rech bdry	72	159	143	254	103	–
6	No-flow bdry	198	–	–	–	–	127

Set		1 {S}	2 {S}	3 {S}	4 {S}	5 {S}	6 {S}
Set	Model	(All values should be multiplied by 1E-4)					
1	Infinite aq	1.25	–	–	1.59	[.48]	.96
2	Vert leak	–	.99	1.40	1.32	.87	–
3	Del yield	–	1.43	.70	1.07	.78	–
4	Partial pen	1.27	.69	.63	.76	.48	–
5	Rech bdry	.75	.81	1.38	1.18	.91	–
6	No-flow bdry	1.90	–	–	–	–	1.63

[ ] indicates a possible, but poor fit.

The diagonal values in the two tables represent the estimates of {T} and {S} using the correct model, off-diagonal estimates use the wrong model. The true solutions for {T} and {S} were 100 and 1E-4 respectively.

The uncertainty from this source can again give rise to a factor of 5 in {T} and as much as 4 in {S}.

(3) Data and subjective uncertainty : data errors arising from the precision of test procedures also gives rise to uncertainties in the estimation of aquifer characteristics. The errors were again estimated by analysis of the synthetic datasets considering only the variation between analysts fitting the same correct model to the data.

DATASET ONE

Set	Analyst Model	True {T}	1 {T}	2 {T}	3 {T}	4 {T}	5 {T}
		(All values in m2/day)					
1	Infinite aq	100	111	119	103	135	113
2	Vert leak	100	96	95	88	95	88
3	Del yield	100	87	88	84	79	40
4	Partial pen	100	119	95	87	103	88
5	Rech bdry	100	103	95	102	111	120
6	No-flow bdry	100	127	151	111	103	117

Set	Analyst Model	True {S}	1 {S}	2 {S}	3 {S}	4 {S}	5 {S}
		(All values should be multiplied by 1E-4)					
1	Infinite aq	1.0	1.25	1.10	1.24	1.43	1.12
2	Vert leak	1.0	.99	.89	.77	.99	1.13
3	Del yield	1.0	.70	.57	.56	.36	.57
4	Partial pen	1.0	.76	.76	.91	.75	.85
5	Rech bdry	1.0	.91	.67	.89	1.06	.58
6	No-flow bdry	1.0	1.63	1.55	.99	1.40	1.70

DATASET TWO

Set	Analyst Model	True	1 {T}	2 {T}	3 {T}	4 {T}	5 {T}
			(All values in m2/day)				
1	Infinite aq	1000	909	1273	1432	1352	1473
2	Vert leak	1000	954	875	1075	994	1020
3	Del yield	1000	936	884	723	565	398
4	Partial pen	1000	875	795	437	517	497
5	Rech bdry	1000	954	954	875	1034	1220
6	No-flow bdry	1000	1273	1432	1193	1034	1729

Set	Analyst Model	True	1 {S}	2 {S}	3 {S}	4 {S}	5 {S}
1	Infinite aq	.10	.06	.08	.08	.09	.08
2	Vert leak	.10	.10	.07	.09	.09	.08
3	Del yield	.10	.08	.10	.14	.07	.07
4	Partial pen	.10	.12	.10	.06	.06	.06
5	Rech bdry	.10	.08	.07	.10	.08	.09
6	No-flow bdry	.10	.10	.10	.09	.12	.18

These largely subjective errors can amount to a factor of 4 for {T} and 3 for {S}.

Taken together, these uncertainties seem to suggest that the data available for modelling is at best an approximate guide to regional formation properties.

2.3 ESTIMATION OF {D} THE DISPERSION COEFFICIENT

In comparison with {D}, the parameters {T} and {S} are relatively well known on a regional scale. Even laboratory attempts to measure {D} are rare and the very best that can be done at present is to make an educated guess at a values for the parameter.

Fried (1975) states that dispersion depends upon a relationship between a number of parameters :

(1) fluid viscosities,

(2) fluid densities,

(3) gravity,

(4) pore velocities,

(5) molecular diffusion coefficients, and

(6) permeabilities.

For water pollution applications, viscosities and densities vary relatively little and gravity can also be neglected as a variable. For practical purposes, the phenomenon of dispersion can be examined in terms of two dimensionless parameters :

(1) the ratio of the dispersion coefficient (D) to the molecular diffusion coefficient (Dm), that is $R = (D/Dm)$, and

(2) the Peclet number (Pe), given by $(u.d/Dm)$, where u is the pore velocity and d is a characteristic spacing of the porous medium often taken to be the square root of the intrinsic permeability or the effective grain size.

The empirically determined relationship between these parameters is shown in Fig. 2.4.2 in Fried (1975) for longitudinal dispersion, that is dispersion in the direction of the velocity vector. Results are primarily derived from experiments using packed beads but a few results for unconsolidated sediments suggests a similar relationship.

Taking into account the linear log-log plot the following relationship can be deduced :

$$R = R' + A.(Pe)^x \qquad (2.3)$$

where R',A and x are constants.

Inspection reveals that x is approximately unity for Peclet numbers greater than 1 and that for Peclet numbers less than 1, R = R'. Thus in simple terms we may write :

$$\{D\} = \{R'\}.Dm \qquad ; \text{ for Pe} < 1 \text{ and Pe} = 1 \qquad (2.4)$$

$$\{D\} = \{R'\}.Dm + A.\{u.d\} \; ; \text{ for Pe} > 1 \qquad (2.5)$$

These relationships are implied for unconsolidated porous media by Harleman and Rumer (1963) and are quoted by Fried (1975). Analogous formulae for consolidated aquifers are suggested by Raimondi et al (1959) and Legatski and Katz (1966). Klotz and Moser (1974) show an experimental inverse relationship between {D} and porosity {n}. This is implied in equation 2.5 since u is inversely related to n (See footnote to equation 2.2). A similar relationship can be deduced for lateral dispersion, that is normal to the velocity vector, when mechanical as well as molecular dispersion is involved :

$$\{D\} = \{R'\}.Dm + B.\{u.d\} \; ; \text{ for Pe} > 1 \qquad (2.6)$$

Values of A and B are very different, Fried (1975) quotes 1.4 to 2.2 for A and 0.025 for B. The value of R' is always less than unity and for unconsolidated granular porous media a value

of 0.6 to 0.7 is usual. For consolidated materials little data is forthcoming and similar values are normally assumed.

Few values of {D} appear explicitly in the literature and those which do have been gathered by Barker and Foster (1981):

{D}(m2/s)*	Species	Medium	Temp	Reference
13	Cl-	Chalk	?	Oakes et al (1976)
3-	Cl-	Sand	35	Stoessell et al (1975)
3-7	Cl-	Soil	25	Barraclough and Rye (1979)
.4-3	Cl-,NO3-	Chalk	?	Mercer (pers comm)
13)			5	
17)	Tritium+	?	15	Mills (1973)
22)			25	

* All values should be multiplied by 1E-9.

The foregoing discussion relates to the estimation of dispersion coefficients based esentially on laboratory experimental data. The same problems of scale that require the field determination of {T} and {S} also apply to {D} and it is strongly argued that field values are necessary for regional models. Very few such determinations have been made up to the time of writing. The field techniques available were reviewed by Fried (1975) :

(1) Single-well pulse technique : where an easily detected tracer is injected into a screened section of well followed by a period of fresh water injection. The tracer pulse is then recovered by pumping. Application of a semi-analytical or numerical model is then used to deduce {D} from the tracer recovery pattern. A detailed description of the technique is given by Fried et al (1972). The values of {D} obtained characterise the area around the well to a radius of 2 to 4 m.

(2) Multiple-well or single-well large scale injection :
where a tracer is injected into an aquifer and spotted at a
series of observation wells. Large volumes are injected and not
recovered. Such tests are very expensive and may themselves
cause pollution unless the tracer is very carefully selected.
The tracer may be allowed to move with the natural flow
velocity of the aquifer or sustained injection may generate a
locally high head gradient. Again semi-analytical or numerical
models are applied to deduce {D} which is representative on a
scale of 20 to 100 m. A rare case history is presented by Oakes
and Edworthy (1976).

(3) Inverse model techniques : cases of natural pollution
are observed and {D} deduced by an inverse modelling technique.
Representative large scale values may be obtained in this case
but a high density of observation wells are required and such
methods are expensive. Fried (1975) refers to an unidentified
case history and gives some experimental results.

From equations 2.5 and 2.6 it can be seen that when
mechanical dispersion predominates and Dm is small compared to
D, we may write :

$${D} = {L}.{u} \qquad\qquad (2.7)$$

where {u} is the flow velocity,
and {L} is called the characteristic mixing length.

Values of {L} are usually quoted from field tests. {L} has

dimensions of length [L] and both longitudinal and lateral values of {L} may be quoted. The few numerical values that are available for various types of test and aquifer include :

L(m) long	L(m) lat	Hydrogeological formation	Reference
12	4	Alluv deps,Lyon	Fried (1975)
1.1	–	Alluv deps,Colmar	Fried (1975)
91	137	Fractured basalt,Idaho	Robertson et al (1973)
0.6	–	Bunter sandstone,Notts	Oakes & Edworthy (1976)
46	14	Alluv deps,Colorado	Konikow (1976)
61	20	Oscala lst,Georgia	Bredehoeft & Pinder (1973)

From values of {D} given in the table above it appears that molecular diffusion is only important when the groundwater velocity is around 1E-9 m/s or less.

Very few numerical estimates of {L} are to be found in the literature and the extent to which any value is representative is unknown. The data analysis to estimate {L} is less rigorous than that used to derive {T} and {S} and uncertainties introduced by choice of model and data errors will be at least of the same order and probably larger than those discussed for the aquifer characteritics. In order to estimate {D}, values of {T} and the flow porosity {n} must be known and these estimates will also involve errors and uncertainties. At best, the numerical values of {D} available are orders of magnitude and will reman so for the forseeable future.

2.4 ESTIMATION OF {q} THE SOURCES AND SINKS

The generalised source terms appearing in equations 2.1 and 2.2 are rather different. In the flow equation (2.1)

sources (and sinks) represent inflows and outflows of water. In the convection-diffusion euation (2.2) sources and sinks represent inputs and outputs of pollutant. These pollutant sources (and sinks) are in practical terms estimated by assigning a concentration to a water inflow or outflow and thus the problems of estimating source terms reduces to one of determining these flows.

Some flows are known very precisely. Well discharges and spring discharges are frequently measured on a regular basis and reliable data are available to the modeller. Water quality for such 'point' sources and sinks is also typicallly well documented.

Other more diffuse source terms are very poorly known. Infiltration from rainfall is estimated by two principal procedures according to Phillips (1978) :

(1) Direct estimation : the rate at which water is absorbed by the ground is measured by some kind of infiltrometer. In the best tests water budgets are calcualated and allowance is made for evaporation and transpiration for large plots. Such data are rare, particularly for uncultivated areas.

(2) Indirect estimation : infiltration is estimated from records of rainfall and evapotranspiration. Precise rainfall statistics with good areal coverage are usually available but measurements of evapotranspiration are rare and estimates are normally made from empirical formulae. Catchment balance

studies provide a check on infiltration estimates over large areas but no independent check on the areal distribution of the parameter is practical. Measurements of the quality of infiltrating waters are not plentiful and a rough estimate must normally be made.

Where inversion techniques are used to deduce {T} and {S} from water level data, these depend critically on the infiltration estimates. Since infiltration depends on such factors as vegetation, cultivation, and geology on a local scale, it is unlikely that distributed parameter estimates are accurate. Another difficulty arises with the temporal variation of infiltration since the lag between the rainfall event and the arrival of the infiltrating water at the saturated aquifer depends on the characteristics of flow through the soil and unsaturated zone which is very largely indeterminate.

Thus, {q} in common with the other 'data' parameters is known only approximately to the modeller using distributed-parameter methods.

2.5 DATA AVAILABILITY FOR DISTRIBUTED PARAMETER MODELS

Bearing in mind the considerable uncertainties in data reliability and availability for distributed parameter modelling of groundwater systems, it is of interest to examine how much data is used in large distributed parameter prediction models. To this end, a review of published models over the past ten years was undertaken to discover the amount of reliable

field data used in the calibration procedures. The results are interesting and alarming :

Parms	Field vals	Model nodes	Modelling method	Model type	Reference
{k}	14	181	A/D hybrd	Flow	Thrailkill (1974)
{k}	6	>100	Elec anal	Flow	Sander (1976)
{k}	>200	900	Elec anal	Flow	Water Res Board (1973)
{k}	12	375	Elec anal	Flow	Gupta et al (1979)
{k}	5	380	Stdy FDM	Flow	Perez et al (1972)
{k}	?	1414	Trans FDM	Flow	Robertson et al (1973)
{T},{S}	25	824	Trans FDM	Flow	Oakes & Skinner (1975)
{T},{S}	33	500	Trans FDM	Flow	Morel (1979)
{T},{S}	19	893	Trans FDM	Flow	Reeves et al (1974)
{T},{S}	8	290	Trans FDM	Flow	Rankine (1981)
{D}	1	1050	Trans FEM	Qual	Bredehoeft & Pinder (1973)
{D}	1	110	Trans FEM	Qual	Guymon (1970)
{D}	1	117	Trans FEM	Qual	Segol & Pinder (1976)
{k}	26	141	Stdy FEM	Flow	Cherry et al (1973)
{k}	26	780	Stdy FEM	Flow	Frind & Verge (1978)

All the tabulated cases represent major regional modelling exercises. It is readily apparent that the amount of field data available for such models is very limited. It is difficult to see how , in many cases, the data justified the application of a sophisticated distributed parameter model. In most cases, the field test data was augmented by use of groundwater level data to infer aquifer characteristics by inversion techniques. The {q} values used for the critical infiltration parameter in such cases is an estimate based on rainfall data.

Conflicting results were obtained by Frind and Verge (1978) when using the data available from a 2-D model and applying it to a 3-D model of the same problem of radioactive waste disposal. Discrepancies arising between the two models were of major importance; the 2-D models suggested that in the event of radioactive waste leakage, the leakage material would be carried to the surface; the 3-D model suggested that it

would be transported to the basal sand aquifer. The authors concluded that the data utilized in the 3-D model, being of 2-D origin, was inadequate to describe the system and that significant 3-D effects might be important. Problems such as changes in stratigraphy and hydrogeologic parameters (notably {D} and {K}) or additional boundary conditions all varying in different vertical sections of the aquifer could account for these results. The conclusion is that reliable 3-D data is needed in order to create worthwhile models of the field system and the implication is that 2-D models may not be capable of successfully predicting system behaviour. But 2-D data is all that is available in most practical problems and very rarely is it reliable and plentiful. The validity of these large distributed-parameter models must therefore be questioned since 2-D models may apparently mislead and reliable 3-D data is virtually unobtainable.

Groundwater modelling relies very heavily on the experience of the modeller in choosing a self-consistent set of values of {T},{S},{D} and {q} which will reproduce observed patterns of the dependent variables c and h. Such sets however are by no means unique and an adequately calibrated model is by no means necessarily a valid one. Very great care must be exercised in the use of predictions from such models. Because of the inherent uncertainty, the cost-effectiveness of large, sophisticated, distributed-parameter models should be seriously considered together with alternative modelling philosophies.

CHAPTER THREE

ANALYTICAL MODELS OF GROUNDWATER SYSTEMS

3.1 ANALYTICAL MODELS

The technique which first comes to mind for dealing with the equations governing groundwater flow and solute transport is the application of analytical solutions. The governing equations are (2.1) and (2.2) and the simpler steady state equations where the time derivative on the right hand side disappears. Analytical solutions are only practically feasible for relatively simple expressions of the convection-dispersion equation. Most of the published solutions are 1-D or pseudo-2-D and treat the convective velocity as an independent variable.

Before the advent and widespread availability of high-speed digital computers, analytical models were the only alternative to electrical and physical analogues. Although they can be replaced by numerical methods for many purposes, analytical methods still have significant applications in a number of areas :

(1) regional problems : analytical models are widely used to solve simple practical problems and to provide preliminary estimates in more complex cases.

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(2) parameter identification : most field and laboratory experiments to determine {T},{S} and {D} rely on analytical solutions.

(3) calibration and validation : many numerical, probablistic and analogue models are calibrated and validated on their ability to reproduce analytical solutions.

Raudkivi and Callander (1976) provide a comprehensive account of groundwater flow analysis; Walton (1970) refers extensively to analytical solutions applied to groundwater resource development and evaluation; Kruseman and DeRidder (1979) give a very full account of analytical solutions for well hydraulics problems; and Fried (1975) discusses analytical solutions of the convection-dispersion equation and their applications.

3.2 REGIONAL APPLICATIONS

Analytical models can be used to solve simple problems or as a first order approximation to 'get a feel' of more complex systems. Since equations (2.1) and (2.2) are linear partial differential equations, solutions to more complex problems may be built up by superposition of fundamental solutions. Linear no-flow and recharge boundary conditions may be simulated using the 'method of images' described by Ferris et al (1962) which involves using signed combinations of fundamental solutions to simulate the required boundary conditions.

Walton (1970) describes a number of practical applications of superposition and image well theory to model regional groundwater abstraction regimes. The first step in the modelling process is to idealise the field situation. This normally involves assumptions of isotropic, homogeneous aquifers and linear boundaries. Before the widespread use of computers quite extensive manual calculations were made with such models. Some typical examples include :

Location	Hydrogeological details	No wells Real	Image
Arcola, Illinois	infinite rectilinear strip, full edge & base barriers, sand and gravel formation.	3	18
San Miguel Basin El Salvador	semi-infinite rectilinear strip, part edge & base barriers, pyroclastics and alluvial deps.	170	170
Assumption, Illinois	semi-infinite rectilinear strip, full edge & base barriers, sand overlain by aquitard.	4	20
Perkin, Illinois	narrow wedge aquifer, 1 edge & base barrier,1 recharge, sand and gravel formation.	4	92
Tallula, Illinois	semi-infinite rectilinear strip, full edge & base barriers, sand and gravel under aquitard.	1	8
North East Illinois	semi-infinite rectilinear strip, 2 edge & base barrier, 1 recharge, sst-dol under aquitard.	6	54

A recent study by Samani (1977) has shown that as the number of superimposed solutions increases, the number of calculations necessary to evaluate the analytical model rapidly approaches those necessary for the equivalent finite difference numerical model. Thus there is a limit to the complexity of problem that are worth analysing by superposition. It is worth noting here

that obtaining a solution within a region by generating the required boundary conditions using a technique of superposition of fundamental solutions of the governing equations is the basis of the indirect boundary element method (BEM) discussed briefly in 5.4.

All the groundwater development examples quoted involve superposition of 'point source and sink' fundamental axisymmetric solutions. For land drainage models, the same image and superposition techniques are used for fundamental solutions involving 'line sources and sinks'. These are described by Raudkivi and Callander (1976) and by Luthin (1969).

Some solutions for 2-D regional flow have been developed. Marino (1974f) gives an analytical expression for the rise and fall of the water-table induced by recharge between two parallel boundaries and Nutbrown and Downing (1976) use solutions to a very similar problem for the analysis of baseflow recession curves. Marino (1974e) also provides 2D-solutions for the growth of groundwater mounds as a result of distributed recharge. Chan et al (1976) and Chan et al (1977) give solutions for wells in rectangualr aquifers and Vandenberg (1977) gives a solution for wells in a semi-infinite strip aquifer. These analytical solutions supersede the image and superposition methods widely used in the 1960's and refered to by Walton (1970).

No practical applications of 2-D solutions to the convection-dispersion equation (2.2) encompassing both lateral

and longitudinal dispersion have been discovered in the groundwater literature at the time of writing though they may exist. Vedat et al (1978) report a solution for steady state 2-D convection with non-uniform infiltration which can be used for prediction of plant nutrient movements in irrigated plots.

3.3 PARAMETER IDENTIFICATION APPLICATIONS

Analytical models are almost always used to deduce aquifer characteristics {T},{S} and {D} from field and laboratory tests. In laboratory tests, boundary conditions are normally prescribed by the experimental procedure and the direction of flow is also controlled. Analytical solutions for standard test conditions are hence of great value.

In field tests, the application of analytical solutions is less obvious. Nevertheless, pumping tests are almost invariably analysed using the analytical solution for transient, confined radial flow to a well in an infinite, homogeneous, isotropic aquifer devised by Theis (1935) or a similar analytical solution of equation (2.1). Similarly, Fried (1975) indicates the possibility of the application of analytical solutions of equation (2.2) under idealised conditions for the estimation of {D} from single and multiple well injection tests.

Analytical solutions for radial flow to wells have been devised for a very wide range of conditions and they are comprehensively reviewed and collated by Kruseman and DeRidder

(1979). The scope of the solutions covers :

(1) confined-unconfined conditions,

(2) partially penetrating wells,

(3) delayed yield from unconfined storage,

(4) anisotropy in {T},

(5) recharge from leaking aquitards above and below,

(6) multi-layer aquifers.

Many more variations in boundary conditions, formation geometry and anisotropy have been investigated.

The problem in applying such solutions is that with each additional refinement new data parameters are introduced and more and more data are required from the field test. In addition, evaluation of the analytical solutions can involve a large amount of arithmetic and some solutions must be evaluated numerically.

Crude 1-D analytical solutions of the convection-dispersion equation for porous media are provided by Marino (1974c); Fried (1975) and DeSmedt and Wierenga (1978). More complex 1-D solutions involving pollutant absorbtion include Marino (1974a,b,d); Selim and Mansell (1976) and Cameron and Klute (1977). Although these models successfully predict the behaviour of transported solutes in unidirectional laboratory experiments, their validity for the analysis of 3-D field tests is very questionable and Fried (1975) recommends the use of distributed-parameter 2 or 3-D numerical models for parameter identification.

3.4 CALIBRATION AND VALIDATION APPLICATIONS

Analytical model solutions provide valuable 'benchmark' solutions for the comparative evaluation of accuracy of numerical and analogue models of all kinds.

Although it is difficult sometimes to find an analytical solution to fit real field or laboratory conditions, almost any idealised conditions can be simulated by distributed-parameter numerical models. Thus numerical simulation of situations for which there is an analytical solution can be readily obtained. Such simulations provide independent checks on the accuracy of numerical models and are thus widely used for calibration and validation.

3.5 LIMITATIONS OF ANALYTICAL MODELS

Whilst not detracting from the use of analytical solutions for many of the problems discussed, the methods do have severe limitations for practical modelling purposes. Nevertheless, many distributed-parameter numerical models are applied to problems which could have been adequately solved in a few minutes with a hand calculator and analytical formula.

The principal limitations of analytical models are those of inflexibility :

(1) Boundary conditions must be uncomplicated and this usually means linear or piecewise linear;

(2) Aquifer characteristics must vary predictably, that is, normally homogeneous and isotropic;

(3) Systems must remain linear such that boundary conditions and aquifer characteristics are invarient with time.

These are very important restrictions but before dismissing the simple analytical approach, the modeller must consider whether the available data justifies the use of a more flexible, sophisticated technique.

In a few cases, very complex analytical solutions, although available, can involve so much computation in their evaluation that a numerical model is a more efficient solution to the practical problem. Many analytical functions are tabulated and presented graphically to avoid the necessity for such calculations.

CHAPTER FOUR

ANALOGUE MODELS OF GROUNDWATER SYSTEMS

4.1 ANALOGUE MODELS

The principal types of analogues used in the simulation of groundwater problems fall into two broad categories :

(1) Physical analogues, which comprise flow-tank models of various kinds including sand-boxes and Hele-Shaw type models; and

(2) Electrical analogues, which comprise resistance and resistance-capacitance networks.

A brief review of recent applications of analogues and their advantages and limitations will be discussed. To obtain realistic practical experience on which to base such a discussion, an experimental steady-state electrical analogue model of drainage from a waste tip into an aquifer with a regional groundwater gradient was developed. Additionally, some limited sand-box experiments were carried out to model pollutant plume development beneath a waste disposal site but quantitative results proved very difficult to obtain and the attempt was abandoned after a few runs.

4.2 SAND-BOX ANALOGUES

Sand-box models represent the porous medium by a granular material (normally sand or gravel) placed in a flow tank; the pore fluid is usually water, often coloured in certain places by dye so that fluid movement can be traced. Pseudo-two-dimensional sand beds are used to represent sub-horizontal flow problems and thin, vertical, transparent-sided tanks are used to represent vertical sections. Occasional 3D-sand-box analogues have been used, having approximately cuboid shape.

The advantages of sand-box models are relatively limited but there are some applications in which they are valuable:

(1) Qualitative demonstrations : sand-boxes find wide and continuing applications in the qualitative demonstration of fluid flow phenomena such as seepage beneath dams, pollutant plume development, streamline illustrations of laminar flow, and filter behaviour. These applications are mainly in teaching.

(2) Particle migration phenomena : sand-box experiments still remain the best method of studying particle migration phenomena induced by fluid flow. Traction of particles in filters and particle movement to produce 'piping' are very difficult to model mathematically.

(3) Solution-deposition phenomena : sand-box models are used with continuing success to examine the migration of salts through porous media. Simulations of subsidence due to solution has also been modelled.

(4) Sources of data : Simple sand-box models have recently been used by Peterson et al (1978) to obtain laboratory data for the calibration and validation of more complex mathematical models.

The advantages of sand-box analogues are thus primarily as qualitative aids in the visualisation of fluid flow problems rather than in their quantitative, practical solution.

The limitations of sand-box models are, in the main, common to all scale modelling situations.

(1) Scaling problems : properties like grain-size and pore-size are not properly scaled and capillary rises and suction problems are very difficult to overcome. Simulated rainfall can disturb particles to significant depths.

(2) Boundary conditions : at low flow rates, minor leaks and seepages from tank seams can be responsible for huge errors since boundary conditions are massively changed.

(3) Measurement accuracy : measurement and maintenance of specified low flow rates is difficult and measurement of head or potential is troublesome because of capillary effects in scaled-down piezometers.

(4) Construction problems : it is virtually impossible to build an anisotropic or inhomogeneous model with pre-specified properties. Problems of compaction and mixing and disturbance during saturation make complex models very difficult to build.

(5) Saturation problems : all sand-box models must be saturated with water at some stage. Ensuring complete saturation is often a problem and air-entrainment can significantly reduce apparent permeability and homogeneity.

The main disadvantages of sand-box analogues lie in the problems of scaling and their overall imprecision both in construction and in making measurements. They are also very time consuming if repeatable quantitative results are required.

4.3 HELE-SHAW ANALOGUES

Hele-Shaw analogues are flow tank models but do not attempt to physically represent the porous medium as a scale model. They exploit the analogy between saturated flow in a porous medium and viscous flow in a narrow space between parallel plates.

Inhomogeneity can be modelled by varying the distance between the plates since the modelled transmissivity is proportional to the square of the plate seperation. Anisotropy is generated by corrugations which relatively restricts flow normal to the ridges. Boundaries in Hele-Shaw models are real

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fluid flow boundaries. No-flow boundaries prevent the passage of the viscous fluid, constant and variable head boundaries are set by controlling the fluid potential, flow boundaries are set by controlling the fluid flow. Sources and sinks require the addition or removal of fluid.

One major advantage of Hele-Shaw analogues is that more than one fluid may be used and thus saline interfaces and pollutant migration problems can be tackled. Their major disadvantages are :

(1) Inflexibility : models are problem specific and a new problem requires rebuilding.

(2) Cost and time : models are time-consuming to construct and the equipment necessary to control and accurately measure fluid flows and pressures is expensive.

(3) Precision of representation : anisotropy and inhomogeneity require very precise, specific measurements of plate seperations to be constructed and maintained. Approximations must be made and only relatively coarse adjustments can be made.

Despite their cost, Hele-Shaw models are valuable particularly for two fluid problems. Recent applications are provided by Marei (1974), Smiles and Stokes (1976), and Bouwer (1978). No experimental work has been carried out in this study using such models but their value in demonstrating two-fluid problems and providing data against which numerical models may be validated is not in doubt.

4.4 ELECTRICAL ANALOGUES

Electrical analogue models of flow through porous media exploit the analogy between subsurface flow under hydraulic gradients and current flow under electrical potential gradients : between Ohm's law and Darcy's law. Hydraulic conductivity is modelled by electrical conductivity, water storage is equivalent to the storage of electrostatic energy in capacitors. Extensive accounts of theory and procedure are given by Walton et al (1963), Domenico (1972) and Herbert and Rushton (1966).

Most large electrical analogue models are based on a resistance-capacitance-network discretisation of the region to be modelled and are two-dimensional approximations. Occasionally 3D-models have been constructed. Steady-state models require only power supplies to maintain boundary conditions; transient models need waveform generators and pulse generators to provide transient inputs together with oscilloscopes to display and store responses. Electrical analogue models achieved their widest application in the mid to late 1960's and in their later stages of development were often interrogated by digital computers to overcome the problems of data collection.

The principal advantages claimed for electrical analogues, for example by Walton et al (1963) and Prickett and Lonnquist (1968), have been almost completely lost with the advent of digital computers.

(1) Flexibility : components are re-usable and new networks can be built up without additional capital expenditure. Digital models are infinitely more flexible, software development is very much easier and faster than rebuilding of hardware devices.

(2) Easy operation : analogues can be subjected to a large number of different inputs and the responses quickly and easily measured. In fact, obtaining potential maps from analogue models is a tedious business even for steady-state models. For transient models, simultaneous reading of the potentials at all network nodes requires a dedicated digital computer. Compared with digital models, analogue operation is complex and time consuming.

(3) Close correspondence to the hydrogeologic system : resistance-capacitance networks can be designed to fit any pattern of permeability and storage coefficient and any boundary conditions. Calibration and validation of analogue models is a long procedure involving frequent replacement of components. Although digital models require a similar number of changes, these changes are in numerical data and are therefore much faster.

(4) Speed and cheapness : analogues are relative cheap to construct and run and results can be rapidly accumulated. Although transient analogues are faster than most digital computers, the collection and presentation of results is not and again numerical methods are superior both is speed and cheapness.

Simple electrical analogues of steady-state, homogeneous, istropic problems can be constructed without the necessity for complex resistance networks by using graphite-coated 'Teledeltos' paper. Such models are very fast and easy to construct and are useful in preliminary investigations of problems with complex boundary topography. Analogue studies of this kind can be a useful prelude to digital modelling and allow the effects of approximations in the representation of boundaries to be rapidly investigated.

One very major limitation of electrical analogues not shared by either sand tank or digital models is their inability to tackle couple flow-dispersion-diffusion problems.

Electrical analogue models are largely a thing of the past though their use still continues. The hybrid electrical-analogue-digital computer used to model the transient response of the Chalk of the London Basin by the Water Resources Board (1973) represents the final stage of complexity and sophistication of such models before their almost complete replacement by digital numerical models. A few later analogue models are to be found in the literature, for example Sander (1976) and Gupta et al (1979), but such examples are increasingly rare.

4.5 EXPERIMENTS WITH ELECTRICAL ANALOGUE MODELS

A simple electrical analogue model was contructed to

simulate flow from beneath a waste disposal tip. The purpose of the experimental work was mainly to gain experience of the technique. However, for relative little effort some useful results were obtained which lend support to the major conclusion of the work as a whole - crude models are much more cost effective than complex models.

The case considered is that of two-dimensional flow in the vertical plane in an aquifer with a horizontal impermeable base and a regional gradient. A localised source of input from the base of tip is superimposed. It is assumed that the waste tip provides a constant source of water. in reality this may represent slow leakage from a perched water-table established in the tip. Infiltration over the remaining area is assumed to be negligible due to efficient field drainage to surface watercourses. The two-dimensional model implies a linear tip normal to the line of section; many spoil disposal tips for mining wastes have this general form.

The experimental equipment used was that employed for routine laboratory demonstations and comprised :

    Graphite-coated 'Teledeltos' paper
    'Electrodag' silver suspension paint
    2 No. DC power supplies (0-20v)
    Variable resistance field plotter (bridge circuit)
    3 No. digital voltmeters
    2 No. digital ammeters

Figures 4.1a and 4.1b show diagramatically the experimental layout for the plotting of equipotentials and streamlines respectively.
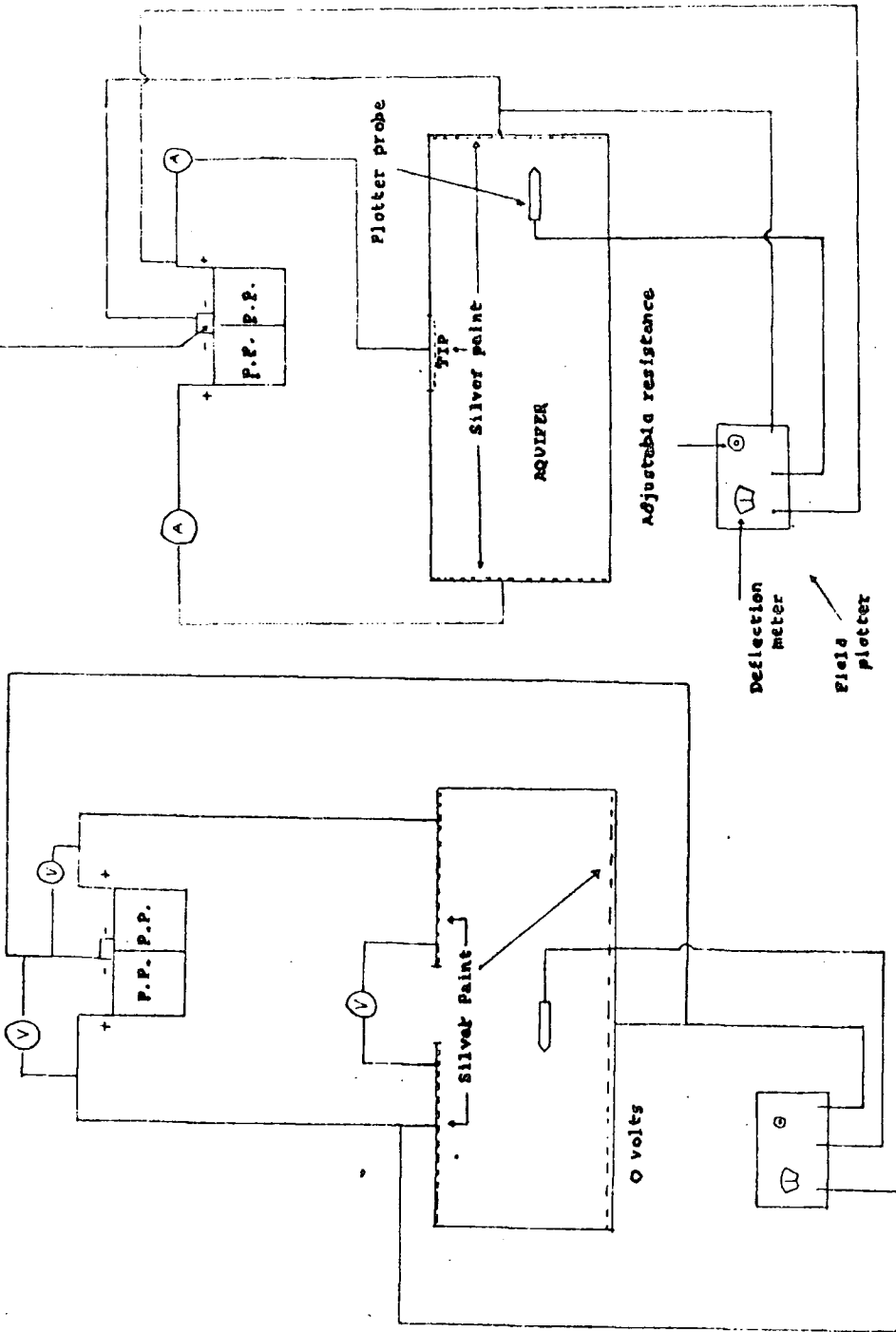
Fig. 4.1a   Experimental layout for equipotential plots

Fig. 4.1b   Experimental layout for streamline plots

For the plotting of equipotential lines, the boundaries marked (a), (c), and (e) in Fig. 4.2 were initially set to constant potential by painting with a silver suspension and applying an appropriate voltage. Boundary (c) was set to zero potential and boundaries (a) and (e) were set to various positive potential values :

Experiment	Boundary (a)		Boundary (e)	
	Potential (volts)	Current (microamps)	Potential (volts)	Current (microamps)
1	+10	+1640	+5	-10
2	+5	+107	+5	+597
3	0	-416	+5	+850
4	+2.5	-362	+5	+1428
5	+1	-980	+5	+2280
6	0	-902	+5	+1802
7	0	-395	+5	+790
8	+2.5	-330	+5	+1148
9	+2.5	-390	+5	+1393

The actual potentials used are irrelevant, only their ratio is important. Checks were made to ensure that the potential drop along the silver painted 'constant potential lines' were minimal then eqipotential lines were plotted using the field plotter to divide the potential drop in ten equal intervals. The field plotter is a simple Wheatstone bridge circuit in which one arm can be set to a fraction of the total p.d. by a variable resistor and balanced against the p.d. to a point on the 'Teledeltos' paper. The currents flowing at the boundaries were measured with the ammeters (see Fig. 4.1a).

For the plotting of streamlines, the constant potential boundaries were made no-flow and vice-versa. This involved cutting a thin strip from the paper with a scalpel to

Fig 4.2   Aquifer representation

120 mm

250 mm

750 mm
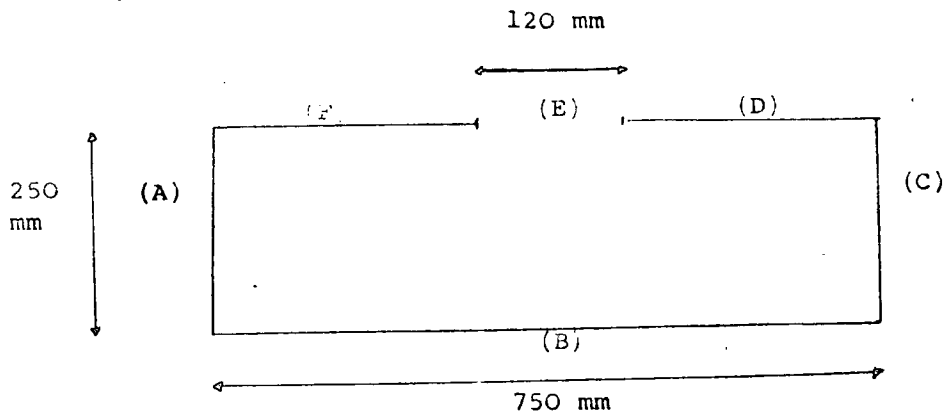
Fig. 4.3   General relationship between i and V
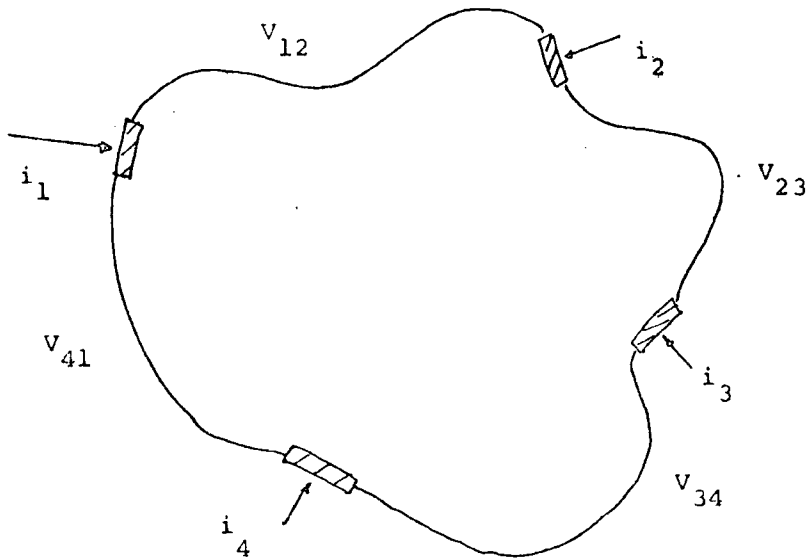
$$i_1 = k(V_{12} - V_{41})$$ $$i_2 = k(V_{23} - V_{12})$$

$$i_3 = k(V_{34} - V_{23})$$ $$i_4 = k(V_{41} - V_{34})$$

remove the paint lines and repainting new boundaries. Strictly speaking the flowlines could have been constructed since they are orthogonal to the equipotentials but in practice it is faster to plot them. The procedure is the same as for equipotential plotting the only problem is deciding on the values of potential for the new constant potential boundaries. Using Ohm's law and Kirchoff's laws it can be shown that the required potential drop between any two new boundaries is proportional to the current at the intervening boundary when it was a constant potential. Figure 4.3 illustrates the required conditions for the general case derived by Domenico (1972) in the groundwater modelling context.

The purpose of the experiments was to help in the formulation of more practical models of pollution from tips and to gain a 'feel' for the problem. The models is crude and many assumptions and approximations are made.

(1) It is implied that flow in the aquifer is parallel to the impermeable base of the formation. A not unreasonable hydrogeological approximation.

(2) It is assumed that the flow from the tip can be represented by a line of constant potential. In reality, the centre of any tip is under a greater normal stress and therefore more compact and perhaps less permeable than the margins. No attempt is made to model this.

(3) It is implied that the three constant potentials are independent. There is no means for them to interact. In many

cases this may be approximately true particularly if the flow from the tip is small compared to the regional flow. In other cases this assumption may not hold.

(4) In experiments 7 and 9, where 0.75 of the formation is saturated, and experiments 6 and 8, where 0.5 of the formation is saturated, only a first order approximation of the shape of the free-surface is made.

The flow-nets produced for the 9 experiments are shown in Figs 4.4a-i. When contaminated water leaks from a spoil heap the model results allow the following tentative conclusions to be drawn :

(1) When the regional flow is high relative to the flow from the tip (Fig. 4.4a) any contaminated water will be swept away at relatively shallow depth.

(2) When regional flow is low relative to flow from the tip (Figs 4.4c,e,f,g) a large but mobile plume of pollutant forms. Although such a plume implies continuous contact between polluted water and the porous medium, chemical reactions may not occur due to the relatively rapid movement of the fluid.

(3) When regional flow and flow from the tip are of similar magnitudes (Figs 4.4b,d,h,i) extensive areas of 'slack' relative immobile water develop. In these areas chemical reaction between polluted waters and the porous medium are possible since long resisdence times are to be expected. Such areas may tend to become anaerobic if the inflow is limited.
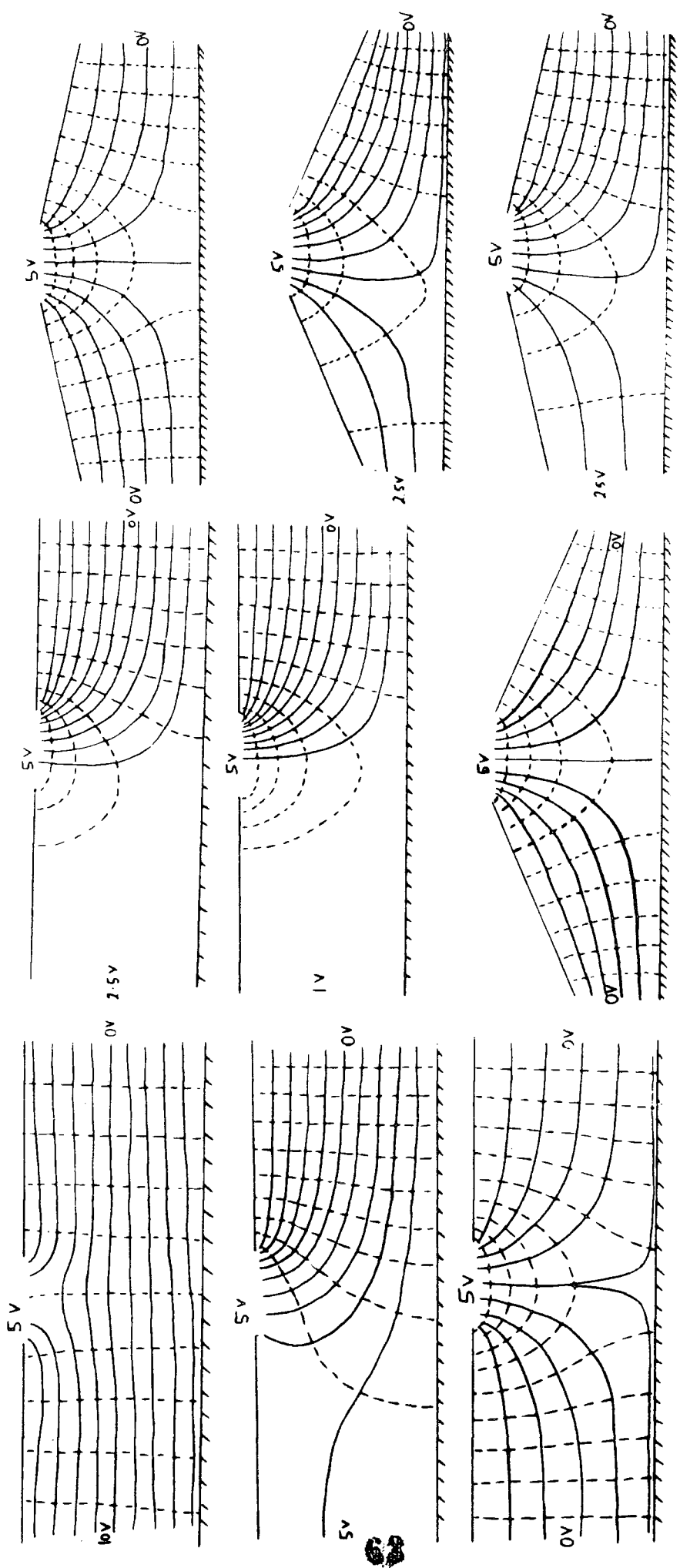
Fig. 4.4a-i Experimentally derived flow nets

These conclusions are relatively obvious even without the model
but the modelling process gives a semi-quantitative aspect to
the conclusion and points the way to more detailed experiments.

NUMERICAL DISTRIBUTED-PARAMETER MODELS OF GROUNDWATER SYSTEMS

5.1 DISTRIBUTED-PARAMETER MODELS

In the various numerical model formulations an attempt is made to predict the dependent variables over a region characterised by properties specified for a finite number of discrete points (nodes) or sub-regions (elements). Where only a few nodes or elements are used in the representation they may be called lumped-parameter models. Where many sub-regions are considered the representations are called distributed parameter models. Although similar formulations are used for both types of model, the formal use of finite difference methods (FDM), finite element methods (FEM) and boundary integral equation or boundary element methods (BEM) is often only acknowledged in the distributed-parameter case.

Sophisticated distributed-parameter numerical methods are widely used in groundwater flow and quality models. According to the review of Prickett (1979), FDM are most popular but FEM are also widely used. Applications of BEM to groundwater problems have only recently appeared in the literature.

5.2 FINITE DIFFERENCE METHOD (FDM)

The FDM technique represents the continuous partial differential equations governing flow and/or solute transport in a region, by a set of approximate difference equations referring to a finite number of discrete points in the region of interest. The approximations implicit in the discretization process introduce errors and a variety of schemes have been devised to minimize and control these errors. Comprehensive discussions of the application of the FDM to groundwater problems are provided by Shamir and Harleman (1967), Remson et al (1971) and Freeze and Cherry (1979). A more detailed mathematical background is provided by many more general texts such as Ames (1977).

A variety of schemes can be used to represent the derivatives in the governing equations but these eventually lead to the reduction of the problem to one of obtaining a solution to a set of simultaneous, linear, algebraic equations.

Depending on the approximation used for the derivatives this set of equations may be :

(1) explicit - yield their solution by direct substitution, or

(2) implicit - require inversion followed by substitution for their solution.

A number of standard methods are employed for the solution of

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these equations including Gauss-Seidel elimination (GSE) and successive over relaxation (SOR).

All the various formulation schemes have associated with them numerical stability and convergence characteristics discussed by Remson et al (1971), Rushton (1973) and Ames (1977) among others. In general, pure implicit schemes are unconditionally stable whereas explicit and semi-implicit schemes such as Crank-Nicholson, have stability criteria dependent on the spatial and temporal discretization intervals. The alternating direction implicit (ADI) method proposed by Peaceman and Rachford (1968) is a scheme frequently utilised in 2-D groundwater models.

In the solution of the dispersion-convection equation a phenomena called 'smearing' can occur where numerical dispersion takes place as a result of the discretization process. This can be eliminated by using the widely applied method of characteristics (MOC) technique proposed by Gardner et al (1964).

The FDM has a long history of application to groundwater problems. Very many examples of FDM applications to practical problems as well as more theoretical investigations are documented in the technical litrature.

In well hydraulics, Cooley (1971) and Rushton (1973) and Rushton and Booth (1976) compare analytical and FDM solutions. Rushton and Chan (1976) use the technique to simulate inhomogeneous, anisotropic flow to wells.

In regional aquifer management, Reeves et al (1974) describe a resource evaluation model for the Triassic sandstones in the Vale of York and Oakes and Skinner (1977) describe a model for a similar aquifer the Fylde area of Lancashire. Rushton and Tomlinson (1975) model the fissured Lincolnshire Limestone aquifer and Morel (1979) applies the method to the Chalk of the Upper Thames basin. Aguardo et al (1977) use the FDM to optimize well spacings for aquifer development.

In groundwater pollution, Bredehoeft and Pinder (1973) investigate chloride pollution in Georgia and Konikow and Bredehoeft (1974) discuss salinity of groundwaters in Colarado. Robertson (1977) reports an application in the control of radioactive wastes in Idaho and Konikow (1976) models chloride pollution from liquid industrial wastes in Colorado. Gorelick et al (1979) model chloride contamination from a river. Lin (1977) compares numerical and analytical solutions of the transient convection-dispersion equation.

5.3 FINITE ELEMENT METHOD (FEM)

The FEM technique solves the partial differential equations governing flow and solute transport in a region by finding those values of the dependent variables necessary to minimise an integral form of the equation. The integral is evaluated by summing the contribution for a finite number of sub-regions or elements.

The concepts of FEM are much more difficult to understand than the FDM concepts. To aid understanding FEM can be regarded as a technique for finding the minimum potential energy system consistent with sources, sinks and boundary conditions.

The integral form of the governing equation is derived by two alternative approaches :

(1) Variational methods : using the principles of variational calculus to derive the functional which must be minimised for the values of the dependent variable to be the required non-trivial solution of the governing partial differential equation. Such procedures are known as Rayleigh-Ritz methods. Neuman and Witherspoon (1971) develop a typical variational formulation for transient 2D-groundwater flow. Guymon et al (1970) provide an example of the development of the 2D-convection-dispersion equations.

(2) Weighted residual methods : where the differences (residuals) between the required solution and a trial solution are systematically eliminated. A weighting function is applied to the nodal residuals and the sum of the weighted residuals is minimised for each element in the region. This procedure clearly involves the minimisation of a sum or integral as in the variational methods. Gray and Pinder (1974), for example, apply a weighted residuals method (Galerkin's procedure) to the case of 2D-transient groundwater flow and an application to the 2D-convection-dispersion equation is discussed by Segol and Pinder (1976).

Because of their more general form and flexibility, weighted residual methods have been increasingly used in preference to variational forms. Galerkin's procedure, widely used in groundwater FEM models, is a particular weighted residual method characterised by the way in which the weighting function is chosen. Unlike FDM, in FEM the dependent variable is represented not only at nodal points but over the entire element or sub-region. This is achieved by interpolation from nodal values (which do not necessarily bound the element concerned). The interpolation function is called a shape function. In Galerkin's procedure the weighting function is chosen to be the shape function.

Extensive texts have been written on FEM, notably Zienkiewiez (1971) and Desai and Abel (1972); however, specific groundwater modelling applications are best covered by Remson et al (1971) and Gray and Pinder (1979).

Variational and weighted residual methods lead to the reduction of the problem to one of solving a set a linear, simultaneous algebraic equations. The methods of solution available are the same as those for FDM formulations and all the problems of stability, convergence and numerical dispersion apply. The extent of such problems and the differences and similarities between FDM and FEM will be discussed further.

Like FDM, FEM also finds widespread employment in groundwater modelling. However, relatively few of the FEM applications are practical and the majority of studies

demonstrate the availabilty of the method rather than its practical applications.

In well hydraulics, Javandel and Witherspoon (1969) discuss the application of variational methods and Reilly (1976) and Chorley and Frind (1978) compare FEM simulations with analytical solutions.

In civil engineering, Desai (1972) analyses 2-D groundwater flow through earth dams.

In regional aquifer management, Wilson and Hamilton (1978) describe an FEM model to predict the effects of opencast mining on regional groundwater flow.

In groundwater pollution modelling, Cherry et al (1973) use a 2-D model radioactive waste disposal in Manitoba and Frind and Verge (1978) re-examine the same problem in 3-D.

Much FEM modelling has been concerned with generalised rather than specific problems. Smith et al (1973) discuss 2-D convection-dispersion and Gupta and Tanji (1976) invesigate the possibility of 3-D models. Frangakis and Tzimopoulos (1979) compare FDM and FEM techniques for 2-D groundwater flow. Narasimhan et al (1978) review the application of FEM models to a wide range of problems in subsurface hydrology. Futagami et al (1976) use FEM coupled with linear programming in a suggested management model for water pollution control. Pickens and Lennox (1976) discuss a sensitivity analysis for a 2-D steady-flow model of transient convection-dispersion.

5.4 BOUNDARY INTEGRAL EQUATION METHOD (BEM)

The BEM technique will only be briefly discussed since it is a relatively new method and at its present stage of development lacks the flexibility that has been achieved by FDM and FEM.

In BEM, the problem of solving the governing partial differential equations for the dependent variables over a region is reduced to one which depends only on the values on the boundary of the region. This has a very large effect on the computational efficiency of the method since the arithmetic required for a 3-D boundary element model is roughly that for the 2-D bounding surface. BEM also has the ability to represent boundaries at infinity which presents problems for FDM and FEM. Hybrid BEM-FEM techniques have been developed to take advantage of the flexibility of FEM and the boundary at infinity representation afforded by BEM. In common with FDM and FEM, BEM formulates a set of linear, simultaneous equations which must be solved. A comprehensive introduction to the BEM technique and its applications is given by Brebbia (1978).

Application of BEM to groundwater modelling is a growing area of research and groundwater flow models have been presented by Liu and Ligget (1978) and Ligget and Liu (1979). These papers indicate the scope of the technique but do not describe examples of its use for practical problem solving. Ross and Koplick (1979) similarly indicate how the method can

be applied to groundwater quality modelling by representing a porous medium by a network of streamtubes in 1-D.

The computational conciseness of BEM offers real scope for microcomputer applications and clearly an area for further research exists.

5.5 LIMITATIONS OF NUMERICAL METHODS

To be of value in groundwater studies, it is necessary to understand the problems and limitations inherent in the application of numerical methods. Brebbia (1978) elegantly shows that FDM, FEM and BEM can all be considered as weighted residual methods for which various degrees of flexibility are permitted in the choice of the weighting functions. This treatment is a convenient framework for the discussion of the general problems common to numerical methods. All formulations finally require the solution of a set of linear, simultaneous algebraic equations. The precise form of these equations depends on the procedure used to derive them but their solution requires :

(1) convergence : truncation errors should not be allowed to grow in an uncontrolled manner.

(2) stability : unstable numerical oscillations should be effectively damped out.

(3) conservation : water or pollutant should be neither

created nor destroyed by numerical errors.

(4) no dissipation : numerical dispersion due to discretisation should be prevented.

(5) accuracy : in addition to preventing errors due to truncation and discretisation, it is necessary that the solution obtained is also free from systematic errors leading to inaccuracy.

Accuracy can be lost in the formulation procedure and a solution can be convergent, stable, conservative, show no dissipation but be inaccurate because of the formulation of the system of linear equations. Accuracy is also a function of the precision with which the independent variables are represented in the model and is closely allied with data reliability.

Explicit solution schemes require care in the choice of the spatial and temporal discretisation intervals to ensure stability. Such schemes have the advantage of simplicity but their use is restricted because of the stability problems which are discussed at length by Shamir and Harleman (1967) and Rushton (1973) among many others. Haverkamp et al (1977) present evidence suggesting that explicit methods are computationally inefficient relative to implicit procedures for equivalent accuracy.

Pure implicit solution schemes are unconditionally stable but the accuracy remains a function of the chosen spatial and temporal discretisation interval and the

formulation procedure. Both Shamir and Harleman (1967) and Rushton (1973) point out the fallacy of accepting results from implicit schemes without checking numerical accuracy. Implicit solutions are favoured for their stability - however large but stable oscillations can and do occur. The popular ADI scheme is not immune from these problems but is recommended by many authors for its computational efficiency.

Numerical dispersion or smearing is a problem found in the solution of the convection-dispersion equation. The problem arises from the approximation in the derivatives used to calculate the velocity term. Two procedures are used to reduce or eliminate the smearing phenomenon :

(1) separation of the convection and dispersion terms so that the processes are modelled consecutively rather than concurrently. This technique involves the method of characteristics (MOC) and is widely used, for example by Konikow (1976).

(2) improvement of the estimate of the spatial derivatives used to generate the velocity term. Chaudhari (1971), for example, overcomes the problem by using a high order finite difference scheme, including more terms in the truncated Taylor series. In FEM schemes, care in the choice of shape function can reduce the problem.

Discretisation errors can lead to numerical inaccuracies and the choice of nodal spacings and time steps is a trade-off between acceptable accuracy and computational

efficiency. It is useful to bear in mind that the acceptable accuracy may change over the region modelled and that acceptable numerical inaccuracy must be influenced by the errors inherent in the data for independent variables.

Numerical accuracy cannot substitute for data reliability and models must be formulated with this in mind. For sensitivity analyses and theoretical studies such problems are not present but in practical, predictive models no amount of mathematical rigour will create or improve the basic data available.

Calibration is an important stage in all modelling execises. A general scheme for a coupled transient flow-convection-diffusion model would perhaps be :

(1) By inversion or trial and error find a $\{T\}$, $\{S\}$ and $\{q\}$ values necessary to produce the observed dependent head distribution;

(2) By inversion or trial and error find a $\{D\}$ distribution necessary to produce the observed dependent concentration distribution.

Gillham and Farvolden (1974) have pointed out the infinity of possible solutions in step (1) if little or no field data is available and Segol and Pinder (1976) report that perfectly acceptable solutions for step (1) totally inconsistent with step (2) are obtainable. The calibration process tends to be an iterative one in which distributions for all the independent

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variables are sought which are consistent with field estimates and observations of the dependent variables. At the end of the calibration stage, Birtles and Reeves (1977) recommend validation of the model with data independent of the calibration dataset. Pilot schemes or large scale field tests can be devised to fulfill the validation role.

Care in the formulation of FEM meshes is of special concern since the node and element ordering schemes critically affect computational efficiency. This arises because of the numerical advantages of inverting sparse matrices with a narrow bandwidth. Accuracy can also be reduced by badly ordered meshes. These problems escalate when 3-D models are considered and seperate programs for mesh generation and optimization are often necessary in such cases.

Costs for running even efficient large FDM and FEM models are not insignificant. Some rough estimates have been made based on published CPU/storage requirements and experience gained during this study. Adjustments have been made to eliminate hardware differences by scaling to equivalent times on an IBM 370/168. In August 1981 commercial use of an IBM 370/168 was costing 27p per CPU sec.

Comparisons are difficult because of uncertainties in program efficiencies, computer operating systems, hardware comparability and many other factors but the CPU time figures and implied costs should give at least an order of magnitude guide.

When comparing the runtimes of various models, it is important to have an idea of the speed of execution of different computers. A linear rating scale is used to compare the performances and the values used were as follows:

Computer type	Rating
IBM 370/168	3250
CDC 6500	1200
IBM 360/75	950
Burroughs B6700	475
Sorcerer microcomputer	3

Hence the IBM 360/75 is considered to be approximately twice as fast as the Burroughs B6700 — see Frind and Verge (1978). Other values were given by the Computer Unit at Durham University (pers. com). The microcomputer figure is derived from the discussion in section 5.7.

Steady state models

CPU time/ node/iter (ms)	Computer	Flow model	Reference
4.9	360/75	2-D FEM sat	Gillham & Farvolden (1974)
22.5	360/75	3-D FEM unsat	Frind & Verge (1978)
28.3	Burroughs	3-D FEM sat	Gupta & Tanji (1976)
68.3	370/168	2-D FEM unsat	Section 5.8

Transient models

CPU time/ node/step (ms)	Computer	Flow model	Reference
0.7	Sorcerer	2-D FDM sat	Section 5.7
2.8	CDC 6500	2-D FDM sat	Davis (1975) [4]
0.6	CDC 6500	2-D FDM sat	Davis (1975) [4]
0.4	CDC 6500	2-D FDM sat	Davis (1975) [1] [2] [3]
0.4	370/168	2-D FDM sat	Section 5.7
18.4	360/75	3-D FEM sat	Frind & Verge (1978)
8.3	360/75	3-D FEM sat	Frind & Verge (1978)
2.4	CDC 6500	2-D FEM sat	Davis (1975) [5]
1.1	CDC 6500	2-D FEM sat	Davis (1975) [7] [8]
0.5	CDC 6500	2-D FEM sat	Davis (1975) [6]

( ) refers to particular algorithm run by Davis.

All times are 370/168 equivalents.

From the above table it can be seen that typical 2-D saturated transient flow models require about 1 ms CPU time per node step. 3-D models appear to need an order of magnitude of time per node step more. For steady state saturated 2-D flow models, about 5 ms per node step is required. Unsaturated flow and 3-D steady state models increase time requirements by a factor of 5 or 10.

5.6 COMPARISON OF FDM AND FEM

Since FDM and FEM methods are very widely used an evaluation of their comparative merits in groundwater modelling is indicated.

FDM schemes are widely criticised for their lack of flexibility. This criticism comes largely from FEM proponents since FDM remains very much the favoured practical technique and many of the implied problems can be overcome. Smith et al (1973) suggest that inflexibility in FDM schemes results in reduced computational efficiency relative to FEM schemes. Freeze and Cherry (1979) among many others point out that FDM requires that nodes be chosen on a rectangular grid and for anisotropy to be modelled, the grid axes must coincide with the principle axes of anisotropy. If two anisotropic formations with different principal axes are present in a flow field, FDM cannot be applied. Guymon et al (1970) indicate the problems of modelling convection and dispersion using FDM. The anisotropy

of dispersivity occurs normal and parallel to the flow velocity vector, thus the grid axes must be realigned to coincide with the dispersivity axes. FDM encounters difficulties in representing free-surfaces where the spatial position of grid points must be flexible, hence Desai (1972) employs FEM for the study of flow through earth dams.

These criticisms are well founded and in complex anisotropic materials, free-surface problems and in transient coupled dispersion (where the principal axes of dispersion may rotate) FEM has advantages. Other objections to FDM may be less serious.

For example, the non-coincidence of point sources and sinks with grid points indicated by Oakes et al (1975) and the imprecise representation of boundaries pointed out by Remson et al (1971)and many others, can be overcome satisfactorily in most cases by grid refinement techniques such as those used by Birtles and Reeves (1977). In many groundwater problems the precision with which the hydrogeological boundary is known is likely to lead to much larger errors than the numerical errors induced by imprecise location.

Many would argue that what FDM loses in flexibility and computational inefficiency relative to FEM and BEM, it gains in conceptual simplicity and user familiarity. FDM programs tend to be easier to 'debug' and more rapid to develop because of the more direct link with the form of the governing partial differential equation. Although FDM can be shown to be computatinally inefficient relative to FEM in some

circumstances, in studies reported by Emery and Carson (1971) and Pinder and Frind (1972), FDM was both faster and more concise for equivalent accuracy.

FEM gains in flexibility are not without cost. Flexibiity requires that shape (or interpolation) functions become more sophisticated and hence the resulting set of equations to be solved present more problems with regard to numerical errors in their solution. The permissible shapes for elements are rather limited when accuracy is required and in FEM mesh design requires as much if not more skill than FDM grid design. This problem was found by Frind and Verge (1978) to be particularly difficult in unsaturated-saturated zone models. FDM grids are rectangular and hence nodal co-ordinates are easily calculated and errors rarely occur. On the other hand, errors in mesh node co-ordinates for complex FEM meshes are a serious source of error reported by Pinder and Frind (1972) and overcoming this problem involves further computational or manual effort.

A useful assessment of various FDM and FEM was made by Davis (1975), who compared the performances of different formulations to a set of simple transient flow problems, for which analytical solutions were available. He concluded that given small enough time step or mesh (grid) spacing, all methods would give rise to accurate results. Methods involving no matrix reduction were comparitively inexpensive and posed no problems in changing {S}, {T} or even the time interval from step to step. The efficiency of all methods involving matrix reduction could be optimized by careful node numbering in order

to minimize the matrix bandwidth. Trial and error fits of the best grid or mesh size were essential to obtain optimum results.

In summary, when selecting between FDM and FEM techniqes it is worth bearing the following points in mind :

(1) For free-surface problems and problems where several sets of axes or rotating axes of anisotropy are present, FEM has the required flexibility.

(2) For conceptual simplicity coupled with simplified program writing and development FDM is superior.

(3) In terms of computational efficiency for equivalent accuracy, the reports in the literature are ambiguous. It seems that FEM is favoured as model complexity increases.

(4) The survey of Prickett (1979) and the impression gained from reviewing the recent literature suggests that practical modellers select FDM unless the inflexibilities of the method prevent its use.

5.7 EXPERIMENTS WITH FDM MODELS

A model developed by Rankine (1980), based on an original program by Pinder (1970) was used to obtain typical run times on an IBM 370/168 mainframe computer. In addition, the original program written by Pinder was rewritten in BASIC

to run on an 8-bit microcomputer in order to compare the run times for equivalent programs. Both programs thus use identical ADI algorithms to set up and solve the equations of flow and difer only in input/output statements and where language differences force minor changes in syntax.

The FORTRAN version run on an IBM 370/168 requires about 0.4 milliseconds CPU/time step/node. The BASIC version run on a Z80A-based microcomputer requires about 800 milliseconds CPU/time step/node. Hence the mainframe is faster by about a factor of about 4000 assuming the microcomputer arithmetic precision is acceptable. A later attempt at running a BASIC version of the program on the mainframe suggested that a factor of 1000 would be a fairer comparison.

Comparisons based on CPU time are rather misleading for microcomputers versus time-shared mainframes. Comparisons based on turn-around time (the time between user submission of the job and its return) are much more meaningful. On this basis, if the NUMAC (Northumbrian Universities Multiple Access Computer) time-sharing system is typical, elapsed time (actual job run time) is on average about 10 times the CPU time. For jobs run from terminal in busy periods (10.00-18.00 hours) this factor can rise to 100. In addition a delay of roughly 30 minutes is involved in the return of hard copy output. For batch-processed jobs, delays depend on the CPU requirement and it is virtually impossible to have a job requiring more than 64 CPU seconds run between 10.00 and 18.00 hours.

In summary, the NUMAC IBM 370/168 mainframe computer

operating time-sharing is intrinsically about 1000 times faster than the Sorcerer microcomputer. Delays in return of output from the mainframe mean that the dedicated microcomputer is faster for problems of less than about 200 node-steps. Additional overheads during mainframe busy periods between 10.00 and 18.00 hours extend the size of the problem for which the microcomputer can be effectively used to perhaps 500 node-steps.

The time to 'debug' and adapt the FORTRAN version of the program to run on the IBM 370/168 was 2 to 3 times that required to prepare the BASIC program on the microcomputer reflecting the advantages of a dedicated machine and an interpretive rather than compiling language. This advantage is significant if models are not to be used for extensive 'production runs' since what is gained on run time can be easily lost in development time.

Data preparation and input time requirements for both FORTRAN and BASIC programs were similar if advantage was taken of the distributed-parameter facilities and parameters and variables specified for each individual node. Initial preparation times of 1-2 minutes per node for a new mesh are realistic for 'real' rather than idealized problems even for the experienced user. Data input for simplified problems was very much faster using interactive microcomputer BASIC programs than mainframe FORTRAN.

5.8 EXPERIMENTS WITH FEM MODELS

A model based on the program developed by Amend (1975) was adapted to run on the NUMAC IBM 370/168 in order to investigate the run time, development time and data preparation time.

Fairly major modifications of the program were required to the mesh-regeneration routines to make the model find the phreatic surface for an arbitary initial mesh. Development time to adapt an original FORTRAN program to the IBM 370/168 was similar to that for the finite difference program discussed in Section 5.7. Data preparation and input times were also comparable.

As far as the user is concerned, the problems of adapting and running existing FDM and FEM software on mainframe and microcomputers are very similar. In both cases, the development and debugging time may be large compared to the 'production time' unless an extensive series of runs are anticipated. Under such circumstances, microcomputer implimentation may have attractions especially if small (<200 node-steps) models are involved.

LUMPED-PARAMETER NUMERICAL MODELS OF GROUNDWATER SYSTEMS

6.1 LUMPED-PARAMETER MODELS

Although partial differential equations describing the flow of water and transport of pollutants through porous media on a macroscopic scale are known, lack of adequate data severely limits the accuracy of any practical predictions made by application of these equations. As a result of the data limitations, doubt can be cast on the accuracy, practical value and, in particular, cost effectiveness of large sophisticated distributed-parameter models. In many cases, it can be argued that very simple models would enable equally valid conclusions to be drawn.

Lumped-parameter models break the groundwater system down into a few sub-units with average properties, taking advantage of as much data as is available. Spatial variations in the dependent variables are not predicted but very large scale behaviour can be simulated much more cheaply and argueably, with equal accuracy, compared with sophisticated distributed-parameter methods.

The application of lumped-parameter models of groundwater systems has been largely neglected and there has

been a marked tendency to use distributed-parameter models in situations where their application was neither necessary nor cost effective.

6.2 LUMPED-PARAMETER MODELS OF GROUNDWATER FLOW

The most basic lumped-parameter of all in hydrology is the well-known catchment water budget equation for a catchment :

$$P = E + Q + G - D \qquad (6.1)$$

where P is the catchment precipitation,

E is the catchment evapotranspiration,

Q is the catchment surface water recharge,

G is the catchment groundwater recharge,

and D is the catchment total discharge.

Most catchment models attempt to find D and the equation is thus written :

$$D = P - (E + Q + G) \qquad (6.2)$$

In the simplest models it is assumed that (E + Q + G) can be expressed as a function of P and hence that a 'black-box' transformation can be used to convert the precipitation time-series into the catchment discharge record. This is the efective assumption of the famous unit-hydrograph concept of Sherman (1932). The form of the necessary function is

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determined by analysis of past precipitation and discharge records.

Implicit in this empirical procedure is the assumption that current discharge is a function of past precipitation and that therefore the system has some storage characteristics. A very simple assumption made about catchment storage is that it is a weighted function of recharge ($R = Q + G$) and discharge (D) :

$$s = c.[x.R + (1-x).D] \qquad (6.3)$$

where s is the catchment storage,

    c is a storage constant with dimension (T),

  and x is a dimensionless weighting factor.

This equation, together with the fact that the first derivative of s with respect to time is $R - D$, forms the basis of the routing equation presented by Muskingum (1940).

Lumped-parameter catchment models are very widely used in surface water flow prediction a typical example being the 'Stanford Watershed Model' described by Crawford and Linsley (1966). The parameters in such models are determined by the calibration procedure and often cannot be directly related to a field measurement or observation. Such models have provided rapid and reliable surface flow predictions but, because of their empirical nature, they are unable to predict groundwater-surface water interactions.

This problem is overcome by use of more realistic lumped-parameter models of sub-surface flow. Gelhar and Wilson (1974) point out the relationship between groundwater parameters and the empirical parameters of the 'linear reservoirs' used in many catchment flow prediction models. The linear reservoir assumes that the discharge is proportional to the storage which in turn depends on the head (h). For sub-horizontal (Dupuit) flow between a barrier and discharge boundary (at head h'), Gelhar and Wilson (1974) show that :

$$D = (3T/(L^2).(h - h') \qquad (6.4)$$

where T is the aquifer transmissivity

and L is a characteristic length of the aquifer.

Continuity requires that the change in storage of the system is equal to the net inflow, thus :

$$R - D = S.dh/dt \qquad (6.5)$$

where S is the aquifer storage coefficient.

Equations (6.4) and (6.5) provide a lumped-parameter model for estimating the discharge from a groundwater system given the recharge.

Birtles and Reeves (1977) suggest the incorporation of a more realistic lumped-parameter groundwater storage element involving vertical and horizontal flow. The model

simulates 1-D horizontal and vertical flow using an explicit finite difference formulation and requires parameters directly related to average {T} and {S} values for a limited number of catchment sub-units. In essence, the model is the same as that of Gelhar and Wilson (1974). Rapid runoff can be simulated by incorporating high {T}, low {S} sub-units. The model is demonstrated by simulation of flows in the groundwater dominated River Hull catchment and it's performance is compared with a 900-node distributed-parameter model for a Triassic sandstone catchment.

6.3 LUMPED-PARAMETER MODELS OF GROUNDWATER QUALITY

The value of lumped-parameter models in this context has been recently reviewed by Gelhar (1976). Solute transport models are based on a mass balance equation of the form :

$$c.dv/dt + v.dc/dt = c'.v' - c''.v'' \qquad\qquad (6.6)$$

where c ,v is the solute concentration and volume,

     c',v' is the net inflow concentration and volume,

and c'',v'' is the net outflow concentration and volume.

If transport is considered under steady flow conditions, then the first term on the left hand side vanishes (since the volume will be invarient). The inflow and outflow terms on the right hand side may include :

(1) convective inflows and outflows,

(2) dispersive gains and losses,

(3) recharge and discharge sources and sinks.

Lumped-parameter quality models divide the groundwater system into a few cells. Gelhar and Wilson (1974) in a model to predict aquifer pollution due to road salting, use a single cell and assume perfect mixing of all sources. Mercado (1976) and Central Water Planning Unit (1976) make similar assumptions for nitrate movement models concerned with irrigation and regional pollution respectively. Both models treat nitrate as a non-conservative species, that is, the nitrate present in the system decays with time. In the model described by Mercado (1976), chloride and nitrate transport is considered, the chloride ion being treated as conservative, that is, no decay with time. Thomas et al (1972) use a lumped parameter water quality in conjunction with an electrical analogue flow model. Solution-precipitation reactions are modelled using solubility product data.

No multiple-cell lumped-parameter groundwater quality models were found in the literature and convective-dispersive inflows and outflows do not seem to have been considered.

6.4 APPLICATIONS OF LUMPED-PARAMETER MODELS

Lumped-parameter models have been relatively little used in groundwater modelling but hold considerable attractions in system analysis and management simulations. The principal areas where their application could be valuable include :

(1) Preliminary models : where data is sparse and approximate predictions of flows and water quality are required, particularly for systems too complex for analytical models.

(2) Long-term simulations : where distributed parameter methods can prove very expensive. Lumped-parameter models may be calibrated by more sophisticated models.

(3) Complex interactive systems models : where interaction between two or more sub-systems is involved. Examples could include :

(a) groundwater-surface water flow interactions,

(b) agriculture-groundwater quality interactions,

(c) rock matrix solution-permeability interactions.

The applications are essentially long-term, complex interactive problems where data is sparse.

6.5 LIMITATIONS OF LUMPED-PARAMETER MODELS

As with other modelling techniques, lumped-parameter models have their disadvantages. The main limitations are :

(1) lack of detail : spatial patterns of drawdown and pollution plumes are not attempted and thus predictions for individual localities cannot be made. Point pollution sources and individual wells are not represented.

(2) approximation of systems : in common with analytical models, the system under investigation is idealised and approximated. In some cases, the variability of a region may be so great as to rule out the lumped-parameter 'average' approximation.

(3) over elaboration : as more and more lumped-parameter cells are added to a model, the difficulties associated with distributed-parameter models grow and the advantages of the lumped-parameter technique are lost. Providing for continuity between model cells eventually grades into distributed-parameter techniques.

Lumped-parameter models are attempts to simulate large-scale, long-term system behaviour involving gross simplification and loss of detail in order to examine general trends and parameter interactions.

6.6 EXPERIMENTS WITH LUMPED-PARAMETER MODELS

A lumped-parameter groundwater flow and solute transport model was developed for interactive use on a desktop microcomputer. The model is conceptually similar to those developed by Gelhar and Wilson (1974) and Birtles and Reeves (1977) and is devised for the evaluation of alternative regional management stategies. It has been applied to the problem of aquifer pollution arising from the widespread application of salt for road deicing but can equally be applied to any dispersed source regional pollution problem.

Combining equations (6.5) and (6.6) by making substitutions for the volume terms in (6.6) : $v = S.h$; $v' = R$; and $v'' = D = a.(h - h')$; gives :

$$S.d(h.c)/dt = R.c' - a.c.(h - h') \qquad (6.7)$$

where $R.c'$ represents a net source term.

The source term includes natural recharge, artificial recharge and any groundwater abstractions. A conceptual diagram of the model which forms the basis of the computer program APPLE is given in Fig. 6.1.

The program APPLE listed at the end of this chapter, solves equation (6.6) by a stepwise, explicit finite difference scheme; advancing the calculation of the dependent variables h and c consecutively. The average value of h over the explicit time step (t) is given by :

$$H = [2S.h + (a.h' + R).t]/[2S + a.t] \qquad (6.8)$$

Now the concentration calculation is advanced to give the average value of c over the time step :

$$C = [2S.H.c + R.c'.t]/[2S.H + R.t] \qquad (6.9)$$

The value of the parameter a in equation (6.8) is given by equation (6.4). In the program APPLE, each source element involved in the parameter R may be represented as a lumped-
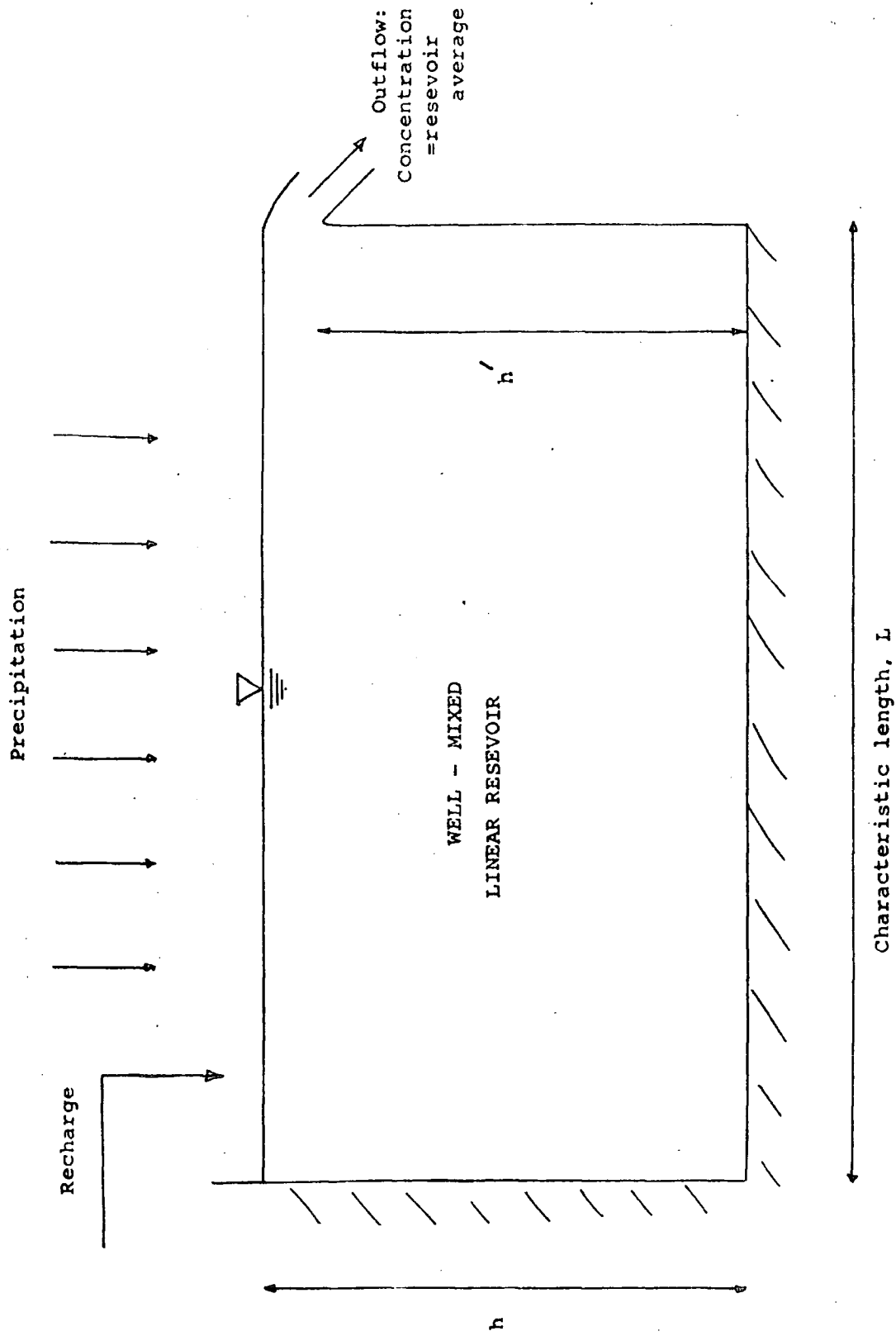
Fig. 6.1   Conceptual diagram of lumped-parameter model
used in APPLE

parameter cell if required so that sources may have variable release rates for pollutant.

APPLE was calibrated and validated by repeating the modelling exercise presented by Gelhar and Wilson (1974). A prediction of aquifer chloride levels arising from salt application is attempted. The concentration of chloride in road run off is taken to be 400 mg/l. An annual growth rate of 10% is modelled for the increase in salt applications over the 18 year period for which data is available. Natural recharge is assumed to be free from chloride. The model was allowed to run for 18 years at 10% growth and then a further 12 years with salt applications maintained steady. Both Gelhar and Wilson (1974) and APPLE predict chloride levels in the test aquifer approaching a steady state values of around 100 mg/l as shown in Fig. 6.2 which is the appropriate to the final steady input rate. The models also correctly predict the observed annual amplitude of water level fluctuations for the aquifer shown in Fig 6.3. In addition to 10% growth, zero growth, 1%, 2.5% and 5% growth simulations were carried out and the results are given in Fig 6.4. For no growth after year 18, line 560 of the program should read :

560 PRINT YR;:IF YR>17 THEN D(2)=0

Following the steady-state simulations, two policy options for salt application afer year 18 were investigated :

(1) reduce salting to original application rate equivalent to 400 mg/l chloride. APPLE line 560 should read :

```
560 PRINT YR;:IF YR>17 THEN C(2)=400
```

(2) stop salting altogether after year 18. APPLE line 560 should read :

```
560 PRINT YR;:IF YR>17 THEN C(2)=0
```

APPLE gives results consistent with those obtained by Gelhar and Wilson (1974) in both cases as illustrated by Fig. 6.5.

The APPLE program was developed, programmed, debugged, tested and calibrated in less than 30 man-hours. Interactive data input to the program typically takes about 60 seconds, the steady-state initial heads are calculated in 25 seconds and 400 water quality time steps require about 320 seconds of CPU time on an 8-bit microcomputer. This exercise clearly illustrates the power of lumped-parameter models on desktop computers as problem solving tools. The 30 man-hours involved in the exercise is trivial compared with most modelling exercises and the very rapid program development, debugging and testing is a feature of dedicated desktop computer operation. The program was written in BASIC, which being an interpreted rather than compiled language, tends to favour rapid program development. A typical input/output dialogue listing follows the program listing of APPLE.
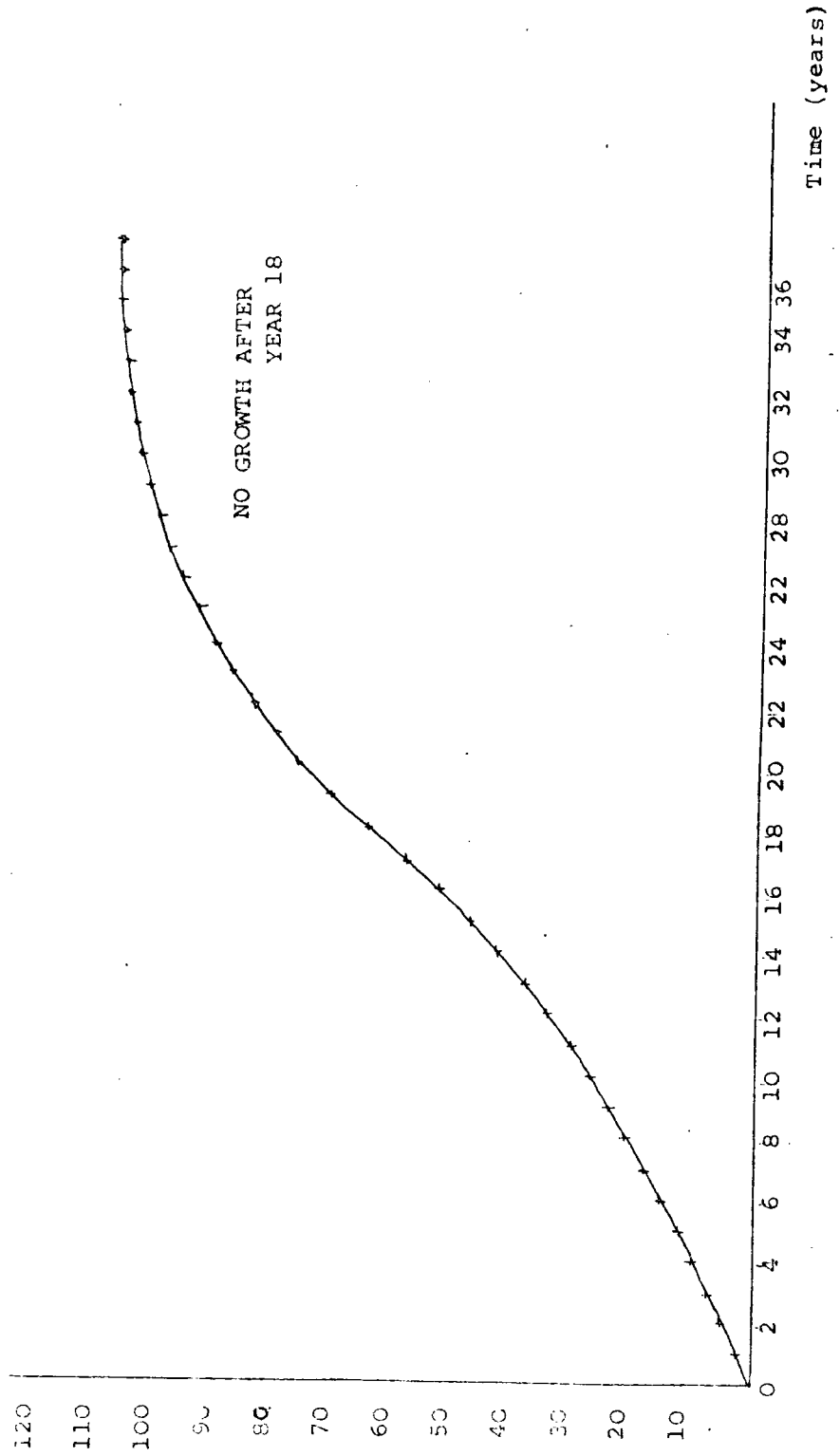
Fig. 6.2   Steady-state chloride concentration (APPLE)

NO GROWTH AFTER
YEAR 18
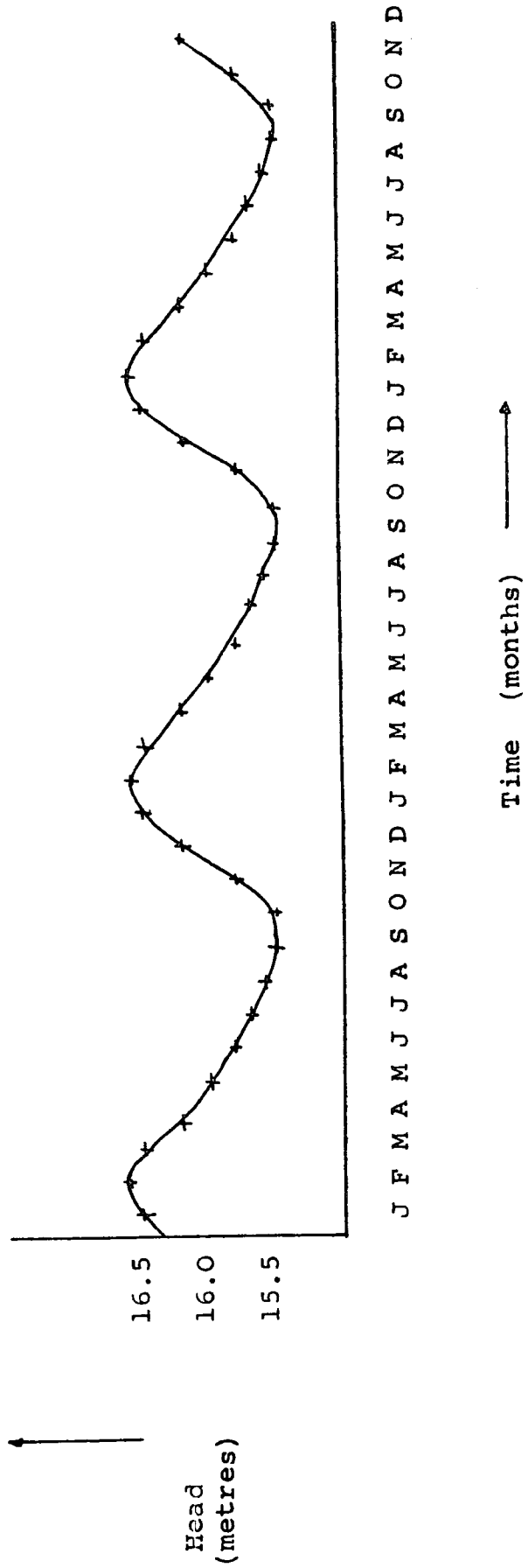
Fig. 6.3   Temporal water level fluctuations (APPLE)

99

Salt
Concentration
(mg/l)

120
110
100
90
80
70
60
50
40
30
20
10

0 2 4 6 8 10 11 12 14 16 18 20 22 24 26 28 30 32 34 36

Time (years)

10% GROWTH

5% GROWTH

2.5% GROWTH

1% GROWTH
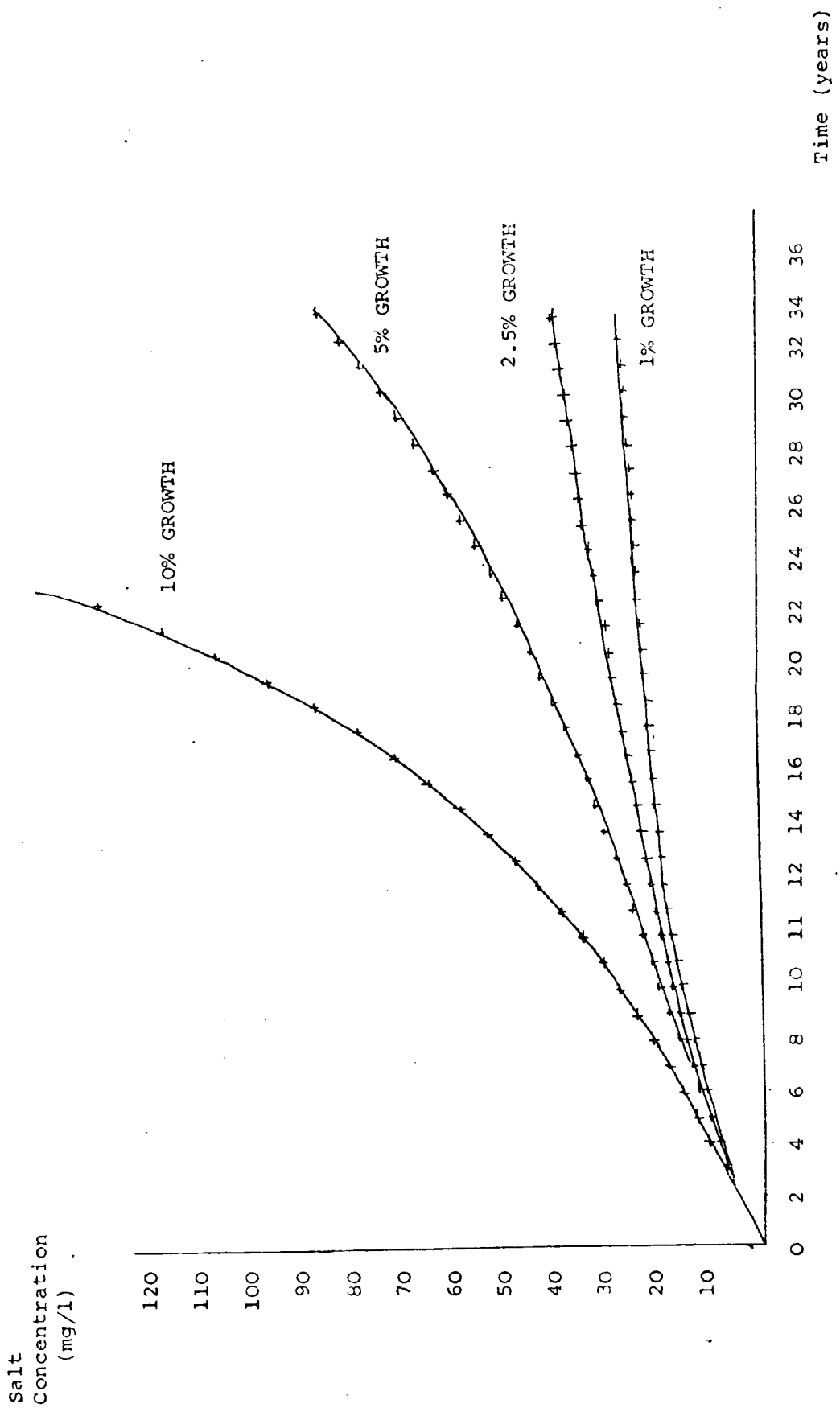
Fig. 6.4   Effect of salting policy on chloride
            concentration (APPLE)
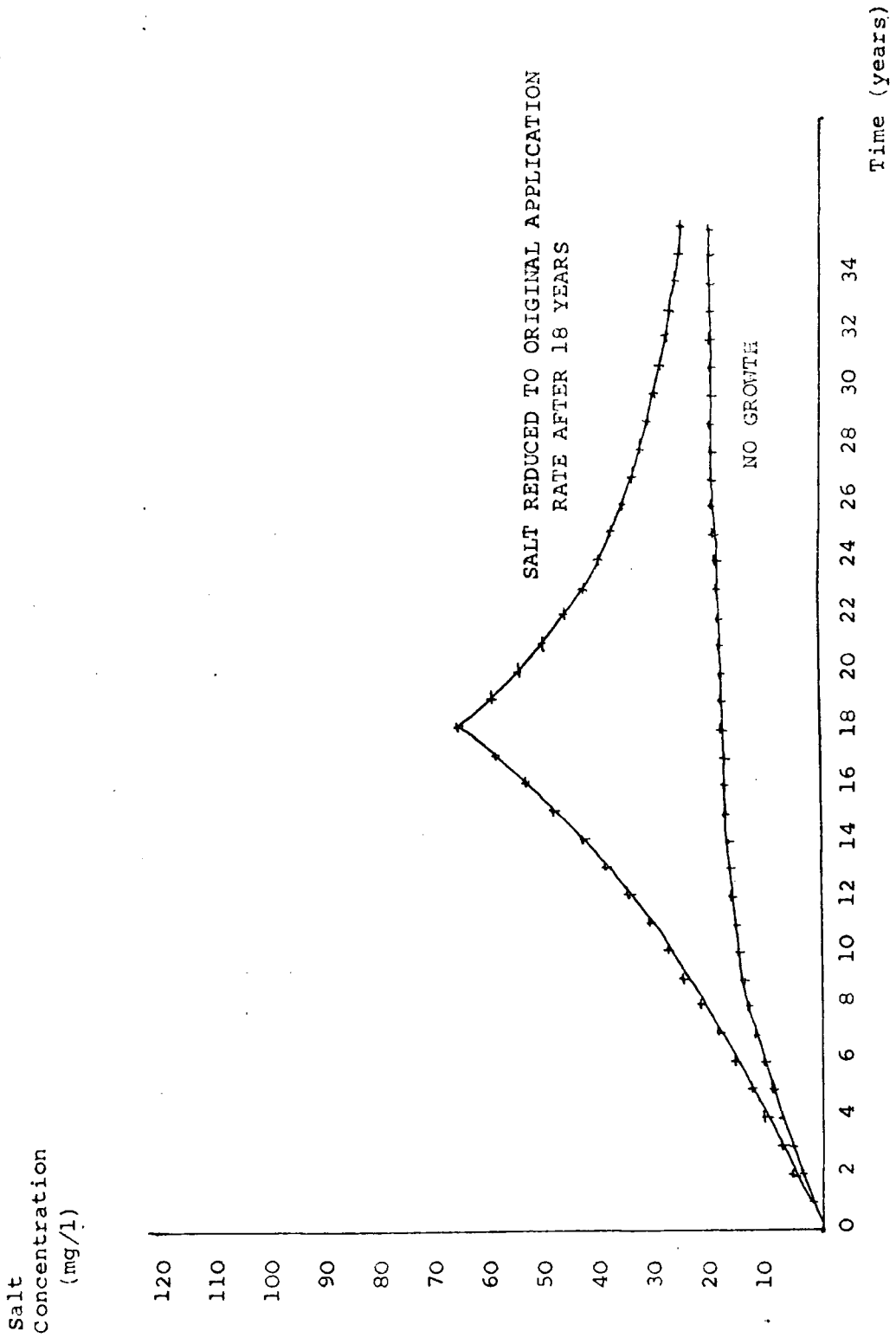
Fig. 6.5   Effect of policy options on chloride
            concentration (APPLE)

```
10 REM ***********************************************
20 REM Main program
30 REM --------------------------------------------------
40 DATA Aquifer Pollution Prediction Lumped-parameter Equation
50 DATA s Model,APPLE (C) Copyright John Bell and Malcolm Reev
60 DATA es (1980)
70 PRINT CHR$(12)
80 PRINT:FOR NI=1 TO 2:READ A$,B$:PRINT A$,B$:NEXT NI:PRINT
90 PI=4*ATN(1):T0=365/4:T1=365/2:T2=365:TR=(T2-T1)/12
100 A$="Enter number of pollution sources"
110 MN=1:MX=10:GOSUB 1100:NP=D:NN=NP+1:NP=2
120 A$="Is the data stored in DATA statements":GOSUB 1300
130 IF R=1 THEN GOSUB 1220:GOTO 220
140 FOR I=1 TO NN:GOSUB 920:NEXT I
150 PRINT:PRINT "ENTER INFILTRATION PARAMETERS"
160 A$="Enter long term average annual evapotranspiration (mm)"
170 MN=1:MX=5E3:GOSUB 1100:AE=D
180 A$="Enter long term average annual rainfall (mm)"
190 MN=AE+1:MX=5E3:GOSUB 1100:AR=D
200 PRINT:PRINT "Infiltration applied as half sinusoid"
210 PRINT:PRINT "Period":INT(100*TR)/100;"months"
220 PRINT:PRINT "ENTER TIME PARAMETERS"
230 A$="Enter start time for run (days)"
240 MN=0:MX=365:GOSUB 1100:TS=D
250 A$="Enter stop time for run (days)"
260 MN=MN+1:MX=100*365:GOSUB 1100:TF=D:TP=TF-TS:YP=INT(TP/365)
270 TP=TP-365*YP
280 PRINT:PRINT "Run is for period of";YP;"years and";TP;"days"
```

```
290 A$="Enter time step for run"

300 MN=30:MX=365*YP+TP:GOSUB 1100:DT=D:YT=INT(365/DT)

310 IF 365/DT<>YT THEN DT=365/YT:PRINT:PRINT "TIME STEP
AMENDED"

320 PRINT:PRINT "Time step will be";INT(100*DT)/100;"days"

330 FOR I=1 TO NN:IF D(I)=0 THEN 360

340 IF D(I)<0 THEN D(I)=1-EXP(LOG(1-D(I))/YT):GOTO 360

350 D(I)=EXP(LOG(D(I))/YT)

360 NEXT I:TS=TS+1E-3*DT:T=TS:PRINT:PRINT "INPUT COMPLETE"

370 PRINT:PRINT "ITERATING FOR STEADY STATE HEADS":PRINT

380 REM----------------------------------

390 REM Steady state head iteration loop

400 REM----------------------------------

410 HS=H(1)

420 GOSUB 790:FOR I=2 TO NN:GOSUB 870:GOSUB 640:H(I)=HA:NEXT I

430 I=1:GOSUB 870:GOSUB 710:H(I)=HA:T=T+DT:IT=INT(T/DT)

440 HP=INT(10*HA)/10:LR=0:QR=0:QC=0

450 LR=0:QR=0:QC=0:IF IT<>YT THEN PRINT HP;:GOTO 420

460 PRINT HP:IF ABS(HS-HA)>0.01 THEN 410

470 PRINT HA

480 PRINT:PRINT "EXECUTING TRANSIENT WATER QUALITY MODEL":PRINT

490 C0=C(1):T=TS:YR=0

500 PRINT "POLLUTANT CONCENTRATION IN AQUIFER (mg/l)":PRINT

510 PRINT "Step";:FOR NS=1 TO YT:PRINT TAB(5+4*NS);NS;:NEXT NS

520 PRINT:PRINT "Year"

530 REM----------------------------------

540 REM Transient quality iteration loop

550 REM----------------------------------

560 PRINT YR;

570 GOSUB 790:FOR I=2 TO NN:GOSUB 870:GOSUB 640:H(I)=HA:C(I)=CA
```

```
580 NEXT I:I=1:GOSUB 870:GOSUB 710:H(I)=HA:C(I)=CA:T=T+DT

590 TS=TS+DT:IT=INT(T/DT):LR=0:QR=0:QC=0

600 IF IT<>YT THEN PRINT TAB(5+4*IT);INT(CA);:GOTO 570

610 PRINT TAB(5+4*IT);INT(CA):IF TS<TF THEN YR=YR+1:GOTO 560

620 END

630 REM*****************************************************

640 REM--------------------------------

650 REM Pollution source head model

660 REM--------------------------------

670 A=3*KA*(HA+H0)/(2*LA*LA):B=2*NA+A*DT:LR=LR+LA

680 HM=(2*NA*HA+A*H0*DT+F)/B:QR=QR+A*(HM-H0)*DT*LA

690 HA=2*HM-HA:CA=CA*(1-DA):QC=QC+QR*CA

700 RETURN

710 REM--------------------------------

720 REM Aquifer head model

730 REM--------------------------------

740 A=3*KA*(HA+H0)/(2*LA*LA):B=2*NA+A*DT:FA=F*(LA-LR)/LA

750 HM=(2*NA*HA+A*H0*DT+FA+QR/LA-QP)/B:HA=2*HM-HA

760 CM=(2*NA*HM*CA+FA*C0+QC/LA)/(2*NA*HM+FA+QR/LA+DA*NA*HM*DT)

770 CA=2*CM-CA

780 RETURN

790 REM--------------------------------

800 REM Infiltration model

810 REM--------------------------------

820 F=0:IF T>365 THEN T=T-365

830 IF T>T1-T0-DT/2 AND T<T2-T0-DT/2 THEN RETURN

840 FY=1-(T2-T1)/365:FM=1E-3*(AR-AE)/365

850 F=DT*PI*FM*SIN(2*PI*(T+T0+DT/2)/365)/(2*FY)

860 RETURN

870 REM--------------------------------
```

104

```
880 REM Set up values from array storage

890 REM-----------------------------------

900 KA=K(I):LA=L(I):NA=N(I):CA=C(I):DA=D(I):H0=H0(I):HA=H(I)

910 RETURN

920 REM-----------------------------------

930 REM Input routine

940 REM-----------------------------------

950 IF I=1 THEN A$="AQUIFER":GOTO 970

960 A$="POLLUTION SOURCE"+STR$(I-1)

970 PRINT:PRINT "ENTER ";A$;" PARAMETERS"

980 RESTORE 990

990 DATA Permeability (m/d),1E-6,1E3

1000 DATA Characteristic length (m),1E-1,1E8

1010 DATA Minimum saturated thickness (m),1,1E3

1020 DATA Initial average head above aquifer base (m),1,1E2

1030 DATA Fractional porosity,1E-3,1

1040 DATA Pollutant concentration (mg/l),0,1E5

1050 DATA Fractional pollutant annual decay constant,-1,1

1060 FOR NI=1 TO 7:READ A$,MN,MX:GOSUB 1100:ID(NI)=D:NEXT NI

1070 K(I)=ID(1):L(I)=ID(2):H0(I)=ID(3):H(I)=ID(4):N(I)=ID(5)

1080 C(I)=ID(6):D(I)=ID(7)

1090 RETURN

1100 REM-----------------------------------

1110 REM Data item read routine

1120 REM-----------------------------------

1130 GOTO 1150

1140 PRINT B$

1150 PRINT:PRINT A$;:INPUT D$:D=VAL(D$):B$="ERROR : "

1160 IF D$<>"0" AND D=0 THEN B$=B$+"number required":GOTO 1140

1170 IF D<MN THEN B$=B$+"DATA < PRESET MINIMUM":GOTO 1140
```

```
1180 IF D>MX THEN B$=B$+"DATA > PRESET MAXIMUM":GOTO 1140

1190 RETURN

1200 REM-------------------------------

1210 REM Fast data read routine

1220 REM-------------------------------

1230 RESTORE 1240

1240 DATA 8.5,520,15,16,.25,0,0

1250 DATA 1,26,5,5,.3,400,-.1

1260 DATA 450,1000

1270 FOR I=1 TO NN:FOR J=1 TO 7:READ ID(J):NEXT J:GOSUB 1070

1280 NEXT I:READ AE,AR

1290 RETURN

1300 REM-------------------------------

1310 REM Yes/no routine

1320 REM-------------------------------

1330 PRINT:PRINT A$;:INPUT R$:R$=LEFT$(R$,1)

1340 IF R$="y" OR R$="Y" THEN R=1:RETURN

1350 IF R$="n" OR R$="N" THEN R=2:RETURN

1360 GOTO 1330
```

Aquifer Pollution Prediction Lumped-parameter Equations Model
APPLE (C) Copyright John Bell and Malcolm Reeves (1980)

Enter number of pollution sources? 1

Is the data stored in DATA statements? N

ENTER AQUIFER PARAMETERS

Permeability (m/d)? 8.5

Characteristic length (m)? 520

Minimum saturated thickness (m)? 15

Initial average head above aquifer base (m)? 16

Fractional porosity? .25

Pollutant concentration (mg/l)? 0

Fractional pollutant annual decay constant? 0

ENTER POLLUTION SOURCE 1 PARAMETERS

Permeability (m/d)? 1

Characteristic length (m)? 26

Minimum saturated thickness (m)? 5

Initial average head above aquifer base (m)? 5

Fractional porosity? .3

Pollutant concentration (mg/l)? 400

Fractional pollutant annual decay constant? -.025

ENTER INFILTRATION PARAMETERS

Enter long term average annual evapotranspiration (mm)? 450

Enter long term average annual rainfall (mm)? 1000

Infiltration applied as half sinusoid

Period 15.2 months

ENTER TIME PARAMETERS

Enter start time for run (days)? 0

Enter stop time for run (days)? 13200

Run is for period of 36 years and 60 days

Enter time step for run? 30

TIME STEP AMENDED

Time step will be 30.41 days

INPUT COMPLETE

ITERATING FOR STEADY STATE HEADS

```
16.3   16.4   16.3   16.1   15.9   15.8   15.6   15.5   15.4   15.5
15.8   16.1
16.5   16.6   16.5   16.2   16    15.8   15.7   15.6   15.5   15.5   15.8
16.2
16.5   16.6   16.5   16.2   16    15.8   15.7   15.6   15.5   15.5   15.8
16.2
```

EXECUTING TRANSIENT WATER QUALITY MODEL

POLLUTANT CONCENTRATION IN AQUIFER (mg/l)

Step Year	1	2	3	4	5	6	7	8	9	10	11	12
0	0	1	1	1	1	1	1	1	1	1	2	2
1	3	3	3	4	4	4	4	4	4	4	4	4
2	5	5	6	6	6	6	6	6	6	6	6	6
3	7	7	8	8	8	8	8	8	8	8	8	8
4	9	9	9	10	10	10	10	10	10	10	10	10
5	10	11	11	11	11	11	11	11	11	11	11	12
6	12	12	13	13	13	13	13	13	13	13	13	13
7	13	14	14	14	14	14	14	14	14	14	14	14
8	15	15	15	15	15	15	15	15	15	15	15	16
9	16	16	16	17	17	17	17	17	17	17	17	17
10	17	17	18	18	18	18	18	18	18	18	18	18
11	18	18	19	19	19	19	19	19	19	19	19	19
12	19	19	20	20	20	20	20	20	20	20	20	20
13	20	20	21	21	21	21	21	21	21	21	21	21
14	21	21	22	22	22	22	22	22	22	22	22	22
15	22	22	22	23	23	23	23	23	23	22	22	23
16	23	23	23	23	23	23	23	23	23	23	23	23
17	24	24	24	24	24	24	24	24	24	24	24	24
18	25	25	25	25	25	25	25	25	25	25	25	25
19	25	26	26	26	26	26	26	26	26	26	26	26
20	26	26	27	27	27	27	27	27	27	27	27	27
21	27	27	28	28	28	28	28	28	28	28	28	28
22	28	28	28	29	29	29	29	29	29	28	28	28
23	29	29	29	29	29	29	29	29	29	29	29	29
24	29	30	30	30	30	30	30	30	30	30	30	30
25	30	31	31	31	31	31	31	31	31	31	31	31
26	31	31	32	32	32	32	32	32	32	32	32	32
27	32	32	33	33	33	33	33	33	33	33	33	33
28	33	33	34	34	34	34	34	34	34	34	33	34
29	34	34	34	35	35	35	35	35	35	34	34	34
30	35	35	35	36	36	36	36	36	36	35	35	35
31	36	36	36	36	36	36	36	36	36	36	36	36
32	37	37	37	37	37	37	37	37	37	37	37	37
33	38	38	38	38	38	38	38	38	38	38	38	38
34	39	39	39	39	39	39	39	39	39	39	39	39
35	40	40	40	40	40	40	40	40	40	40	40	40
36	41	41	41	41	41	41	41	41	41	41	41	41

READY

CHAPTER SEVEN

STOCHASTIC MODELS OF GROUNDWATER SYSTEMS

7.1 STOCHASTIC TREATMENT OF GROUNDWATER PARAMETERS

All the modelling techniques described in previous chapters are deterministic in character. That is, if the aquifer characteristics, boundary conditions, sources and sinks are fixed then the model will always generate identical results. A run of the model is exactly reproduceable.

A major source of limitation for deterministic models has been the uncertainties present in the data used in their construction. In many cases it has been argued that the modelling techniques may be 'too good for the data'.

Stochastic approaches to modelling seek to use the information available on data reliability by incorporating appropriate random variations in the data parameters. The traditional approaches to the modelling of groundwater systems have always been deterministic but Freeze (1975) has pointed out the value of the stochastic approach. Stochastic groundwater models generate a range of results for repeated runs of identical problems, the variation in output arising from the uncertainties in the data. Freeze (1975) regards deterministic models as special cases of stochastic models when

all data parameters are perfectly known and have zero variance. He also points out the dangers inherent in the deterministic assumption.

DeRidder (1974) has indicated the stochastic nature of source and sink {q} terms in groundwater models. The fact that data for {T}, {S} and {D} takes the form of sample, local observations taken to be representative of large or very large regions supports the contention that these parameters too are best regarded as random stochastic variables. Bearing in mind the large uncertainties in data parameters for groundwater flow and quality models refered to in the discussion of data reliabilty, the stochastic approach has obvious attractions.

Freeze (1975) studied the sensitivity of a system involving a homogeneous non-uniform porous medium where parameter values were selected by a Monte-Carlo technique from the same probability distribution at all spatial locations. Simple saturated 1-D flow was investigated. It was concluded that the variance of the stochastic parameters had a significant influence on system response. The system did not behave in the same way as the equivalent deterministic model employing uniform homogeneous mean parameter values. Smith and Freeze (1979) use a Monte Carlo parameter assignment technique coupled with some spatial smoothing to investigate the sensitivity of 2-D steady state flow models to non-uniform assumptions. It is concluded that the equivalent uniform model does not have the mean non-uniform parameter value.

A similar Monte-Carlo parameter selection technique has been employed by Heller (1972), Mercado (1976) and Schwartz (1977) in groundwater quality models. In this work, it is shown that a marked change in the dispersion characteristics occurs between uniform and non-uniform homogeneous porous media. This work confirms the empirical and intuitive conclusions of Theis (1967) and Mercado (1967). A more detailed analysis of the problem is presented by Matheron and DeMarsily (1980) and Gelhar et al (1979) where it is concluded that 'the longitudinal dispersivity approaches a constant value which is dependent on statistical properties of the medium'. Smith and Schwartz (1980) and (1981) maintain that large-scale dispersion should not be modelled as a diffusion phenomenon. Macroscopic dispersion is cast as a process related to spatial heterogeneity in {T} and consequent velocity perturbations.

These important findings must cast doubt on sensitivity analyses which assume aquifers to be uniform media. The variance of parameters may have great significance in the prediction and analysis of macroscopic behaviour.

7.2 LIMITATIONS OF STOCHASTIC MODELS

The stochastic approach is not however without limitations. The same criteria of usefulness must be applied as those employed for deterministic models. Accuracy, speed, flexibility and most of all cost has to be considered. It is undeniable that the equivalent deterministic model is faster

and cheaper to run than its stochastic counterpart. The modeller must decide if the extra information provided by the stochastic approach justifies the increased expenditude of resources in predictive models. In sensitivity analyses, the decision is more likely to be as to whether the modeller can afford to ignore non-uniformity. Dettinger and Wilson (1981) in a study of prediction uncertainty in 2-D transient groundwater flow models conclude that 'the prediction uncertainty is a function of the magnitude of the parameter uncertainty and sensitivity of the predictions to the parameters'.

7.3 REGRESSION MODELS OF GROUNDWATER SYSTEMS

The introduction of the concept of random variables for data parameters is a relatively recent innovation in groundwater modelling though it has been commonplace in other fields. This concept, however, does not change the basic view of the modelling process as one of solving the physical equations of flow and dispersion (2.1) and (2.2). The mechanism for these processes is assumed to be adequately represented by these equations. Such models, where the governing equation for the process is known, may be called 'mechanistic' models.

There are many processes, particularly when interactions occur between different systems, where the governing equations are not known. In these cases, where the system response to known inputs has been observed but the precise nature of the internal operation of the system cannot be represented by a set of governing equations, a model is

required to predict future outputs. This is a very common problem and regression models are used to find the best estimate of the function necessary to transform inputs to outputs. In this case the system output is regarded as a random variable dependent on the precedent inputs.

Regression models are very commonly applied to the analysis of surace water flow and quality though applications in the field of groundwater modelling are lees common. However they represent an alternative approach to modelling to be evaluated alongside 'mechanistic' models.

Phillips (1978) describes a multiple regression technique for forecasting groundwater levels from rainfall and infiltration estimates. The predictor equations take the form :

$$L' = \text{Sum } \{a.I\} + \text{Sum } \{b.L\} + c.R \qquad (7.1)$$

where L'   is the groundwater level one time step on,

  I   represents infiltration for n preceding time steps,

  L   represents water levels for m preceding time steps,

  R   represents rainfall for current time step,

  a,b,c are empirical coefficients,

  and m,n   are integers.

This is a typical general regression model including both regressive and autoregressive elements.

A general approach to simulating river water quality from groundwater and surface run off sources using regression

models is presented by Page and Warn (1974). A more sophisticated river water quality model is proposed by Birtles (1977). River flow is broken down into effluent flows, direct run-off and aquifer baseflows. The total river load for any quality parameter is assumed to be given by :

$$Mp = Sum \{Qe.Cep\} + Sum \{Qb.Cbp\} + Qr.Crp \qquad (7.2)$$

where Mp   is the total load of quality parameter p,

     Qe   is one of n effluent flows,

  and Cep is the corresponding concentration of p,

     Qb   is one of m groundwater baseflow discharges,

  and Cbp is the corresponding concentration of p,

     Qr   is the run-off flow,

  and Crp is the corresponding concentration of p,

  and m,n are integers.

Equations similar to (7.2) can be formulated for each quality parameter in turn. Water quality and river flow records mean that a large number of simultaneous estimates of M values are available and these can be used to obtain least squares estimates of Q and C. The model can then be used as a predictor for water quality changes resulting from changes in Q.

7.4 LIMITATIONS OF REGRESSION MODELS

Regression models have two outstanding advantages :

(1) conceptual and computational simplicity, and

(2) cheapness and speed in prediction.

Regression models are very easy to program and after calibration, prediction is simply a matter of evaluating an explicit formula.

The chief limitations of regression methods are also well-known :

(1) large amounts of data are required for calibration to identify empirical coefficients,

(2) there is no guarantee that empirical coefficients are not specific to the dataset from which they were deduced,

(3) predictions can only be made for datasets very similar to the calibration dataset.

If possible checks should be made by splitting calibration datasets to ensure that coefficients do not vary wildly. Models should also be validated on datasets totally independent of those used in calibration. All the sources of variation in the inputs used in predictive runs must have been present in the calibration runs.

7.5 EMPIRICAL MODELS FOR DECISION MAKING

Regression models, in essence, summarise past

experience and use that experience to make predictions. In order to formulate a regression model, however, it is necessary to have a large amount of complete quantitative data from which empirical coefficients can be deduced.

There are many situations in a groundwater context where decisions must be made on the basis of experience when that experience is both incomplete and qualitative. For example, in the selection of abstraction well sites, waste disposal sites and in the estimation of the effects of mining or agricultural operations on groundwater quality and flow. A method of rationalising such experience in the form of a model enables the non-expert to review a complex situation, be prompted as to the salient parameters, and come to a preliminary decision.

A decison-assisting model may be constructed by the following steps :

(1) assembling all the case history data, subjective opinions and rules of thumb,

(2) identifying all the different potential outcomes of the decision process,

(3) structuring the data into a set of observational factors which mitigate for or against each particular outcome,

(4) quantifying the relative influence of observational factors for each outcome as weighting or predisposing factors,

(5) ordering the outcomes for particular case histories and reviewing quantitative weightings to calibrate the model.

This procedure was used in the formulation of the model MINES which forecasts the likelihood of acid mine drainage resulting from a particular mining operation and the probable chemical character of the effluent. The procedure adopted can be seen, with hindsight, to have considerable similarities with the construction of a group of models combining digraph theory with stochastic processes and called transition digraph models. These models are described by Roberts (1976) in an environmental context.

7.6 RANDOM-WALK SIMULATION OF DISPERSION

Dispersion in porous media arises from two principle sources :

(1) molecular diffusion : due to random molecular motions within the fluid phase, and

(2) hydrodynamic dispersion : due to random fluctuations of flow velocity through the porous medium on a microscopic and mesoscopic scale.

Thus the manifestation of dispersion on a macroscopic scale arises, argueably from small-scale random motions. The analogy between solutions to the diffusion equation and random Brownian

motion is widely exploited in physics and is discussed exhaustively by Port and Stone (1978) in relation to potential theory. The simulation of diffusion by a random-walk process is also used in biology as described by Okubo (1980).

Consider the diffusion process in 1-D. In any given small time period (t') a 'particle' will move a short distance (x') to the left or right. If the medium is isotropic, the probabilities of left or right movement will be 0.5. After the time increment t' the population made up of all the 'particles' will have moved, half to the left and half to the right. In the next time increment, each individual particle again moves either left or right independently of its previous motion. Thus on average, 25% of the population will find itself a distance of 2.x' from the origin as the population spreads further. After a large number of time steps, n.t', the distribution of 'particles' is not uniform since as n becomes large the probability of a particle finding itself a distance n.x' from the origin is very small (0.5 to the power n in fact). After a large number of random left or right motions a typical particle will be a distance m.x' from the origin. To get there it will have moved (a) steps left and (b) steps right such that :

$$n = a + b \qquad \text{and} \qquad m = a - b \qquad (7.3)$$

or alternatively :

$$a = (n + m)/2 \qquad \text{and} \qquad b = (n - m)/2 \qquad (7.4)$$

The number of possible paths to this typical position can be

shown by combinational theory to be :

$$n!/(a!.b!) = n!/(\{(n + m)/2\}!.\{(n - m)/2\}!) \qquad (7.5)$$

The total number of possible paths for a 'particle' is 2 to the power n, hence the probability of a particle being at a distance m.x' from the origin after n time steps of length t' is given by :

$$P(m,n) = (0.5)^n.n!/(\{(n + m)/2\}!.\{(n - m)/2\}!) \qquad (7.6)$$

This is the well-known binomial distribution which for large n is known to closely approximate the Gaussian or normal distribution :

$$\lim \{P(m,n)\} = \{2/(\pi.n)\}^{0.5} . \exp\{-m^2/(2.n)\} \qquad (7.7)$$

Replacing the discrete variables by continuous variables, m.x' becomes x and n.t' becomes t and defining :

$$D = \lim \{x'^2/(2.t')\} \qquad , \text{ for small } x' \text{ and } t' \qquad (7.8)$$

where D is the diffusion or dispersion coefficient.

Equation (7.7) can now be written for the continuous variables :

$$P(x,t) = \{1/(4.\pi.D.t)\}^{0.5} . \exp \{-x^2/(4.D.t)\} \qquad (7.9)$$

The solution of the diffusion equation for a point source in an

infinite, homogeneous, isotropic medium with an intitial source
concentration of Co at x = 0 is :

$$C(x,t)/Co = \{1/(4.n.D.t)\}^{0.5} . \exp \{-x^2/(4.D.t)\} \qquad (7.10)$$

The analogy between the diffusion-dispersion process and the
random-walk Markov model is thus apparent in the similarity of
equations 7.9 and 7.10.

Random-walk simulations have one very major
computational advantage over other modelling techniques. The
spatial and temporal distribution of the dependent concentraton
variable can be generated by sequential logical operations. No
arithmetic is necessary. This technique has been applied to a
series of groundwater pollution problems and results are
reported in detail in the description of the DIFAN model. No
reference to previous applications in the field of groundwater
modelling has been found in the literature.

The use of random-walk simulations promises to
overcome the difficulties inherent in deterministic numerical
models associated with the non-uniform character of aquifer
parameters reported by Smith and Freeze (1979) and Smith and
Schwartz (1980) amongst others.

PART TWO

NEW MODEL DEVELOPMENTS

COMPARATIVE EVALUATION OF MODELLING METHODS

8.1 CLASSIFICATION OF MODELLING PROBLEMS

There are essentially four classes of problems to which groundwater modelling techniques can be applied :

(1) Preliminary evaluation studies (PE) : where some kind of assessment must be made as to whether a real problem worthy of more detailed investigation exists. Such evaluations must be made on a large number of occasions and rapid decisions are often required. The techniques employed must therefore be simple and fast.

(2) Parameter identification studies (PI) : where estimates of aquifer or fluid characteristics are to be deduced from field or laboratory observations. Again large numbers of these studies are required so methods cannot be overelaborate; however, techniques should point out the degree of ambiguity or potential error in the resulting parameter estimates.

(3) Response prediction studies (RP) : where the outcome of a proposed course of action on a particular system is to be predicted. Such models can become routine management tools and be in regular use. Sophisticated techniques may be required in

some cases when computational efficiency will be an important consideration.

(4) Sensitivity analysis studies (SA) : where the dependency of system response on specific parameters or groups of parameters is investigated. Such studies may vary considerably in their scope but in their most complex form represent the area of application for very sophisticated techniques.

For each of the four classes of problem, the application may be :

(a) Simple (S) : a linear problem with simple boundaries and parameters constant or showing a simple pattern of variation involving the behaviour of only one isolated, independent system, or

(b) Complex (C) : a general, possibly non-linear, problem with arbitary boundaries and parameter inhomogeneity and anisotropy perhaps involving several interactive systems.

(c) Global (G) : concerned with large scale response of regional variables such as total outflows and average pollution levels, or

(d) Local (L) : concerned with individual sites and wells within the modelled region.

These two pairs of qualifying terms expand the four basic problem classes to 16 problem types :

Problem Class	Problem Type			
	Simple		Complex	
	Global	Local	Global	Local
Preliminary Evaluation	PEGS	PELS	PEGC	PELC
Parameter Identification	PIGS	PILS	PIGC	PILC
Response Prediction	RPGS	RPLS	RPGC	RPLC
Sensitivity Analysis	SAGS	SALS	SAGC	SALC

This somewhat arbitary classification of problems will be of use when reviewing and comparing the application of the various modelling methods.

8.2 REVIEW OF APPLICATIONS OF MODELLING METHODS

In order to compare and evaluate the relative usefulness of the various types of groundwater model, the main applications of each type will be summarised to provide the basis for discussion.

Analytical models are useful for preliminary problem evaluation, particularly when point sources and sinks are involved. Most parameter identification problems, particularly for idealised laboratory experiments and field tests where simple boundary conditions can be assumed as a first approximation, are best tackled by fitting analytical models. Very simple regional response prediction problems can be solved with analytical models but as the complexity increases the

computational effort involved rapidly approaches that of distributed-parameter numerical models which are much more flexible. Perhaps the most important use of analytical models is to act as an independent check on the accuracy of other modelling procedures.

Physical analogue models are inflexible and suffer from problems of scaling material properties. Their major area of application is in the demonstration of fluid flow and transport phenomena for teaching purposes. In one respect, physical analogues still provide a valuable research technique. Fluid flow and particle interaction problems, such as the particle traction 'piping' problems and surface subsidence problems arising from particle migration and solution of the porous medium skeleton, remain difficult to model by other methods and physical analogues provide the most feasible modelling technique.

Simple electrical analogues using 'Teledeltos' paper are fast to prepare and allow very flexible boundary geometries. They remain useful in the preliminary evaluation of both regional and local steady state flow problems. Resistance-capacitance networks for transient flow problems have been entirely superseded by distributed-parameter numerical models which are superior in terms of flexibility, preparation time and cost. Both physical and electrical analogue models require considerable space and laboratory back-up facilities.

Complex parameter identification problems are very much the province of distributed-parameter deterministic

numerical models. System sensitivity analysis problems are also best served by distributed-parameter numerical models but for these applications parameters should be treated as stochastic variables. Distributed-parameter models for response prediction are valuable but recent work on data reliability suggests that very good field data is necessary for calibration if the considerable resource expenditure involved in distributed-parameter calibration and prediction is to be justified. Although 3-D models are technically feasible, data limitations are likely to inhibit their practical application. Of the major formulation schemes for distributed-parameter models, FDM is most widely applied to practical problems even though FEM programs have been available for a considerable time. Distributed-parameter numerical models seem to be grossly over-used in circumstances where other simpler models could have been applied equally effectively and much more rapidly and cheaply.

The use of lumped-parameter models in groundwater studies is a neglected area, possibly due to the unthinking application of distributed parameter FDM and FEM packages. They provide an excellent means for tackling response prediction and sensitivity analyses of 'global' variables (representative of whole catchments or regions). Lumped-parameter elements are well suited to evaluating complex system interaction problems. By using sensitivity analysis, lumped-parameter models can make the fullest possible use of limited data whilst requiring only modest computational resources.

Regression models are very valuable for 'patching'

gaps in data records and making response predictions involving very limited extrapolation. They rely heavily on extensive and uninterupted data sequences for their calibration and are often misused by application outside the range of their calibration data. There is also a tendency to validate such models by their ability to regenerate the calibration data and not an independent dataset. For short term prediction and extrapolation, regression and autoregression models have proved very simple cheap and efficient methods.

The necessity to treat aquifer parameters as stochastic variables is a problem receiving a great deal of research attention in the early 1980's and system sensitivity to assumptions of non-uniformity are particularly important in convection-dispersion problems. Stochastic distributed-parameter models are now a major tool in sensitivity analysis problems.

8.3 MICROCOMPUTERS AND GROUNDWATER MODELLING

The raid upsurge in the availability of cheap desktop microcomputer systems is likely to have a profound effect on computer usage for modelling purposes. Reeves and Lucas (1980) and Mido (1981) have pointed out some of the numerous applications that cheap microprocessor technology has made feasible in the geological sciences.

The present generation of desktop microcomputers are limited in their arithmetic power. Many use very slow software

arithmetic and almost all use 8-bit words and high precision arithmetic requires special software. Microcomputers, therefore, though capable of running large distributed-parameter FDM and FEM models, are not well suited to the task and many hours of CPU time are required. This situation is likely to change quite rapidly with the development of 16-bit micros with hardware arithmetic units.

Microcomputer development has presented a large number of non-expert computer users with a cheap powerful calculating device but applications software is scarce. In the groundwater context such non-experts will include managers, engineers and scientists concerned with making day to day decisions of a practical nature. The kind of computer model required in these circumstances must obviously be written for interactive terminal use and also be :

(1) conceptually simple, or if complex the sophistication must be transparent to the user,

(2) very well protected against mistaken or nonsensical data input by error and range checking routines,

(3) able to produce concise and easily assimulated output preferably in the form of a graphic display or a selected decision option.

The review of modelling together with the availability of desktop microcomputers highlights three potential areas where new groundwater modelling techniques

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could be introduced or neglected methods further developed :

(1) Lumped-parameter catchment and regional management and planning models,

(2) Decision-assisting models to provide a systematic basis for technical and resource management decision-making,

(3) A new distributed-parameter technique free from the requirement for extensive 'number crunching' for technical problem evaluation.

8.4 LUMPED-PARAMETER MANAGEMENT AND PLANNING MODELS

An obvious area for the development of lumped-parameter models is in the area of resource management and planning, where some objective means of comparative evaluation of the long-term consequences of alternative management stategies on the groundwater system and interdependent systems such as agriculture is needed.

The program NIPREM has been developed, from an original model developed by Reeves (1977). It comprises a procedure for the prediction of groundwater and surface water nitrate levels resulting from changes in land use and agricultural practice.

Some significant developments of the structure of the model have been made but the major development has concentrated

on developing NIPREM as an interactive input prompting package for a small microcomputer. The package is entirely self-explanatory and self-contained and offers extensive 'default' options to the user. Users require little or no computing experience and all but the most gross and very subtle input errors are detected and referred to the user for amendment. NIPREM actually requires a very large database of parameters extracted from very diverse literature sources. All these can be amended by the knowledgable user but sensible assumptions are made automatically for the non-expert. Even if the results generated by NIPREM are inaccurate, the process of running through the package makes the user aware of the soil-water-nitrogen system and the complex interactions involved.

Other problems which may benefit from similar treatment include :

(1) pollution by herbicides and insecticides.

(2) pollution by leaching of mining wastes.

(3) pollution due to salt used for road deicing.

This latter problem is relatively simple and was tackled as an example of lumped parameter modelling in 6.5 using the program APPLE.

A considerable number of day to day decisions have to be made on the basis of experience or rather subjective qualitative evidence. Such decisions can be aided by structuring the information in a systematic way and providing a framework on which to base data collection and evaluation.

Probability-based models have been developed to deal with decision-making problems where a large body of data exists in a qualitative or semi-quantitative form. A model formulation procedure has been suggested and the model MINES developed to forecast the likelyhood of acid mine drainage problem occuring in a specific situation. Such logical decision-assisting procedures have not previously been applied in a groundwater modelling context. The model developed can be regarded as a kind of digraph or transition digraph model similar to those described by Roberts (1976) although it was developed informally rather than from the formal background of mathematical statistics.

Other groundwater problems which could be treated in this manner include :

(1) siting abstraction wells for dewatering or water supply purposes.

(2) preliminary selection and comparative evaluation of potential waste disposal sites.

(3) forecasting agricultural pollution from slurry disposal and similar localised sources.

8.6 STOCHASTIC RANDOM-WALK DISTRIBUTED-PARAMETER MODELS

Distributed-parameter numerical models require large amounts of arithmetic calculation and are thus not suitable for interactive implimentation on the present generation of 8-bit desktop microcomputers. A technique suitable for microcomputer simulations would therefore be of value.

Random-walk simulation as a means of modelling dispersion has been investigated using the program DIFAN which combines reasonable accuracy with very rapid and therefore cheap computation. The technique has proved valuable for rapid evaluation of regional and local problems and has a flexibility comparable with many distributed-parameter numerical methods. Random-walk simulations have not previously been reported in a groundwater pollution context.

DIFAN is in fact fast enough to support an animated video display to show the time development of pollution plumes and the transient paths of pulse pollution sources.

The random-walk simulation technique has other potential applications in groundwater modelling :

(1) Regional response prediction models.

(2) simulation of fracture permeability.

(3) simulation of absorption, solution, and precipitation reactions within porous media.

The method is in fact more promising for modelling microscopic and mesoscopic effects but certainly provides a reasonable simulation of macroscopic dispersion for preliminary problem evaluations.

8.7 COMPARATIVE EVALUATION OF MODELLING METHODS

The methods, including the newly developed random-walk and decision-assisting stochastic models, can now be classified in terms of their usefulness for a particular application:

Problem Type	Anal	Phys Anal	Elec Anal	DP Num	LP Num	Stoc Num	RW Stoc	DA Stoc	Corr Stoc
PEGS	R	N	?	N	R	N	R	R	?
PELS	R	N	?	N	N	N	R	N	?
PEGC	N	N	N	N	R	N	N	R	?
PELC	N	R	N	R	N	N	N	N	?
PIGS	R	N	?	?	R	N	N	R	?
PILS	R	N	?	R	N	R	?	N	?
PIGC	N	N	N	N	R	N	N	R	?
PILC	N	N	N	R	N	R	N	N	?
RPGS	?	N	?	?	R	N	?	N	R
RPLS	?	N	?	R	N	R	?	N	?
RPGC	N	N	N	?	R	N	N	?	R
RPLC	N	N	N	R	N	R	N	N	?
SAGS	N	N	?	R	R	R	?	N	N
SALS	N	N	?	R	N	R	?	N	N
SAGC	N	N	N	?	R	?	N	N	N
SALC	N	N	N	R	N	R	N	N	N

Where R indicates a recommended technique worthy of serious consideration, ? indicates a possible technique which may occasionally prove useful, and N indicates a technique not recommended on grounds of applicability, efficiency or expense.

NIPREM : A LUMPED-PARAMETER NITRATE POLLUTION MODEL

9.1 INTRODUCTION TO NIPREM

NIPREM is a computer program for the prediction of soil and water nitrogen levels of concentration which can be used to simulate the behaviour of the soil-water nitrogen system.

The program has two distinctive parts : a soil-nitrogen mass balance model element and a hydrological model element. Both models require calibration and validation since the equations they use are empirical functions to fit observed data. Parameter values and a test data set are provided by the program which is interactive and self explanatory. Sources of parameter and data information in the literature are fully detailed.

NIPREM is designed as a predictive tool for planning and monitoring the influence of land use and fertilizer practice on water supplies.

9.2 HISTORICAL DEVELOPMENT OF THE NITRATE PROBLEM

In recent years, those responsible for water supply in England and Wales have become increasingly concerned by the apparent upward trend of nitrate levels in many surface water and groundwater sources of supply.

High concentrations of nitrates in water have for some time been associated with the rare disease called infantile methaemoglobinaemia. The formation of carcinogenic nitrosamines from nitrates is also a potential health hazard. The implications of nitrates in water supply for public health have recently been reviewed by Shuval and Gruener (1975) and Windle-Taylor (1974).

In groundwater from the Chalk aquifer, Foster and Crease (1974) reported levels of up to 12 mg/l nitrate as nitrogen in east Yorkshire, Sumner (1973) and Davey (1974) levels of up to 14 mg/l in north east Lincolnshire, Green and Walker (1970) levels of up to 23 mg/l around Eastbourne and Foster (1976) levels of up to 17 mg/l in the Isle of Thanet. For the Permo-Triassic sandstone aquifer, Satchell and Edworthy (1972) and Seven-Trent Water Authority (1978) have reported levels of up to 27 mg/l in Nottinghamshire and Reeves et al (1974) levels in excess of 22mg/l in north Yorkshire. In a survey of 92 Chalk wells and 161 Permo-Triassic sandstone wells for which long term records are available, the Cental Water Planning Unit (1977) reported significant rises in nitrate level in 14% of the Chalk wells and 51% of the sandstone wells.

Nitrate concentrations reported by the Water Research Centre (1974), in the river Thames have increased from an average of 4 mg/l in 1968 to 9 mg/l in the last quarter of 1973; and in the river Lee over the same period average levels have risen from 6 to 11 mg/l. In January 1974, peak levels of 21 and 14 mg/l respectively for the raw water intakes on the rivers Lee and Thames by Fish (1974) causing abstractions to be temporarily suspended. Other rivers are reported to have increasing nitrate levels. These include the Great Ouse between 1957 and 1967, the Chelmer and Blackwater from 1958 to 1968, the Yorkshire Ouse between 1963 and 1967 (Owens,1970) and the Frome from 1965 to 1972 (Casey,1975). Tomlinson (1970) showed significant upward trends for nitrate in the rivers Manifold, Dee, Tyne and Tees between 1953 and 1967 but concluded that there was little evidence of a general increase in the rivers Stour,Rother, Wensum, Severn and Thames.

Since the World Health Organisation recommend 11.3 mg/l nitrate as nitrogen as an upper limit these obsevations and trends present a serious water resource pollution problem.

9.3 NITROGEN IN THE ENVIRONMENT

The primary source of nitrogen is atmospheric dinitrogen gas. A relatively small number of organisms directly fix dinitrogen in the soil. A small amount of nitrogen is fixed by electrical storms but chemically fixed nitrogen applied as inorganic fertilizer is an increasingly important source.

The top 150 mm or so of soil contains 0.075% to 0.5% nitrogen equivalent to 1500 to 10000 kg/ha. Light cultivated soils have the lowest nitrogen content, heavy clay soils beneath permanent grass and woodland the highest.

Most soil nitrogen is held in organic matter in a relatively immobile form. This nitrogen is gradually mineralised and together with mobile inorganic nitrogen, is taken into plant tissues as they grow.

Nitrogen immobilised in plant tissue enters the food chain of animals where it is used for growth. Eventually it returns to the soil in excreta and as dead matter.

Mineralised mobile nitrogen is subject to biological and chemical denitrification and may be converted to dinitrogen and returned to the atmosphere. Nitrogen in mobile form is also subject to leaching by percolating waters and can be washed into the surface and subsurface drainage systems.

9.4 QUANTIFICATION OF SOIL NITROGEN SOURCES

Nitrogen is accumulated in soils by fixation, addition of animal excreta and application of inorganic fertilizers. Input to soils from the latter source has increased markedly over England and Wales since about 1940 as demonstrated by estimates made by the Central Water Planning Unit (1977) :

Source (thousand tonnes per annum)

| Period | Atmospheric | | Wastes | | Inorganic | Total |
	Fixation	Rainfall	Animals	Humans	Fertilizers	
1938-39	1183	263	608	173	50	2277
1940-49	1202	238	544	182	88	2254
1950-59	1290	258	668	196	183	2595
1960-69	1273	261	778	221	494	3027
1970-72	1230	242	806	228	728	3234

These figures are consistent with the estimates made by Cooke (1976) for nitrogen availability.

Rainfall on average over England and Wales contributes about 16 kg/ha each year. Such estimates can be obtained from records of rainfall quantity and chemical quality. The areal variation of quantity is documented by the Meteorological Office. Surveys of rainwater chemical quality have been carried out by Lawes et al (1882), Stevenson (1968) and Cawse (1974). All have the same broad conclusions. Rainfall in rural areas contains from 1 mg/l nitrogen in the west to 2 mg/l in more eastern areas. Urban areas receive an additional concentration of about 4 mg/l over rural areas.

Biological fixation of atmospheric dinitrogen over England and Wales averages the equivalent of 80 kg/ha. The amount fixed locally is heavily dependent on the vegetation :

Land use	N fixed (kg/ha)	Reference
Tillage	50	Allison (1965)
Clover & rotation grasses	250	Henzell & Norris (1962)
Permanent grass	75	Whitehead (1970)
Rough grazing	75	Stewart (1966)
Urban	0	Whitehead (1970)
Woodland & other rural land	75	Jenkinson (Pers. Comm.)

Waste sources of nitrogen from recycled animal excreta depend on population and have shown a progressive increase from an average of about 50 kg/ha prior to 1940 to about 70 kg/ha by the mid-seventies. These estimates are based on the work of Cooke (1976) :

Animal type	N production (kg/head)
Cattle	50
Pigs	18
Sheep	10
Humans	4.5
Poultry	0.3

Inorganic fertilizer application to soil has increased very markedly since 1940 when the average over England and Wales was about 4 kg/ha to about 50 kg/ha by the mid-seventies. Local application rates depend on farm type as defined by Church et al (1968) and crop type. Typical application rates for arable, mixed arable/dairy, dairy and livestock and upland farms are given in Fig. 9.1 for the period 1944 to 1970 after Yates and Boyd (1964), Church and Webber (1971) and Yates et al (1944).

The information sources above, together with land use and livestock population statistics, enable estimates of nitrogen sources to the soil to be made over any sub-area for which the statistics are available.

9.5 LUMPED-PARAMETER SYSTEM MODEL

A system dynamics model to predict surface and

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Fig. 9.1a   Inorganic fertilizer application rates
              for arable land 1944-66
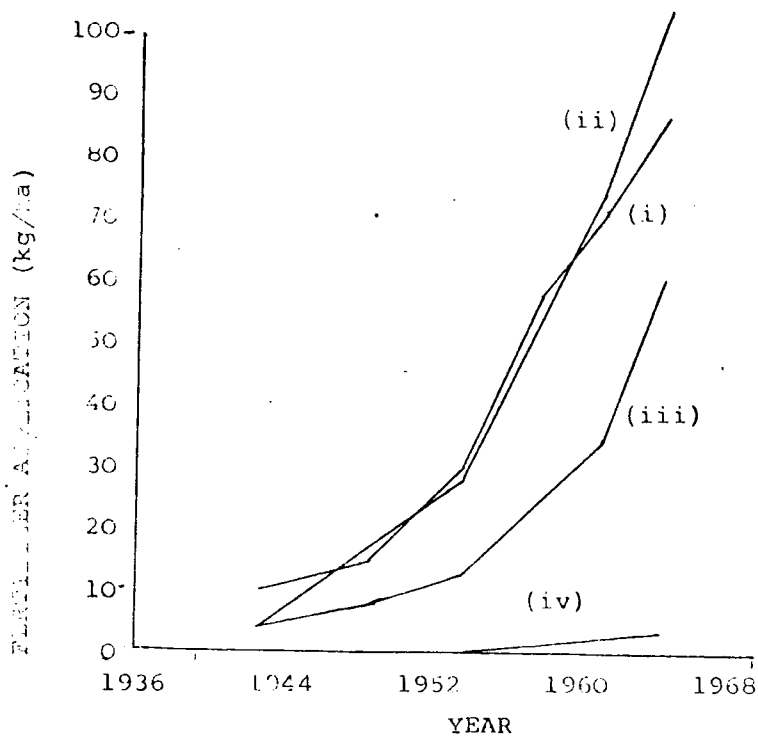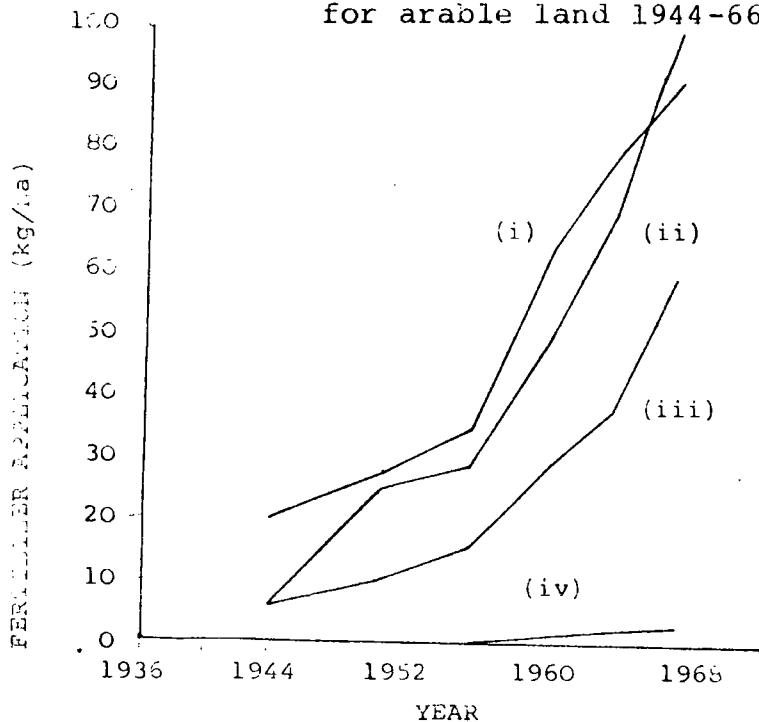
Fig. 9.1b   Inorganic fertilizer application rates
              for mixed arable/dairy farms 1944-66

(i) TILLAGE   (iii) PERMANENT GRASS

(ii) CLOVER / ROTATION GRASS   (iv) ROUGH GRAZING

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Fig. 9.1c   Inorganic fertilizer application rates
              for dairy farms 1944-66
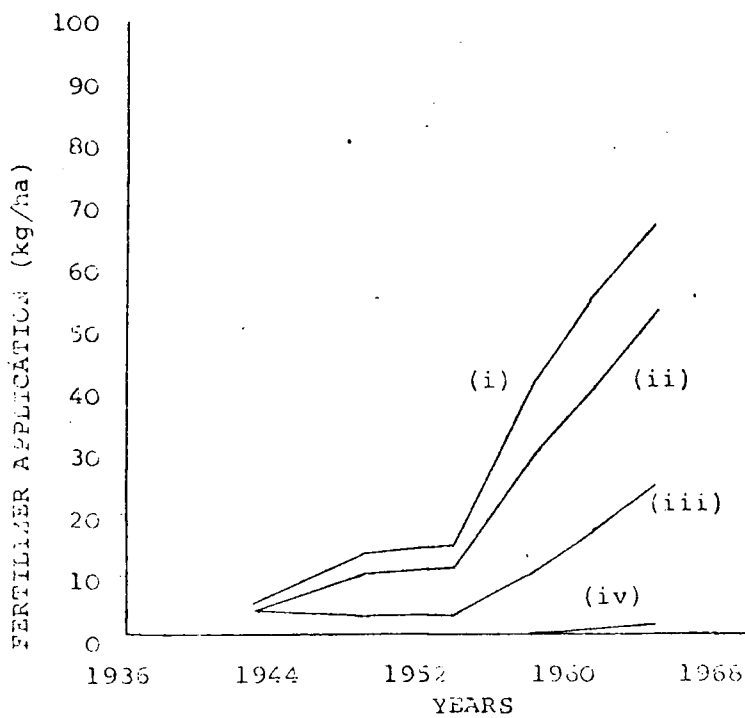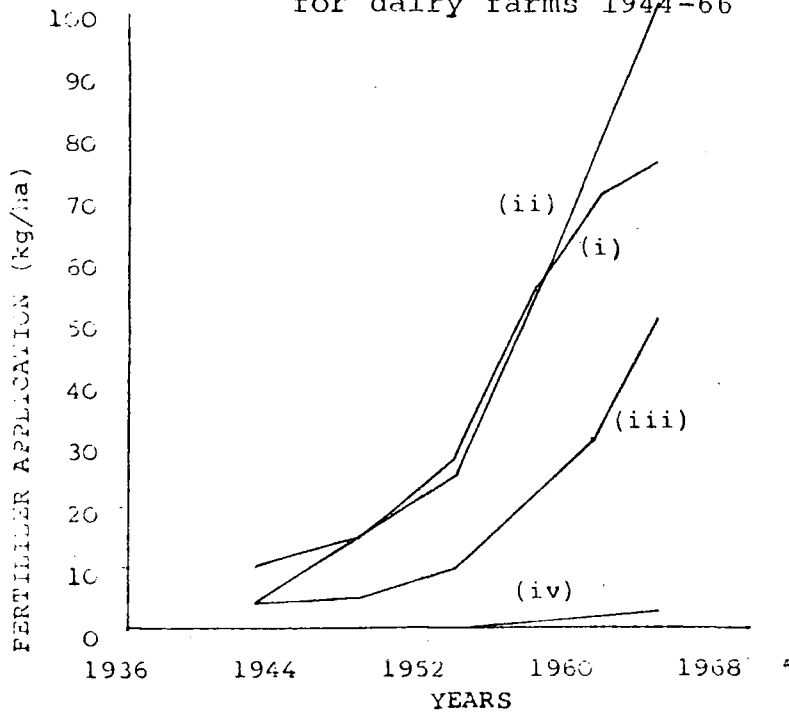
Fig. 9.1d   Inorganic fertilizer application rates
              for livestock/upland farms 1944-66

groundwater nitrogen concentrations called NIPREM has been
devised. Precursors of the present model have been described by
Reeves (1977) and the Central Water Planning Unit (1977).

The computer program, given in Appendix II, is
written in BASIC and is self explanatory. User input is
prompted but default values of all parameters and constants are
supplied together with a default dataset. The program NIPREM
was written for implimentation on a small microcomputer but
would also run on a mainframe computer with minor amendments.
No graphical output is used to ease program transfer but VDU
display routines specific to the Exidy Sorcerer microcomputer
have been written.

The system model is in two distinct parts. A soil
nitrogen balance model which computes the amount of nitrogen
leached and a hydrological model which simulates runoff,
unsaturated and saturated groundwater flow.

9.6 SOIL NITROGEN MODEL ELEMENT

A schematic representation of the processes
considered by the model is given in Fig. 9.2. The inputs are
sub-divided into mobile and immobile forms of nitrogen and
translated into outputs by a series of simple equations. In
formulating these empirical equations very simple functions were
used wherever possible.

Biologically fixed dinitrogen was assumed to enter
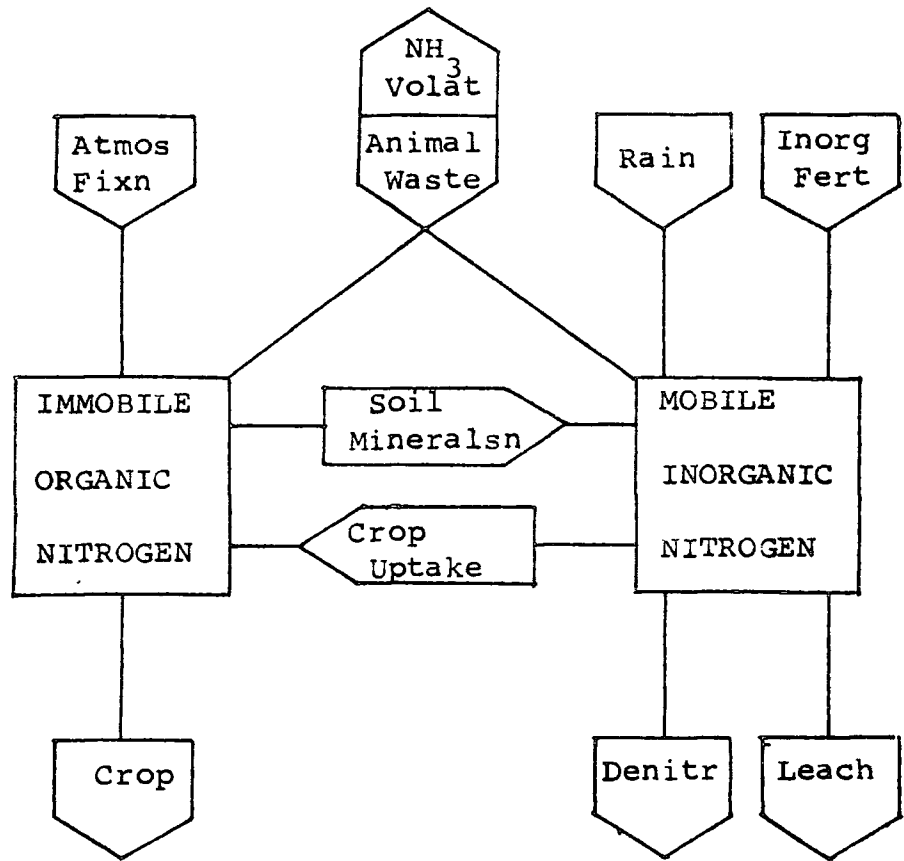
Fig. 9.2   Processes operating - soil nitrogen model

the system in immobile organic form and was incorporated into the 'pool' of nitrogen present in soil organic matter (SOM). Whitehead (1970) suggests that natural dinitrogen fixation is supressed by the addition of some nitrogenous fertilizers and stimulated by others. Quantitative data was not available and it was initially assumed that suppression and stimulation effects could be neglected. To allow for the effect, it is suggested that the estimate of fixed nitrogen be multiplied by the ratio of organic to inorganic inputs raised to some power :

$$FE = ((AF + AW)/(K5.RI + FI))^{K4} \qquad (9.1)$$

where FE is the fixation enhancement factor,

  AF represents the biological fixation input in kg/ha,

  AW represents the organic animal waste input in kg/ha,

  RI represents the inorganic rainfall input in kg/ha,

  FI represents the inorganic fertilizer input in kg/ha,

 and K4 and K5 are empirical, calibration parameters.

The power K4 may be set to a number very much less than one to leave AF virtually unchanged. Increasing K4 increases the strength of the suppression-stimulation effect. Values of K4 greater than one are not permited. K5 is set during the calibration procedure and allows weighting of the nitrogen received in natural rainfall. Since rainfall is necessary to mobilise inorganic fertilizer nitrogen, this weighting parameter was incorporated and was found empirically to be essential for successful calibration. A value of about 3 is normal.

Inputs from animal wastes were assumed to be partly mobile and partly immobile. Volatilisation losses were estimated using data derived from Gardiner (1965) and Richardson (1976). The partition of the remainder was based on the data of Berryman (1970) and the humification coefficients given by Kolenbrander (1974). Inputs from rainfall and inorganic fertilizer sources are assumed to be wholly mobile.

Mineralisation of SOM makes a further contribution to the mobile 'pool'. The proportion of SOM mineralised increases with the volume of infiltration and depends heavily on soil type. Annual proportions between 0.5 and 4% are observed for British soil, the lower values being associated with clay soils and the higher values with light sandy soils according to Tinsley (1969). A suitable function was determined by trial and error experiment to be :

$$FS = K6.(RR/RA).EXP(-(K5*RI + FI)^{K1/SQR(PH)}) \qquad (9.2)$$

where FS   is the proportion mineralised annually,

RR   is the annual residual rainfall in mm,

RA   is the long term average annual rainfall in mm,

PH   is the soil effective grain size in mm,

EXP is the exponential function,

SQR is the square root function,

and K1, K5 and K6 are empirical, calibration parameters.

The empirical constants K1, K5 and K6 are determined by the calibration procedure. K5 also appears in equation (9.1) and is

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a weighting factor for natural rainfall nitrogen. K6 determines the maximum value of the function and K1 the sensitivity to soil type. Classification of soil types in England and Wales are given by Avery et al (1975) and corresponding guide values for effective grain sizes have been estimated (in millimetres) based on the classification of Chiang and Petersen (1970) :

Soil texture	I	II	III	IV	V	VI	VII
	Well-drained			Mod	Mod-poor	Poor	V.poor
	deep > 1m	mod .5-1m	shall <.5m	drain	drain	drain	drain
Clays	.002	.001	.001	.001	.001	.001	.001
Silts,loams, mixed sand-clay	.05	.02	.02	.02	.01	.01	.001
Silts,loams on fractured rock	.05	.05	.02	.02	.01	.01	.001
Well-sorted sands,gravels	.2	.2	.2	.2	.1	.1	.001
Sands,gravels on fractured rock	.5	.5	.5	.5	.2	.1	.001

The soil texture type classification is based on the UCS sub-divisions shown in Fig. 9.3. Assigning a single value for the parameter PH is difficult and the tabulated values are designed to act as a starting point for model calibration. The significance of soil drainage characteristics is very important since poorly drained soils are characterised by high fines contents even when of an apparent sandy or gravelly nature. Some laboratory determined values of effective grain sizes are a useful adjunct in the estimation of PH :

100 0

45

Clay

50

Silty
clay

Sandy
clay

30

Silty
clay
loam

Sandy clay
loam

Clay loam

18

10

Sandy loam

Sandy silt
loam

Silt
loam

100

Sand   L.s.

100   85   70   50   20   0

L.s. = Loamy sand
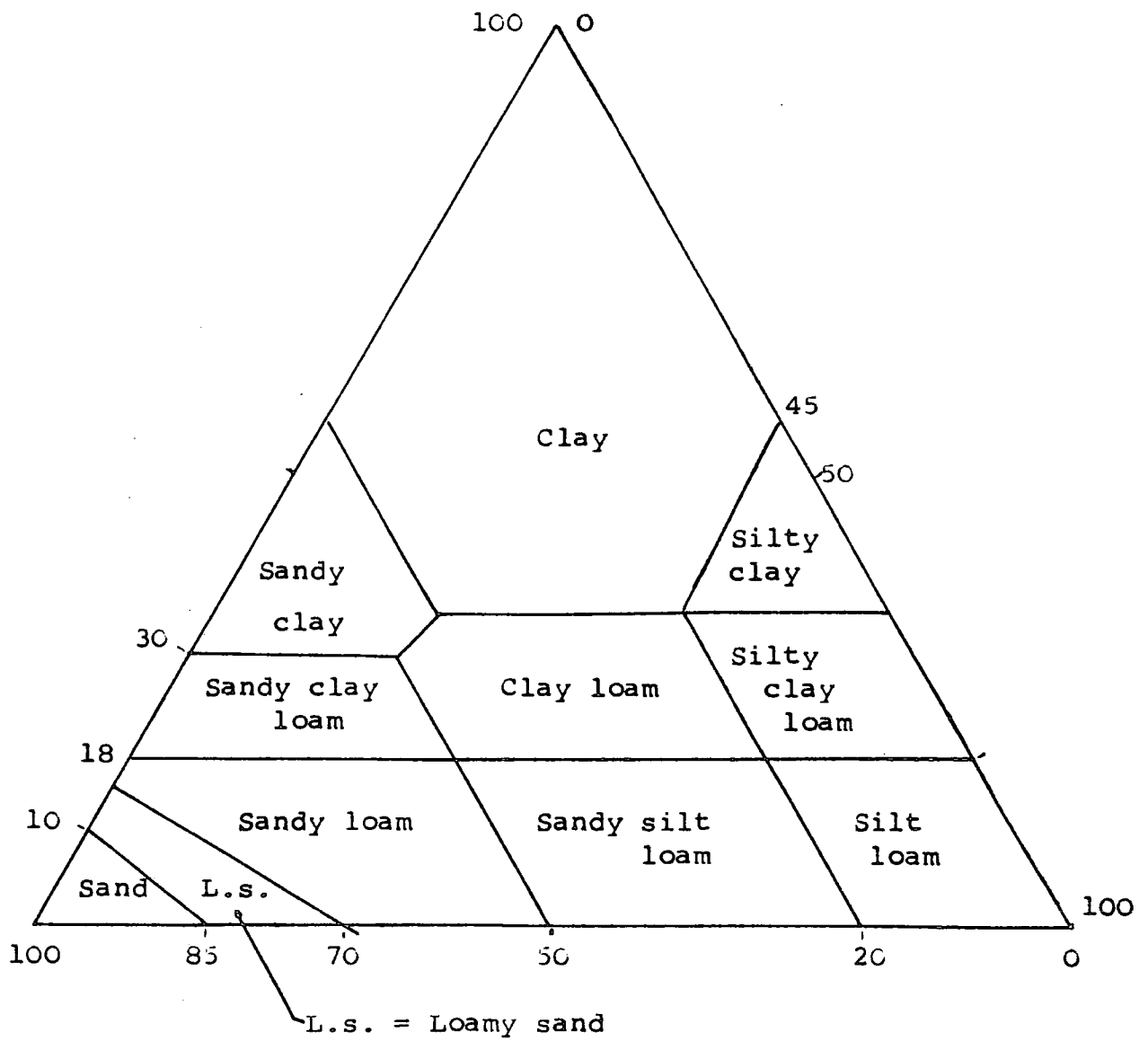
Fig. 9.3   UCS - soil classification table

Soil Type	Locality	Effective grain size (mm)
Beach sand	Hartlepool	0.07
Beach sand	Seaham Harbour	0.2
Coarse brown sand	Leighton Buzzard	0.58
Medium coarse white sand	Leighton Buzzard	0.33
Poorly graded river sand	Durham	0.1
Sandy gravel	?	0.35
Unconsolidated sands	Hetton-le-Hole	0.34-0.80
Unconsolidated sand	Frodsham	0.40
Sandy loam	?	0.035
Silt clay/loam	?	<0.005
Silty clay	Birtley	0.004
Silty clay	?	0.001

The major process of uptake of mobile nitrogen is by metabolic usage by plants. The proportion utilised in this way is a function of crop type and appropriate uptake factors were gleaned from the experimental data of Johnston (1976) and Whitehead (1970). Part of the mobile nitrogen remaining after plant uptake is leached. An empirical equation was devised to reproduce the leaching rates reported by Kolenbrander (1973) as a function of soil type, residual rainfall and nitrogen source. The function chosen was of the form :

$$FM = TANTH(K2.RR.SQR(PH).(RR/RA)) \qquad (9.3)$$

where FM is the fraction of remaining mobile nitrogen leached,

   RR is the annual residual rainfall in mm,

   PH is the effective grainsize of the soil in mm,

   RA is the average annual residual rainfall in mm,

   TANTH is the hyperbolic tangent function,

   SQR is the square root function,

and K2 is an empirical, calibration parameter.

The constant K2 is determined empirically from the observed data. The TANTH function ensures that FM lies between 0 and 1 and is sigmoidal in form.

Any residual mobile nitrogen after leaching is assumed to be retained in the soil. There is very little empirical data available on rates of denitrification but the model permits an annual percentage loss to occur at different rates for the unsaturated and saturated zones. A proportion of that mobile nitrogen removed in plant growth is returned to the soil after harvesting as immobile organic debris. The fraction of material removed was estimated from the report of Johnston (1976) and added to the immobile SOM 'pool'.

The model as described operates on an annual basis but can be modified to operate on any time step for which data can be obtained. All the functions described above are arbitary and are suggested as reasonable mathematical representations of empirical observation. They are however only suggestions and users may wish to replace or modify them.

9.7 SOIL NITROGEN MODEL ELEMENT CALIBRATION AND VALIDATION

In order to assign values to the various constants in the empirical equations some simple systems on which detailed measurements were available were simulated. The two systems used for this purpose were the Broadbalk continuous wheat experiment described by Johnston and Garner (1969) and the Park grass experiment described by Warren and Johnston (1964). The

values of constants were adjusted so that model values of SOM, crop uptake of nitrogen, leaching losses, and other losses were in broad agreement with the observations.

Calibration Run 1 : Broadbalk Continuous Wheat Experiment

Nitrogen source	Field data (kg/ha/a)		Model results (kg/ha/a)	
	Unfert	Fert	Unfert	Fert
Atmospheric fixation	?	?	55	54
Rainfall	5	5	5	5
Animal wastes	–	–	–	–
Inorganic fertilizer	–	145	–	145
TOTAL INPUT	5+	150+	60	204
Crop uptake	25	78	24	79
Denitrification etc	?	?	22	78
Leaching	12	48	13	48
TOTAL OUTPUT	37+	126+	59	205
Soil nitrogen	3108	3428	3111	3413

The slight inbalance between model inputs and outputs is due to rounding to the nearest integer for the tabulation.

Calibration Run 2 : Park Grass Experiment

Fertilizer Application (kg/ha/a)	Crop Recovery (kg/ha/a)	
	Observed	Modelled
–	74	78
145	203	186
290	304	294
435	395	403

The calibration runs enabled values to be assigned to the empirical parameters K1 to K6 and for reasonable agreement to be obtained between model and observation.

Validation of the model was acheived by testing the performance of the model on experiments not used in the calibration procedure. The Hoosfield continuous barley

experiment described by Warren and Johnston (1967) and the experimental grassland systems described by Whitehead (1970) were used in this case.

Validation Run 1 : Hoosefield Continuous Barley Experiment

Fertilizer Application (kg/ha/a)	Crop Recovery (kg/ha/a)	
	Observed	Modelled
–	38	37
48	57	63
96	90	88
144	110	114

No parameter adjustment was permitted after the initial calibration runs and the 'fit' of the validation run is a reasonably idependent test of the model.

Validation Run 2 : Whitehead Grassland System

Nitrogen source	Field data (kg/ha/a)				Model results (kg/ha/a)			
	No Fert	Ino Fert	Org Fert	Both Fert	No Fert	Ino Fert	Org Fert	Both Fert
Atmospheric fixation	290	10	280	10	290	10	282	10
Rainfall	10	10	10	10	10	10	10	10
Animal wastes	–	–	180	220	–	–	180	220
Inorganic fertilizer	–	340	–	340	–	340	–	340
TOTAL INPUT	300	360	470	580	300	360	472	580
Crop uptake	200	235	245	300	202	236	239	288
Denitrification etc	0	55	90	170	0	63	63	158
Leaching	0	10	0	15	0	10	0	22
TOTAL OUTPUT	200	300	335	485	202	309	302	468
Net gain to soil	100	60	135	95	98	51	170	112

The agreement between model and observation is acceptable bearing in mind the uncertainties inherent in the observations. By 'fine tuning' the empirical parameters an improved 'fit' could be obtained but could not be justified by the reliability

of the data used in calibration and validation. Similar 'fits' were obtained during calibration and validation of a precursor of NIPREM is fully documented in the report of the Central Water Planning Unit (1977).

9.3 HYDROLOGICAL MODEL ELEMENT

Leached nitrogen leaving the soil must pass down through the unsaturated aquifer to the saturated zone or run off to a surface watercourse. The precise mechanism of unsaturated flow, particularly in relation to the Chalk aquifer, is in doubt. The relative merits of the 'piston displacement' model of Smith et al (1970) and the 'pore-fissure diffusion' model of Foster (1975) have been discussed by Reeves (1979). However the flow occurs, it is likely that the observed effects are rather similar and can be represented by a slow downward displacement of nitrate with a proportion of rapid direct fissure flow to the saturated zone.

The unsaturated flow model thus comprises : a downward displacement element, representing intergranular flow; and a bypass element, representing fissure flow. For each time increment in the model, a proportion of the flow is displaced downwards a distance dependent on the quantity of flow and the aquifer intergranular effective porosity. This addition to the top of the unsaturated 'column' causes an equal volume to be displaced into the sturated zone at the base of the 'column'. The remainder of the flow is assumed to travel as a rapid fissure component bypassing the displacement column. The model

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is illustrated in Fig. 9.4.

The saturated zone model is represented by a 'homogenised reservoir'. Additions are made by displacement or bypass flow from the unsaturated zone and the average nitrogen content of the 'reservoir' recalculated after each addition.

The soil run off and groundwater discharge in each time increment are combined to estimate surface water quality. The proportion of run off flow to percolation may be specified as data.

In summary, the model for run-off, unsaturated flow and saturated groundwater flow thus provides :

1. a profile of nitrate content through the unsaturated zone,

2. an estimate of nitrate content in saturated groundwater flow, made up of slow displacement and rapid bypass elements,

3. an estimate of river water nitrate content, made up of run off and groundwater flow elements.

The model is thus very simple and additional sophistications can be incorporated if the usage and available data would justify the increased complexity.
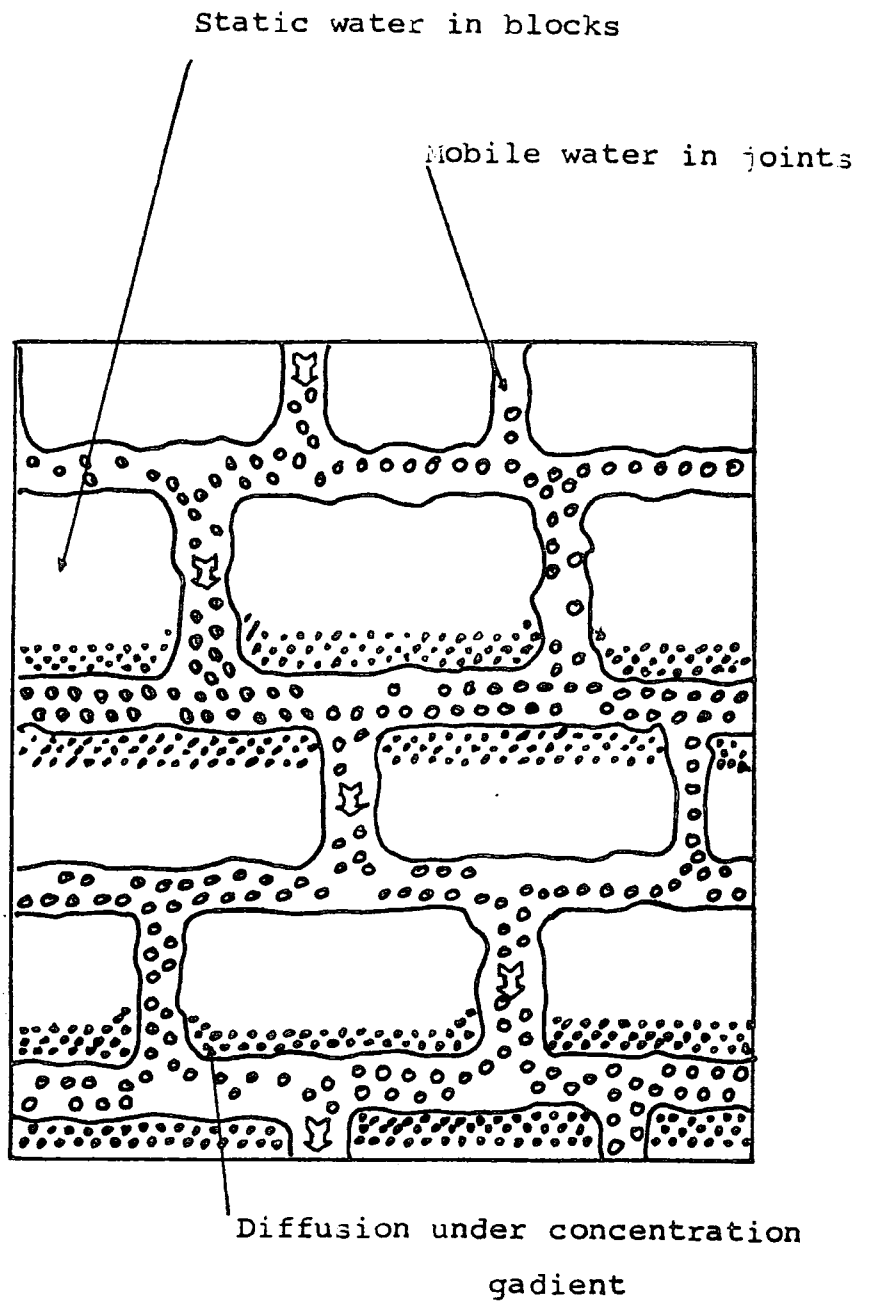
Static water in blocks

Mobile water in joints

Diffusion under concentration gadient

Fig. 9.4   Schematic view of unsaturated zone flow
             assumed in NIPREM

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Parameter values for the hydrological model can be readily estimated from the characteristics of rivers and aquifers. The unsaturated zone nitrate profiles reported by Young et al (1976) provided suitable data for calibration and validation of the unsaturated zone and groundwater elements. The results of a validation run are plotted in Fig. 9.5. The profile is simulated for the New Hampshire North Field of Bridget's Farm. NIPREM was run from a model start time of about 1935 in order to obtain the 1974 profile shown in the figure. Prior to the modelled time interval an equilibrium cereal growing system was assumed. The predicted nitrate profile is in general agreement with the observations, particularly when sampling variability and data reliability are considered.

The river water quality model was calibrated and validated using the empirical observations of Tomlinson (1970). Figure 9.6 shows the results of an attempt to simulate nitrate levels in the Essex River Stour between 1953 and 1969. The river represents a fairly typical eastern England Chalk catchment. For the simulation, rainfall data was taken from British Rainfall (1939-69) and fertiizer application rates for arable land were estimated from Fig. 9.1. The agreement between model and observation was considered satisfactory.

9.10 PARAMETER SENSITIVITY CONSIDERATIONS

The models contain a very large number of parameters,

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Fig. 9.4   Schematic view of unsaturated zone flow
             assumed in NIPREM
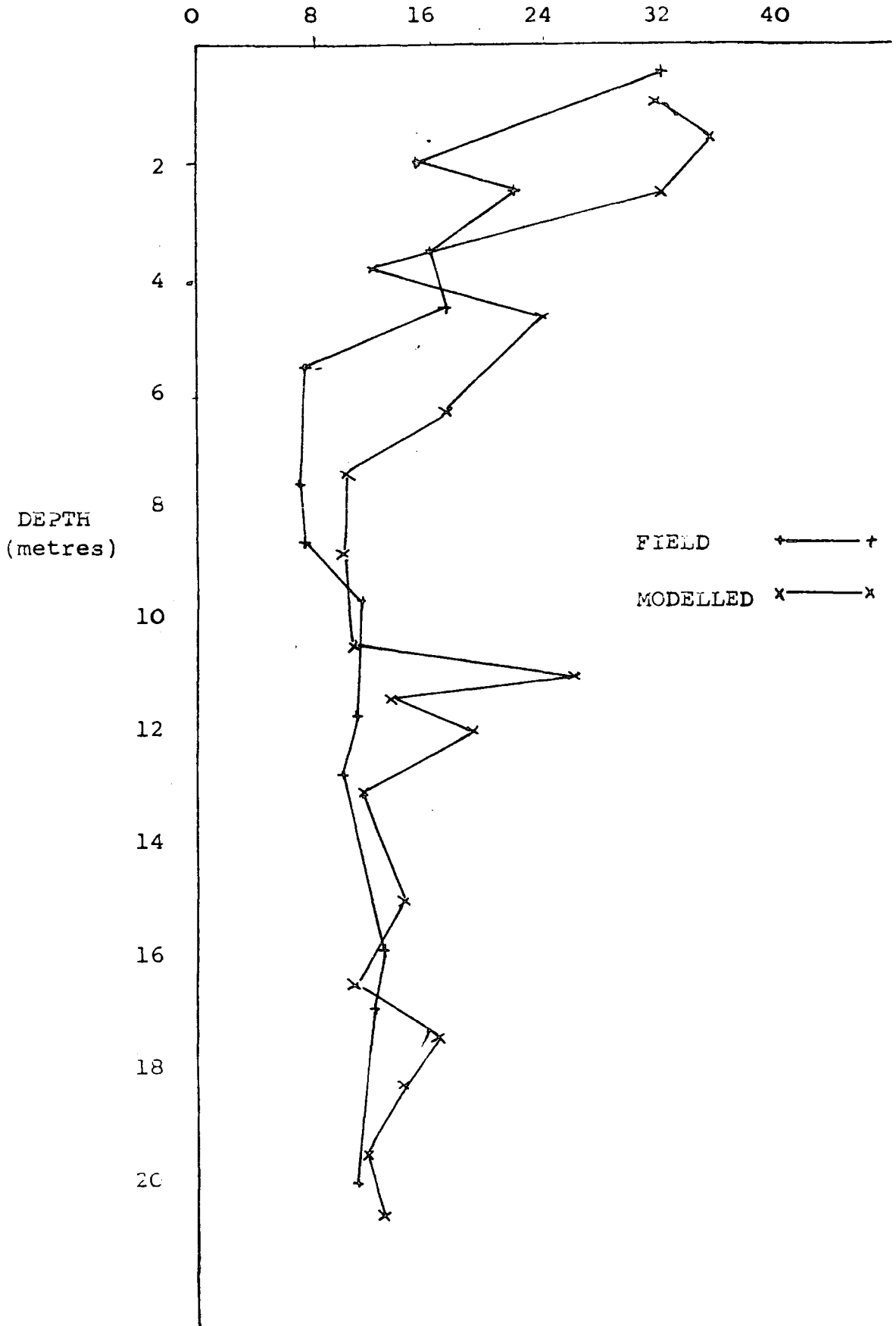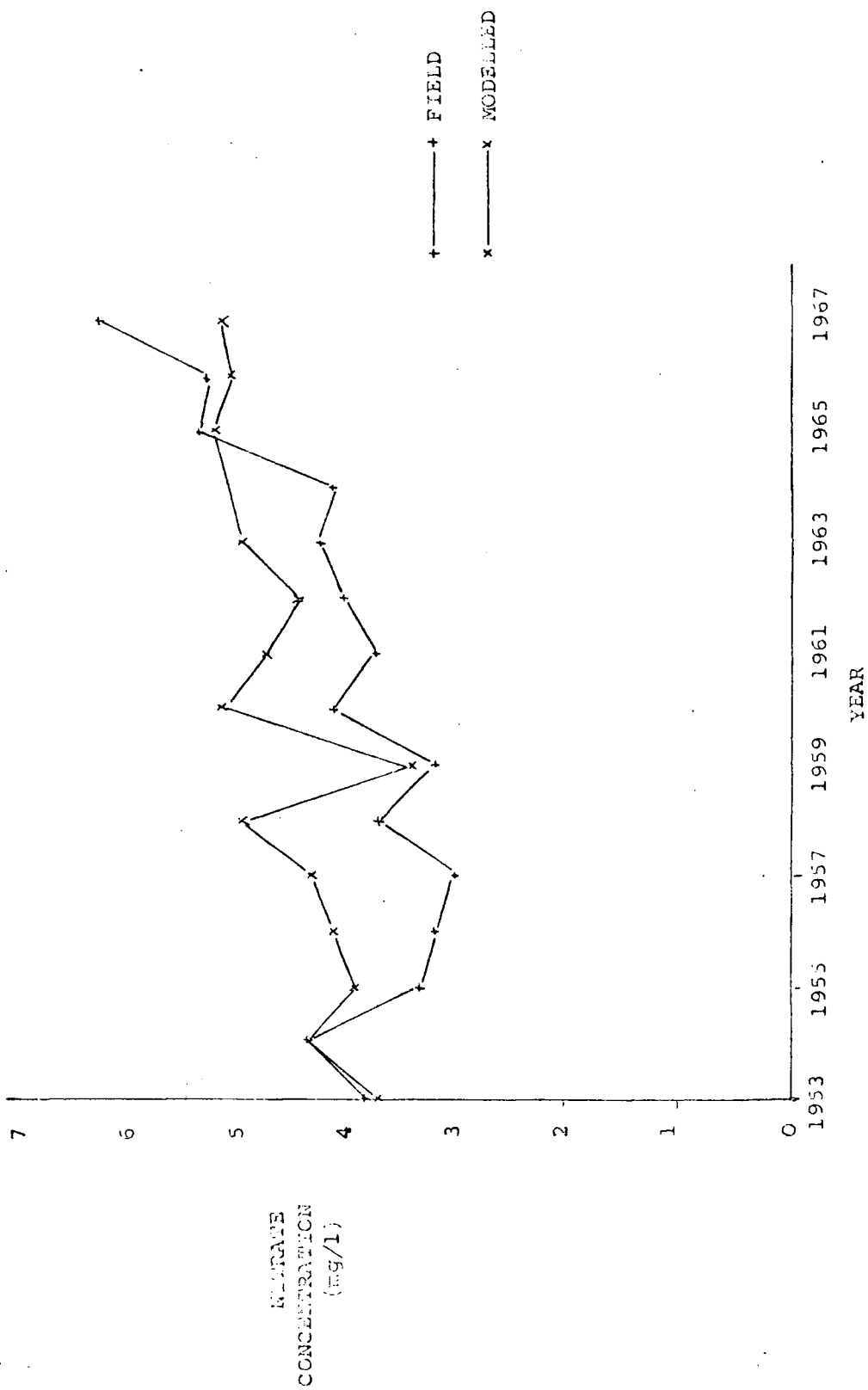
Fig. 9.6   River water quality model – results
            compared with those of Tomlinson (1970)

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over 25, and discussion of a full sensitivity analysis is not feasible. The model can of course be used to check any parameter causing concern. Some parameters, however, those least well known with high sensitivity in respect of SOM nitrogen and leached nitrogen, are worthy of discussion to draw attention to critical parts of the model where care is needed in its application. Equations (9.1), (9.2) and (9.3) are particularly difficult to calibrate and are discussed very briefly.

In equation (9.1) there is little data to support any large variation in FE, thus the value of K4 should be small (<0.1). Increasing K4 has the effect of increasing the nitrogen fixed in the system and in particular the SOM nitrogen level. The value for K5 is normally about 3 and is more easily fixed in equation (9.2) since FE is normally assumed to be close to unity.

In equation (9.2), K1 and K6 can be quite closely fixed in order to simulate the empirical observations of mineralisation rates but SOM nitrogen and leachate nitrogen are very sensitive to the value of FS. K5 is readily found if data with and without fertilizer application is available.

In equation (9.3) the value of K2 can be derived by using the function to simulate empirical observation but leachate nitrogen is very sensitive to the value of FM which largely depends in turn on the value of the grain size parameter PH.

Both equation (9.2) and (9.3) contain the soil grain size term PH. In both cases the square root function is used to suppress the function sensitivity to the parameter. A LOG function, for example, could have been chosen to give a similar effect. The functions for FE, FS and FM are not sacrosanct and if they are found wanting they should be amended to a more suitable form. Any changes made in either the form of eqautions or parameters in the model make it necessary to repeat the calibration and validation procedures.

Additional parameters relating to uptake of nitrogen by various crops are included in the model and can be adjusted to a limited extent. The listing of NIPREM in Appendix II contains all the parameter values used in the calibration and validation runs that have been discussed. DATA statements prefaced by REM statements are used to carry most of this information.

9.11 APPLICATION OF NIPREM FOR PRACTICAL PREDICTIONS

NIPREM is designed to be of use in studies of the environmental effect of changes in land use and fertilizer usage in respect of soil and water nitrogen. It is recommended that the model be calibrated and validated on independent data sets for any application. The quality of any predictions is largely dependent on the quality of the calibration-validation procedure. The level of SOM nitrogen (the parameter SN) tends to a constant value in systems in equilibrium. The model finds the equilibrium value for the initial input data by iteration.

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This value is often known or can be estimated to check model performance. Elements of the model may be modified to exclude unnecessary parameters or include new parameters as required. The time increment used in NIPREM is one year but minimal amendment is needed for the program to operate on daily, weekly or monthly data.

A forerunner of NIPREM was used to predict national trends in surface and groundwater nitrate contents as reported by the Central Water Planning Unit (1977). NIPREM itself has been used for agricultural economic studies of fertilizer usage at the University of Manchester.

9.12 NIPREM : CONCLUSIONS

Simple lumped-parameter system dynamics models like NIPREM have wide applications in the field of environmental planning. Their construction clarifies and exposes interactions in complex systems, their calibration and validation identifies areas where data or reseach is required and their predictive use allows potential environmental hazards to be forseen at an early stage when remedial action is feasible. NIPREM is a first attempt at bringing together aspects of agricultural science, soil science, hydrology and geology in a form of use to regional and national planners.

CHAPTER TEN

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MINES : A MODEL TO FORECAST MINE WASTEWATER QUALITY

10.1 INTRODUCTION TO MINES

Mining operations remove large volumes of rock at or beneath the surface and expose fresh rock surfaces to the atmosphere both underground and in surface spoil heaps. The minerals present at the newly exposed rock surfaces are abruptly subjected to a major change in their chemical and physical environment and because of the disequilibrium created undergo mechanical and chemical degradation. This process is called weathering and the chemical weathering of mine wastes is often accelerated by the partial physical breakdown resulting from the mining operation.

As a direct consequence, large quantities of water soluble compounds may be released and dissolved in percolating groundwaters and surface waters. Such waters will also carry away as suspended solids the smaller particles generated by mechanical and chemical weathering. The breakdown of the mineral pyrite is a particularly important aspect of weathering in both coal and metalliferous mines since acid ferruginous drainage waters can be produced.

Acidic and ferruginous drainage waters are found in a

number of situations in mining operations :

(1) in underground workings,

(2) in surface workings (open pit and opencast),

(3) in and around mine spoil heaps, and

(4) in and around mineral stock piles.

The problem is that the severity of the acid ferruginous drainage pollution depends on a large number of interrelated chemical, biological and physical factors involving geological, geotechnical and hyrological aspects.

MINES is an attempt to use some aspects of simple statistical theory to forecast the likelihood and type of drainage for specific cases.

10.2 CHEMICAL CONSIDERATIONS

Although the detailed mechanism of pyrite (including marcasite) oxidation is not fully understood, all authors concerned with acid mine drainage problems seem to agree that :

(1) oxidation of pyrite {FeS_2} is the root cause of the problem, and

(2) oxidation leads to the release of hydrogen ions, and

ferric hydroxide {Fe(OH)3} resulting in an acid ferruginous solution or suspension.

Disagreement seems to exist over the identification of the oxidising agent and the role of bacteria in the process.

The most commonly accepted series of chemical equations describing pyrite breakdown according to Porges et al (1966) and Down and Stock (1977) may be summarised :

(1) oxidation of sulphide to sulphate :

$$2.FeS2 + 7.O2 + 2.H2O ---> 2.Fe++ + H+ + 4.SO4-- \qquad (10.1)$$
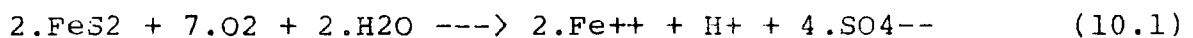
(2) oxidation of ferrous to ferric iron :

$$4.Fe++ + O2 + 4.H+ ---> 4.Fe+++ + 2.H2O \qquad (10.2)$$
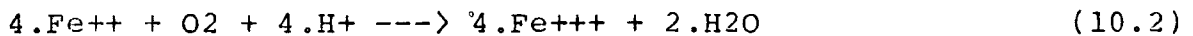
(3) precipitation of 'ochre':

$$Fe+++ + 3.H2O ---> Fe(OH)3 + 3.H+ \qquad (10.3)$$
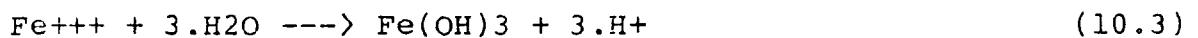
In the breakdown of sedimentary rocks, the release of sulphuric acid results in solution of calcium and magnesium, particularly from carbonates but from silicate minerals also. In addition, acid conditions result in the preferential leaching of any heavy metals (zinc, cadmium, nickel, zinc, etc) from the rocks. Hence the reactions result in an increase in hydrogen, ferrous, ferric and heavy metal cations in solution and sulphate anions.

Reaction (10.1) is the critical stage occuring at the surface of the solid crystalline mineral phase. Reactions (10.2) and (10.3) are responsible for the characteristic red-brown discolouration of drainage water known as 'ochre'. These latter reactions occur at sites remote from the mineral surace and according to Barnes and Remberger (1968) and Smith and Shurmate (1971) have no bearing on the rate of pyrite oxidation.

10.3 BIOLOGICAL CONSIDERATIONS

Barnes and Romberger (1968), Down and Stocks (1977) and Olson et al (1979) discuss bacterial involvement in the oxidation of pyrite. From these discussions bacterial involvement in the oxidation process itself seems unlikely but they may well act as catalysts. The presence of the bacteria Thiobacillus ferro-oxidans is commonly associated with acid mine drainage conditions and it is said to promote the more rapid oxidation of pyrite. Other bacteria found in acid mine drainage environments include T. thio-oxidans and Ferrobacillus ferro-oxidans.

Considerable controversy exists over the oxidising agent involved in pyrite breakdown and the role of bacteria. Barnes et al (1964) suggests that there is both field and laboratory evidence for pyrite breakdown in the absence of oxygen and Barnes and Clarke (1964) suggest that water may be the oxidising agent. Brock and Gustafson (1976) have pointed out the role of ferric ions as oxidising agents. In an attempt

to resolve these conflicting views, Smith (1974) has suggested the following reaction sequence :

(1) initial pyrite oxidation by oxygen :

$$2.FeS2 + 7.O2 + 2.H2O ---> Fe++ + 2.H+ + SO4-- \qquad (10.4)$$
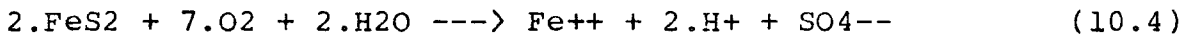
(2) slow bacterial oxidation of Fe++ by T.ferro-oxidans :

$$4.Fe++ + O2 + 4.H+ ---> 4.Fe+++ + 2.H2O \qquad (10.5)$$
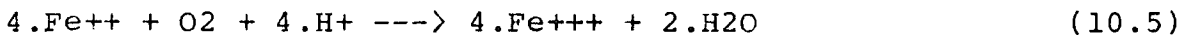
(3) rapid use of Fe+++ to oxidise further pyrite :

$$2.Fe+++ + FeS2 ---> 3.Fe++ + 2.S \qquad (10.6)$$
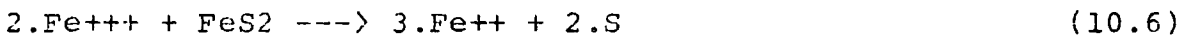
(4) if O2 absent, sulphur oxidation by Fe+++ :

$$2.S + 12.Fe+++ + 8.H2O ---> 12.Fe++ + 2.SO4-- + 4.H+ \qquad (10.7)$$
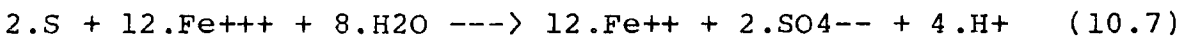
(5) if O2 present, sulphur oxidation by T.thio-oxidans :

$$2.S + 3.O2 + 2.H2O ---> 2.SO4-- + 4.H+ \qquad (10.8)$$
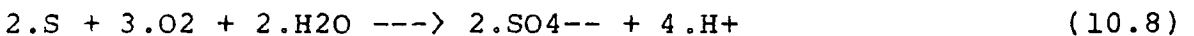
(6) oxidation of Fe++ as drainage as and when Eh rises :

$$4.Fe++ + O2 + 10.H2O ---> 4.Fe(OH)3 + 8.H+ \qquad (10.9)$$
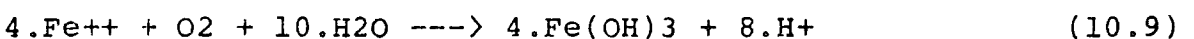
Only a very small amount of oxygen is required to initiate reaction (10.4) and regenerate Fe+++. Bacteria speed the reactions but are not essential, similarly the presence of

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excess oxygen speeds the reaction but is not essential.

10.4 PHYSICAL CONSIDERATIONS

Iron sulphide occurs as two minerals with different crystal structures, the common mineral pyrite and the rarer mineral marcasite. Marcasite although rare is more readily oxidised than pyrite. Henceforth the term pyrite will be used to imply both of the iron sulphide minerals.

Reviews of acid and ferruginous mine drainage by Barnes and Romberger (1968) and Glover (1976) tend to be in broad agreement on the factors controlling the rate of the critical oxidation reaction (10.1).

The rate of pyrite oxidation increases with falling grain-size and increasing Eh. Large brassy pyrite crystals do not readily oxidise, whereas for crushed or finely disseminated material the oxidation is very fast. The presence of water at the mineral surface increases the rate of reaction but saturation may limit the free passage of oxygen to the mineral surface and inhibit the reaction. Increase in temperature also increases the rate of oxidation, as does the removal of free hydrogen ions. A steady flow of water past the mineral surface favours oxidation by supplying fresh oxygen and removing the products of oxidation which tend to accumulate and inhibit further reaction.

The mineral composition of the host rock and

associated rocks may have an important influence on the oxidation reaction rate. The presence of carbonates tends to increase the rate of pyrite oxidation by removing hydrogen ions. Carbonate tends to favour the precipitation of ochre since ferrous ion stability is reduced as the pH rises. Secondary ion exchange reactions may occur with clay minerals.

Coal mining spoil heaps tend initially to be alkaline and acid drainage problems may appear after a long delay. Lack of compaction, steep slope angles, and mineral segregation tend to promote pyrite oxidation in older, loose-tipped, tall, conical, spoil heaps. Continual overtipping prevented much reaction in all but the final surface layers. In newer, compacted tips segregation is not present but extended periods between the placement and compaction of layers allows oxidation to occur at more surfaces according to Spears and Taylor (1972). Studies made on the mechanical breakdown of colliery spoil by Struthers (1964) suggest that a typical weathering sequence in Britain is :

(1) intensive chemical weathering immediately on exposure the atmosphere and moisture,

(2) generation of large quantities of soluble weathering products from a layer down to 1 to 1.5m during the first year,

(3) drainage water concentrations attaining their highest levels in late summer and autumn from a low in early spring,

(4) gradual decline in the generation of soluble products

following the first year of exposure.

Spears and Taylor (1970) suggest that the physical breakdown of colliery spoil is restricted to the breakdown of a few non-detrital minerals, particularly pyrite, ankerite and some swelling or mixed layer clays. They further conclude that the rate of chemical breakdown is much less than the rate of physical degradation.

Combustion is a problem in coal mines and spoil discard heaps. The oxidation of pyrite is a very strongly exothermic reaction and the proximity to combustible carbonaceous material may lead to spontaneous burning if the heat generated cannot be dissipated sufficiently quickly. Combustion promotes the rapid oxidation of pyrite and burnt spoil often contains large quantities of sulphate minerals which may be leached by percolating waters.

The movement of water through underground mine workings is a complex problem. Exit of water from mines takes place predominantly be two mechanisms :

(1) removal in pumped artificial drainage.

(2) percolation to the zone of saturation and removal by saturated groundwater flow.

Within a mine complex patterns of unsaturated and saturated flow zones will be continually fluctuating due to variations in the pumping regime and the natural rise and fall of groundwater

levels in response to infiltration. Soluble products tend to be flushed out in early spring following the winter infiltration season. Most of the products of pyrite oxidation are carried by unsaturated 'weeping' and unsaturated oxygenated groundwater circulation will be largely responsible for carrying oxygen to the site of reaction at the mineral surfaces.

In spoil heaps, most of the flow will be unsaturated oxygenated vadose seepage. Flow will be concentrated in the less compact surface layers and occasional high intensity rainfall pulses will tend to flush out accumulated soluble weathering products from time to time.

10.5 POLLUTION ASPECTS OF ACID AND FERRUGINOUS DRAINAGE

Problems arising from the existence of acid and ferrugnous drainages (AFD) are discussed by Glover (1976) :

(1) In the mine - AFD can cause serious corrosion of metallic components in mining equipment. In addition, the sulphate released leads to the rapid weakening and breakdown of concrete and mortar. Ochreous scale often leads to fouling of pumping equipment and pipework.

(2) In the spoil heap - AFD renders the surface layers infertile and prevents stabilising colonisation by trees and grasses. Gravel and pipe drains become clogged by ochreous deposits leading to blocking and subsequent stability problems.

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(3) In stock piles - AFD will attack concrete hard standing and bunkers.

(4) In surface watercourses - AFD destroys the pre-existing ecology causing very large changes in turbidity, pH, Eh and the levels of toxic metals in solution.

(5) In urban drains and sewerage systems - AFD may lead to structural failure due to sulphate attack of concrete and mortar, blockages by ochreous deposits, and the pH change may destroy and render ineffective biological wastewater treatment processes.

Mine wastewaters arising from pyrite oxidation have very variable compositions depending on the conditions at the site of oxidation and the subsequent history of the water during transport to the sampling point. Glover (1976) recognises five principle water quality classes :

(1) Acid drainages with insignificant ferric or ferrous iron in solution.

(2) Acid drainages with significant ferric iron in solution.

(3) Acid drainages with significant ferrous iron in solution.

(4) Neutral drainages with significant ferrous iron in solution.

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(5) Neutral drainages with significant ferric iron in suspension.

10.6 SUBJECTIVE PROBABILITY MODEL FORMULATION

There are many situations in a groundwater context where decisions must be made on the basis of experience when that experience is both incomplete and qualitative. For example, in the selection of abstraction well sites, waste disposal sites and in the estimation of the effects of mining or agricultural operations on groundwater quality and flow. A method of rationalising such experience in the form of a model enables the non-expert to review a complex situation, be prompted as to the salient parameters, and come to a preliminary decision.

A decison-assisting model may be constructed by the following steps :

(1) assembling all the case history data, subjective opinions and rules of thumb,

(2) identifying all the different potential outcomes of the decision process,

(3) structuring the data into a set of observational factors which mitigate for or against each particular outcome,

(4) quantifying the relative influence of observational factors for each outcome as weighting or predisposing factors,

(5) ordering the outcomes for particular case histories and reviewing quantitative weightings to calibrate the model.

This procedure was used in the formulation of the model MINES which forecasts the likelihood of acid mine drainage resulting from a particular mining operation and the probable chemical character of the effluent.

To construct the program MINES it is necessary to use the statistical concepts of 'subjective probability', 'relative likelihood' and 'conditional likelihood'. Much work in the field of probability and statistics deals with the derivations of the probabilities of certain complicated events from the specified probabilities of simpler events. One obvious problem arising out of this is the need to initially assign values of probabilities on which all subsequent calculations are based. Sometimes this is easy since the probabilities can be assigned objectively on the basis of extensive experience and observation. On the other hand, there are some occaisions when it would be difficult to find two people who would agree on even an approximate figure. The probabilities assigned in MINES are the subjective estimates of the author based on an assessment of the theoretical and case history literature.

The MINES program, listed in Appendix III, is divided into to two parts :

(1) Identification : makes the decision on the probability of acid or ferruginous mine drainage being a problem.

(2) Classification : decides on the relative probabilities of the various classes of mine drainage water quality.

The first part of MINES interrogates the user to determine the conditions prevalent at the site of current interest. Questions (9 in this case) are posed sequentially and the user is asked to select from a list of optional replies (4 are offered). Initially MINES assumes that the probabilities of the occurrence or absence of acid or ferruginous mine drainage are equal. MINES also assumes that the degree to which an answer to one question affects the overall outcome is independent of the other answers to all other questions. This asumption can either be removed if there is evidence that it is untrue, or the questions modified to ensure that the assumption is valid. In response to each reply option selected the probabilities are modified by an amount determined by the programmer's subjective estimate of the change in the 'relative likelihood' of the two outcomes. After all responses have been treated in this way, the relative probabilities for the occurence and absence are examined and the user informed of the outcome.

There are a number of ways in which the final probabilities may be calculated:

(1) Additive scheme : where the first step is to assign a probability weighting to each question $P(q)$ ensuring that Sum

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{P(q)} over all questions is not greater than 0.5. A weighting factor for each option (Ao) is then assigned such that no value of Ao exceeds unity. Ao is assigned a positive value for options favouring the occurence of AFD and a negative value for those options favourable to no AFD. Setting Ao to zero implies that the option is neutral in its implication. The products Ao.P(q) define a set of probability increments to be added to the initial 0.5 assumption as a result of each user selected response. Thus the final probability of occurence is given by :

$$P(AFD) = 0.5 + \text{Sum} \{Ao.P(q)\} \qquad 10.10$$

where Ao represents weighting factors for the options,
and P(q) represents the question probability weightings.

(2) Multiplicative scheme : where all question response options are assigned a predisposing factor which quantifies the extent to which the option response increases the probability of AFD occurence. The factors (Fq) must be positive. Fq > 1 is favourable to AFD occurence, Fq < 1 mitigates against it. Fq = 1 is neutral. The Fq values for the user selected options act as multipliers to give the final probability estimate thus :

$$P(AFD) = Fq!/(1 + Fq!) \qquad 10.11$$

where Fq represents selected question predisposing factors,
and Fq! the factorial product for all questions (F1.F2.F3...)

MINES uses a multiplicative scheme for ease of programming and greater flexibility. Changes in data can be made independently

since the only limitation on Fq values is that they are non-negative.

The second part of MINES to predict the most likely water quality class is only operative if P(AFD) at the end of the first program phase is greater than 0.5. All five class options are assigned an intitial probability of 0.2 and the user is asked to respond to a further set (in this case 8) of multiple choice questions. A multiplicative scheme is used to modify the probabilities according to the response option selected by the user.

10.7 MODEL CALIBRATION AND VALIDATION

MINES was calibrated by assigning values for all predisposing factors on the basis of a subjective interpretation of the theoretical and case history data, summarised in sections 10.2, 10.3 and 10.4. A summary of the extensive data made available to Rae (1977) and used in an evaluation of the use of mine drainage waters as potential resources was also used in calibration.

Relatively few well-documented case histories are to be found in the literature but those for which published information is available were investigated and as much additional information as possible collected. MINES was validated on the basis of its ability to correctly forecast mine wastewater quality in these cases.

Results of validation runs on MINES:

DISUSED MINES:

Area	Effluent Observed	MINES %Probabilities 1 2 3 4 5	Reference
Pennsylvania (Anthracite)	pH 3 or 4 plus Fe++/Fe+++	9 15 47 3 23	Barnes et al (1964)
Cardiganshire (Pb/Zn)	pH <2.5 plus Fe+++	0 44 22 16 16	Fuge (1972)
Girvan (Coal)	pH <4 plus Fe++/Fe+++	0 34 25 12 25	SDA (1980)
Co. Durham (Coal)	pH 7.8 plus Fe+++	0 0 0 95 2	Cairney et al (1975)

TAILINGS DUMPS

| Ontario (Base metals) | pH 2.0 plus Fe+++/Fe++ | 49 16 24 1 8 | Hawley et al (1971) |
| Appalachians | pH 2.6-3.3 | 8 27 40 3 20 | Emrich et al |

KEY to MINES predictions:

1 Free acid (sulphuric)

2 Acidic containing ferrous iron

3 Acidic containing ferric iron

4 Neutral containing ferrous iron

5 Containing ferric iron in suspension

Notes:

(1) SDA refers to Scottish Development Agency

(2) Percentage probabilities sum may not equal 100 due to the rounding-down procedure.

(3) In many cases, the studies referenced concentrated on stream, rather than on effluent sampling. This particularly affects the apparent oxidation state of the iron, such that when MINES predicts ferrous discharge, ferric compounds may in fact be reported in the reference.

A typical, anotated run-time dialogue from MINES is included in

Appendix III.

10.3 MINES : EVALUATION AND CONCLUSIONS

The procedure used to devise MINES is a very simple one and the program is trivial. It can be argued that the simple multiplicative scheme adopted to calculate probabilities is naive and unjustified. Against this is the fact that MINES appears quite successful as a forecaster. Many with experience of mine drainage problems would argue that MINES merely states the obvious. But this is the whole point of the program. MINES is a summary of expertise built into a simple question and answer format for the non-expert.

With hindsight, and following the rather informal and empirical development of MINES, the similarity of the modelling process to that used in the development of transition digraph models by Roberts (1976), was noticed. The formal procedure described by Roberts is clearly superior to the ad hoc methods used for MINES but it still remains a useful model.

At worst MINES reminds the user of the pertinant questions to ask in areas where mine drainage might present a problem. At best it guides the user to a reliable conclusion about the likelihood of a pollution problem arising and the probable nature of that problem in water quality terms. MINES uses a microcomputer for a task to which it is well suited and it is strongly argued that programs of this type, however trivial, can form a valuable source of reference, advice and decision guidance for the busy technical manager and planner who cannot afford to spend days and weeks in literature searches and case history reviews.

DIFAN : A STOCHASTIC RANDOM-WALK MODEL FOR DISPERSION

11.1 INTRODUCTION TO DIFAN

Pollution of groundwater by domestic wastes, mining wastes and agricultural wastes can be modelled by a variety of numerical solutions to the diffusion/dispersion equations. Finite difference methods (FDM), finite element methods (FEM) and boundary element methods (BEM) are widely used for simulation and prediction.

Pollution simulation can also be achieved by a simple stochastic random-walk model involving logical rather than arithmetic operations. Such models are very rapidly executed on 8-bit microcomputers and animation speeds can be attained. DIFAN is such a program written as a series of Z80 assembler routines called from BASIC. Animation of this kind cannot be generated on many mainframe computers which operate time sharing systems.

All models require a means of displaying the results and for 'time-developments' animated graphics are the ideal presentation medium. Animated displays of the results of solution of large sets of simultaneous equations on-line, as the calculations proceed, would require an array processor or

dedicated mainframe computer and for pollution simulation and prediction is not economically viable. Secondary processing on a microcomputer to generate animated displays from distributed-parameter numerical models are a feasible proposition but random-walk simulation provides a means of direct on-line animation.

Animation, whether displaying numerical or stochastic model results, may be created on microcomputers by movement of blocks of memory in and out of the memory-mapped video display area. In the case of secondary processing, pre-prepared full screen (2 Kbytes) images can be updated by transfer from disk a maximum of 15 times a second using the Engineering Geology Laboratories microcomputer system. Stochastic random-walk models will compute and display a new screen image in about a second.

11.2 ANIMATION CONSIDERATIONS

The methods of animation described are specifically for the Exidy Sorcerer microcomputer but the method is the same in principle for any memory mapped display. The speeds quoted were achieved with the 4MHz cycle frequency Zilog Z80A microprocessor and may not be possible with some other CPU chips.

The Sorcerer video display comprises 30 lines of 64 bytes each. Each byte in the video display consists of an 8 x 8 dot matrix character. Each character is stored as a code which

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refers to an 8 byte graphics character storage area. The 8 x 8 matrix is the bit pattern stored in these 8 bytes. Figure 11.1 shows how the ASCII code 45H refers to the bit pattern necessary to generate the letter E on the screen.

The full screen thus comprises 1920 bytes. The Sorcerer has up to 48 Kbytes of Random Access Memory (RAM), thus some 25 full screen images can be stored. The screen image can be updated by a machine code routine in about 8 milliseconds (ms). However, assuming 8 updates per second is sufficient for animation, a time sequence of only about 3 seconds (24 images) can be held in RAM. It is clear that for extended animation sequences screen images must be either transferred from disk or generated on-line.

Disk transfer times from Micropolis minifloppy drives for a screen image cannot be faster than about 120 ms or about 8 images per second. Disk capacities are about 128K at single density, equivalent to 68 images or an 8 second animated sequence; and 300K at double density, equivalent to 160 images or a 20 second animated sequence. Animation by sequential display of pre-processed screen images from disk is thus just about feasible. Half screen animations of minute duration could be possible with two double density disk drives. The software for such a process requires considerable knowledge of the disk DMA transfer capability but is complicated rather than difficult.

On-line generation of screen images can only be attained with Z80 assembler routines. The program DIFAN updates

Fig. 11.1   Character representation
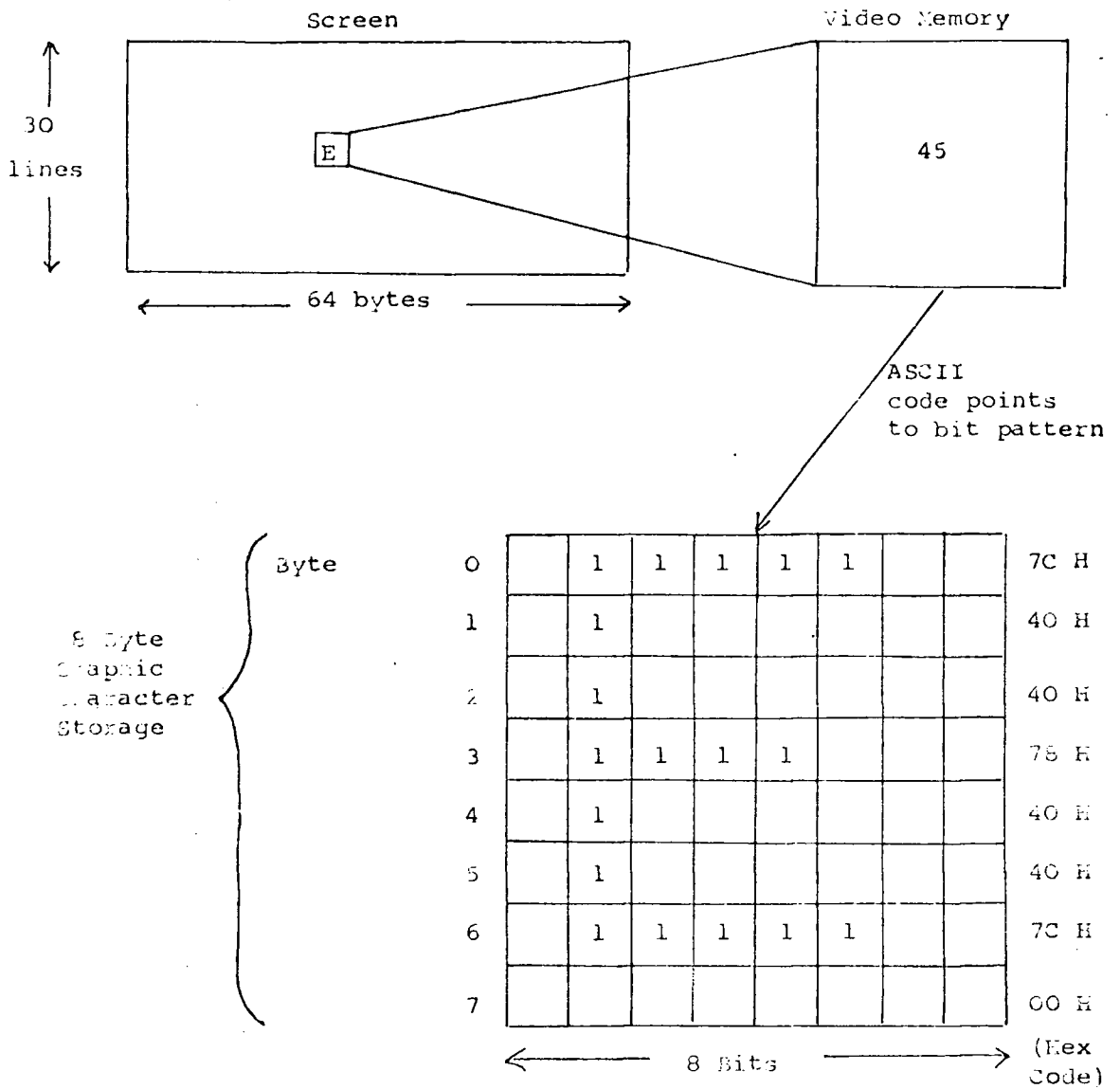
a half screen image in around 1 second and gives a reasonable impression of animation. The program operation will be discussed in some detail.

11.3 RANDOM-WALK STOCHASTIC MODEL

A stochastic technique of randomly displacing and mixing each sub-area of a model has been adopted to simulate diffusion and dispersion. The arithmetic necessary is minimal and the process is largely one of logical comparison. By using a series of Z80 assembler routines supervised by a BASIC program which handles all interactive input/output, the fast simulator/predictor model DIFAN has been devised which gives the impression of an animated display.

In DIFAN the sub-areas used in the simulation coincide with the 64 x 30 memory-mapped video display characters. Each 8 x 8 dot matrix block (we will call a pixel) in the half screen video display represents a level of pollutant concentration. A listing of the BASIC supervisor program DIFAN and the various Z80 assembler routines it calls are given in Appendix IV.

The version of DIFAN listed is not the most general and many of the features described in the text are not present. The reasons for these omissions include :

(1) The general model is under continuing active development and no 'final' or 'complete' version exists.

(2) The arguments made here are about the modelling principles involved in DIFAN rather than a specific description of the program or particular application.

(3) A full listing of DIFAN with the many options tends to conceal the fundamental simplicity of the program.

(4) Z80 assembler code is not very 'transportable' and is only useful for the general reader if extensive documentary comments are included. These comments are very time consuming to write.

For all these reasons, it was thought better to list a fully documented operational version of DIFAN rather than a poorly documented 'development stage' with possible errors.

The convection dispersion process is broken down into its consituent covective and dispersive parts for the purposes of the model simulation used in DIFAN.

Consider a 'slug' of pollutant in a 2-D aquifer. It requires a 4 bit random number to simulate the random convective displacement part of the process :

(1) bit 3 decides if there is any up-down motion,
(2) bit 2 decides if there is any left-right motion,
(3) bit 1 decides up or down,
(4) bit 0 decides left or right.

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There are 16 possible patterns for 4 bits :

    (1) 4 for no motion.   (0000 0001 0010 0011)

    (2) 4 for left or right motion.   (0100 0101 0110 0111)

    (3) 4 for up or down motion.   (1000 1001 1010 1011)

    (4) 4 for diagonal motion.   (1100 1101 1110 1111)

Thus the slug may occupy any of the 9 locations shown in the figure after a random displacement. This can be regarded as the convective part of the convection-dispersion process.

To simulate the diffusion-dispersion part of the process, some mixing assumption must be made which meets the requirement that pollutant mass is conserved. The simplest such assumption is that the concentration at the new and original slug locations are the average of those prior to the displacement. This assumption is used by the listed version of DIFAN but any assumption consistent with mass conservation may be used and the mixing algorithm can be varied very easily. In quantitative applications the flexibility provided by a general mixing rule is necessary for calibration, where convection-dispersion rather than dispersion is modelled.

All displayed pixels are sequentially subjected to a 'pseudo-random' displacement by the routine PIXDIS. The direction of the displacement is decided by testing bit 0 and bit 1 of a random number as illustrated by Fig. 11.2. The pixel at the original location and that at the displaced location are then replaced by pixels representing the "average" concentration of the two, by the routine PIXALT, as shown in

Fig. 11.2   Basic random displacement model

Modelled Area

UP TO
30
BLOCKS

Current Pixel

Displaced Pixel

← UP TO 64 BLOCKS →

| 0 | 1 | 0 | 1 | 0 | 1 | 0 | 1 |
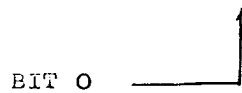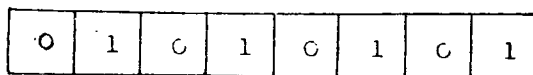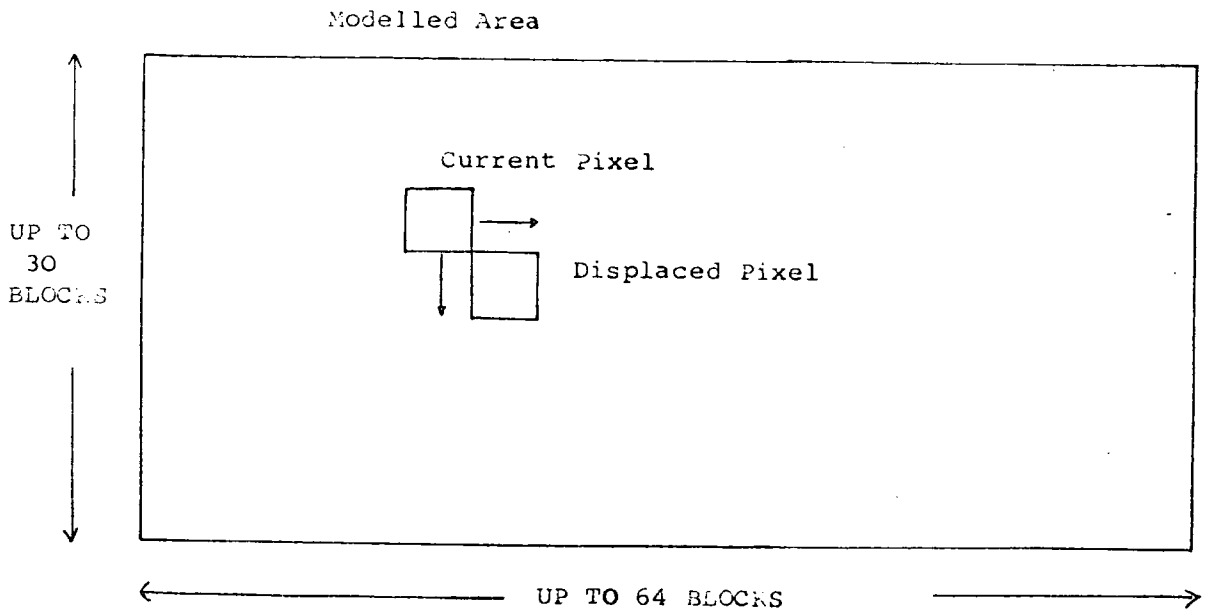
BIT 0

Test Bit 0:

0   ↓   Down

1   ↑   Up

Test Bit 1:

0   ←   Left

1   →   Right

Fig. 11.3. This simple "mixing" assumption has the advantage of simulating the diffusion-dispersion with minimal arithmetic calculations.

11.4 INITIAL CONDITIONS AND SOURCES

Initialisation of the model consists only of loading the appropriate video display locations with the pixel representing the source concentration. A scale of pixels representing a series of concentration steps between the source level and zero are held in memory. For presentation purposes, the visual density increases with concentration. All display locations other than the source or sources are loaded with the zero concentration pixel, a "blank", as Fig. 11.4 illustrates. This initialisation is carried out by the routine SETUP.

For a limited-life source, the source pixel is updated every cycle for the life of the source. For a periodic source, the source pixel is updated every "n" cycles. For a continuous source, the source pixel is invariable updated. For a growing source, new source pixels are introduced with each update cycle. Thus, the time and shape of the pollutant source handled by DIFAN is extremely flexible. Source refresh operations are carried out by the routine PIXREF.

11.5 PHYSICAL BOUNDARY CONDITIONS

In addition to the flexible source boundary

Fig. 11.3   Basic mixing model
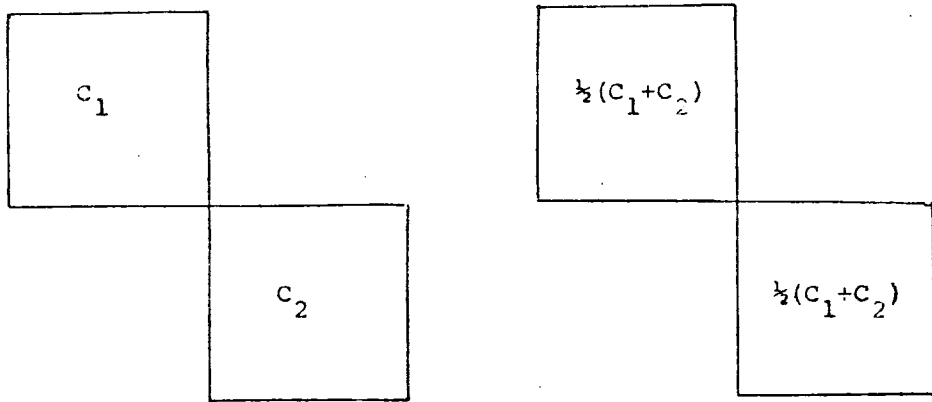
Fig. 11.4   Source simulation

Modelled Area
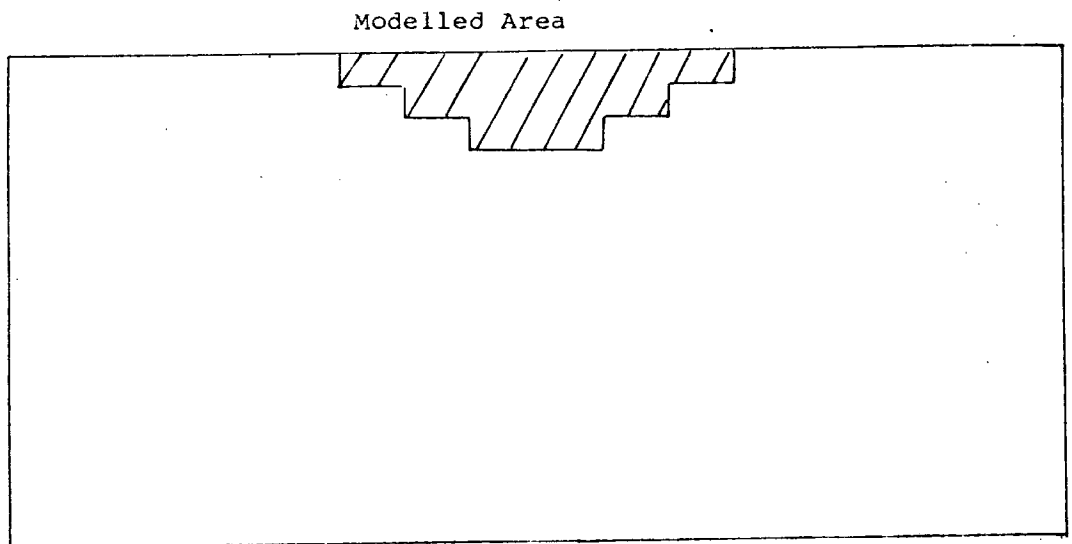
Continuous Update or Short Term Update

conditions, two types of physical boundary are allowed. At a barrier boundary attempted displacements are internally reflected. At a free boundary displacements are not displayed but absorbed into a memory 'buffer' which behaves and is updated in the same way as the display area of the model. Figure 11.5 illustrates the two boundary conditions. Any attempted displacement outside the display area is either reflected or absorbed into a buffer. Physical boundaries are controlled by the routines BDRYL, BDRYR, BDRYU and BDRYD for left, right, up and down respectively.

DIFAN, in its current form, displays all the modelled region as an animated display. Since the display area is limited, so is the size of the modelled region. However, this limitation is largely mitigated by the ability to precisely represent boundaries at infinity ('free' boundaries). The version of DIFAN listed in the Appendix IV has only barrier boundaries since it is intended only as a 'animated display' model for teaching purposes and events outside the 'display' were not considered.

11.6 INHOMOGENEITY AND ANISOTROPY

Simulation of inhomogeneity is achieved by varying the update frequency for sub-areas within the display area by reference to a data byte set up in the BASIC supervisor program. In Fig. 11.6, zone 1 is updated every cycle, zone 2 every other cycle. At each update bit 0 of the data byte is read and the update aborted if the bit is not set. The data

Fig. 11.5   Boundary simulation

Modelled Area

Invisible Buffer for Infinite Boundary

Modelled Area

Final position of pixel

Original pixel position

Attempted position of pixel

Reflection at a Barrier Boundary

Fig. 11.6   Inhomogeneity

Modelled Area

Zone 2
Update Every
Other Cycle

Zone 1
Update
Every
Cycle

Zone

CYCLE
ONE

| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |

Homogeneity
Data Byte   1

| 0 | 1 | 0 | 1 | 0 | 1 | 0 | 1 |
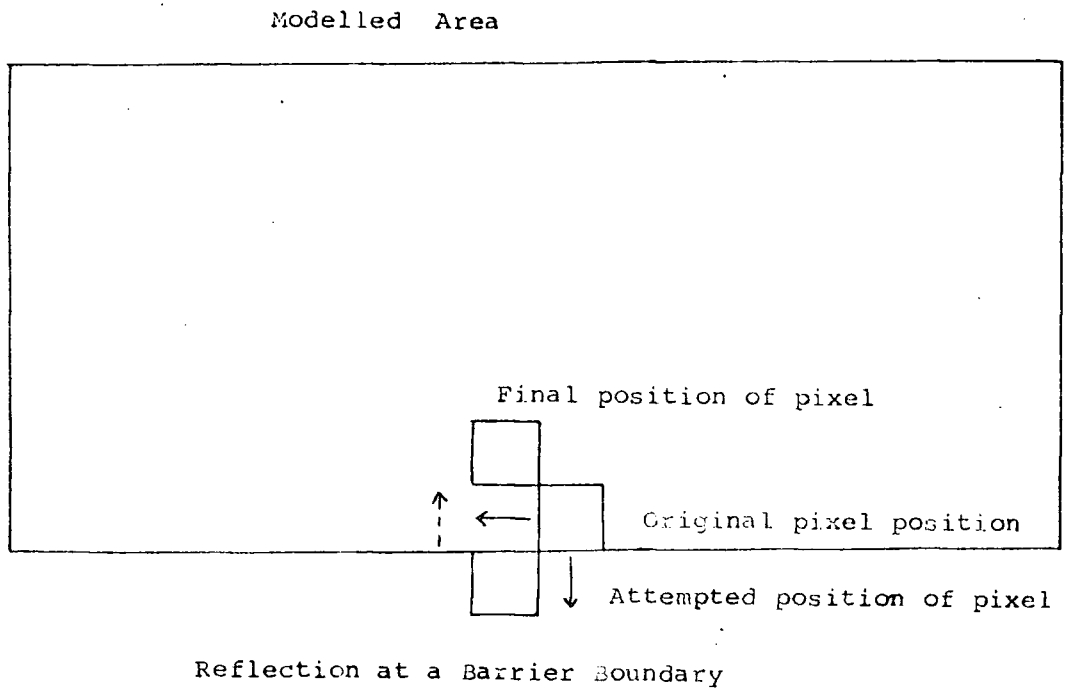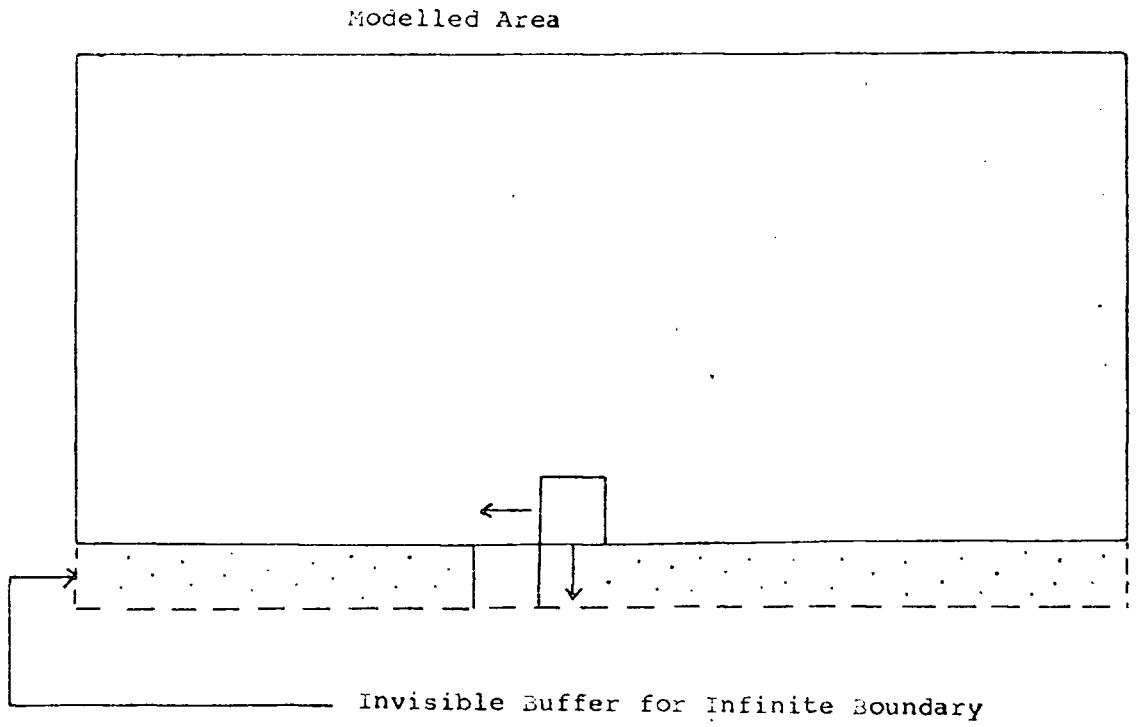
Homogeneity
Data Byte   2
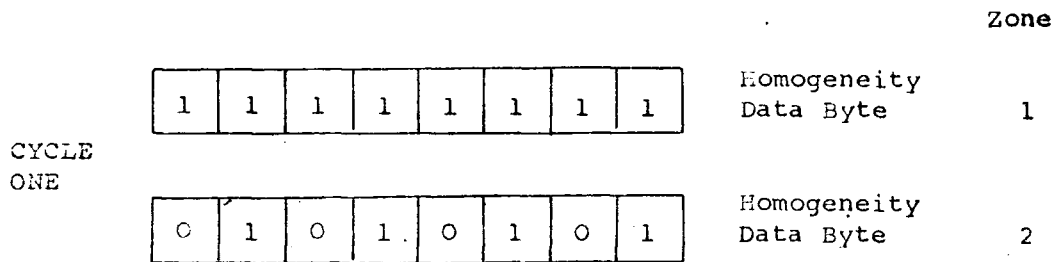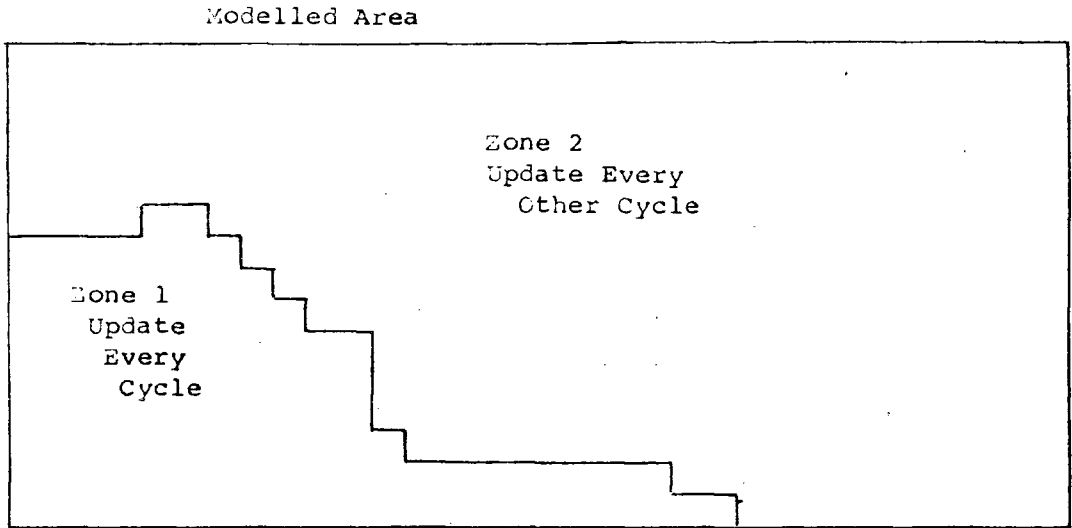
Test Bit 0, then rotate byte left

CYCLE
TWO

| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |

Homogeneity
Data Byte   1

| 1 | 0 | 1 | 0 | 1 | 0 | 1 | 0 |

Homogeneity
Data Byte
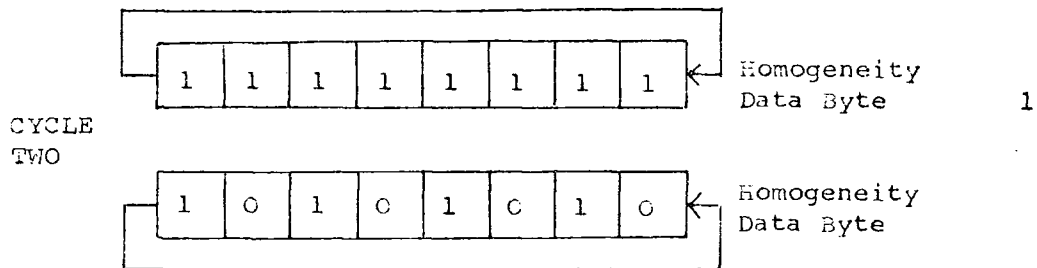
byte is rotated one bit left every update cycle.

Simulation of anisotropy is similarly acheived by reference to data bytes set up from the supervisor program. The up/down data byte(s) allow displacement only if bit 0 of the up/down byte is set. Similarly left/right displacement is permitted only when bit 0 is set in the left/right byte(s). Data bytes are rotated left one bit each cycle. The data byte settings in Fig. 11.7 will ensure essentially horizontal dispersion from right to left across the display. No upward movement is allowed and only slight downward and left to right spreading can take place. The data bytes RIGHT, LEFT, UP and DOWN can be set from the supervisor program.

The precision with which inhomogeneity and anisotropy can be modelled depends on the length of the data bytes. Currently 8-bit bytes are used but 'finer tuning' could be acheived using 16 or perhaps 32-bits if necessary.

11.7 QUANTITATIVE SIMULATION USING DIFAN

The display generated by DIFAN is dimensionless. The length of a time step is implied by the convective velocity in quantitative simulations and a general 'mixing rule' can be used so that the balance between convection and dispersion can be preserved. If dispersion is slow relative to convection then the spatial increment by a 'particle' (x' in section 7.6) during a convective step will be less than the convective displacement. The program to simulate convection and dispersion

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Fig. 11.7   Anisotropy

Modelled Area

| O | O | O | O | O | O | O | O | Up Data Byte

| O | O | O | O | O | O | O | 1 | Down Data Byte

| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | Left Data Byte
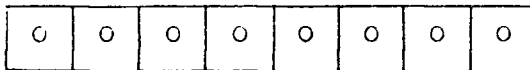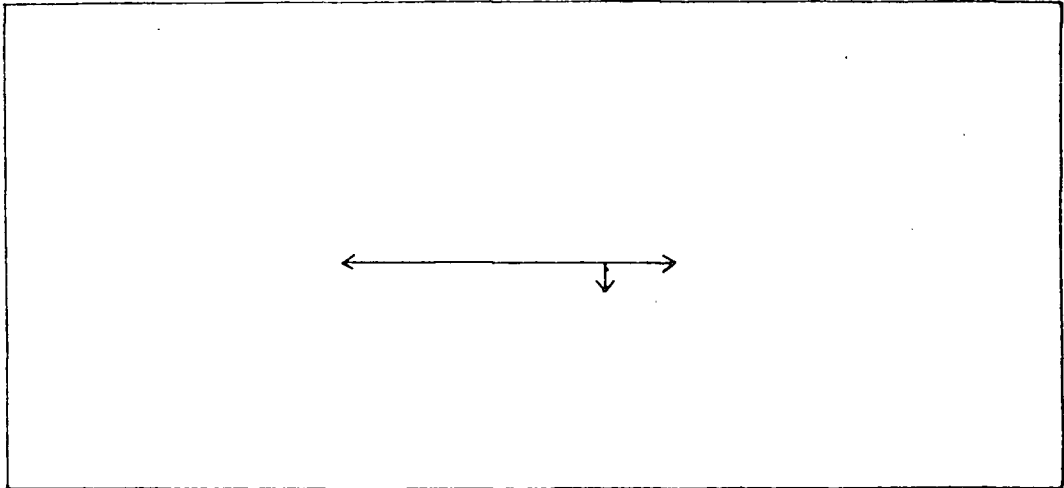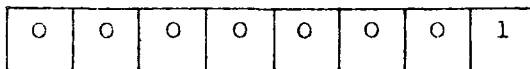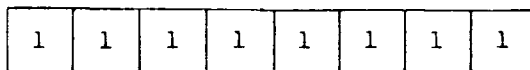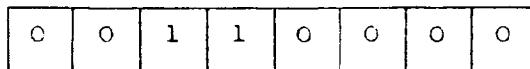
| O | O | 1 | 1 | O | O | O | O | Right Data Byte

Up Data Byte - Never Active

Down Data Byte - Active 1 cycle in 8

Left Data Byte - Active Every cycle

Right Data Byte - Active 1 cycle in 4

remains under development and two approaches are being compared for speed and accuracy. They are best summarised as :

(1) convect and partially mix every step; or

(2) convect every step, mix on some.

The second alternative has the attraction of being easy to program without using arithmetic and is most likely to be used.

DIFAN, at present, requires that the principle axes of anisotropy are invarient and parallel to the rectangular sub-area boundaries. Anisotropy is modelled by DIFAN by manipulating 2 bits (bits 1 and 0) of the convective displacement 4 bit random number. A much more sophisticated representation can be obtained by :

(1) using bits 3 and 2 in addition to 1 and 0.

(2) updating the anisotropy data byte each time step.

These two options permit flexibility in the orientation of the principle axes of anisotropy and rotation of the axes with time. DIFAN remains under constant development and these features will subsequently be incorporated and tested.

If the dimensions and dispersion coefficients are specified and inhomogeneity and anisotropy ratios are known then a real time scale can be assigned to the DIFAN model. A BASIC program to acquire the appropriate information from the

user and calculate the real time scale is a trivial programming task.

11.8 DIFAN : EVALUATION AND CONCLUSIONS

The quantitative validity of DIFAN was checked by comparing concentration patterns with analytical and numerical model studies in the literature. Marino (1974d) provides a useful set of 1-D experiments for this purpose. Because DIFAN generates only approximate contours at concentration intervals equivalent to the source divided by a power of 2, exact comparison is difficult. Figure 11.8 shows the agreement between DIFAN and the analytical and numerical solutions of Marino (1974d). The numerical results presented by Oakes (1976) for idealised aquifers were used to evaluate DIFAN for the 2-D case. DIFAN was used to generate the steady state plume pattern for a rectangular source in a homogeneous isotropic aquifer. The results of DIFAN are compared with those of Oakes (1977) in Fig 11.9. Thus, the random-walk simulations of DIFAN seem to be acceptable in both a qualitative and quantitative sense.

Figures 11.10 and 11.11 show typical screen images to illustrate the flexibility of the model. In Fig. 11.10 anisotropic dispersion from a borehole source in plan is shown and in Fig 11.11 a cross-section simulation of anisotropic dispersion from a landfill site is illustrated.

An attempt was made to apply DIFAN to a practical problem by simulating the observed behaviour of the Cl-
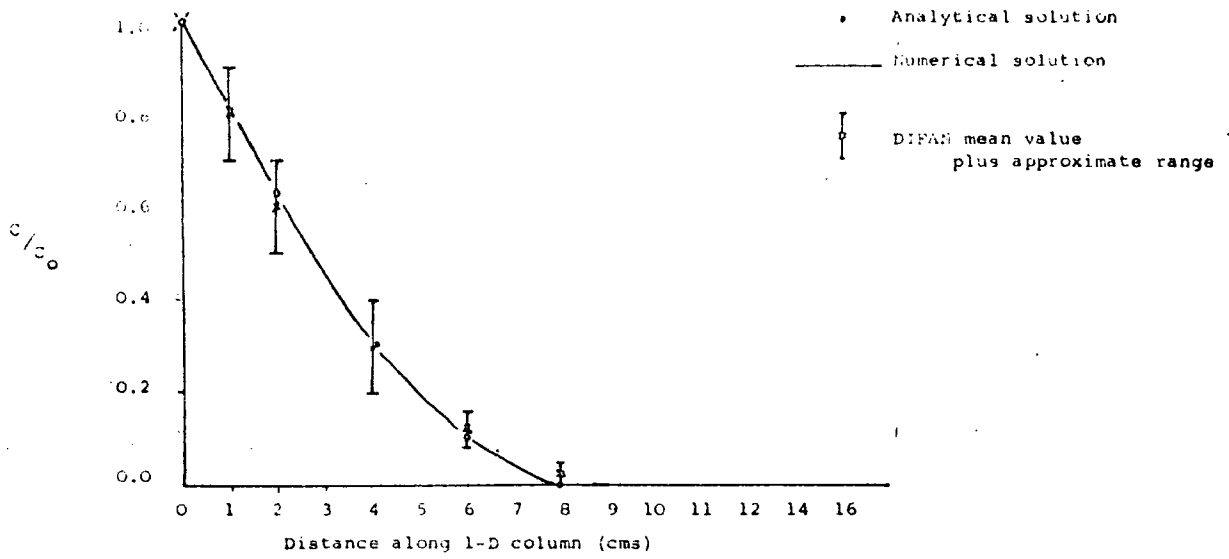
Fig. 11.8   Results of 1-D calibration runs against
Marino (1974d)

Fig. 11'.9   Results of 2-D calibration run against
                 Oakes (1976)
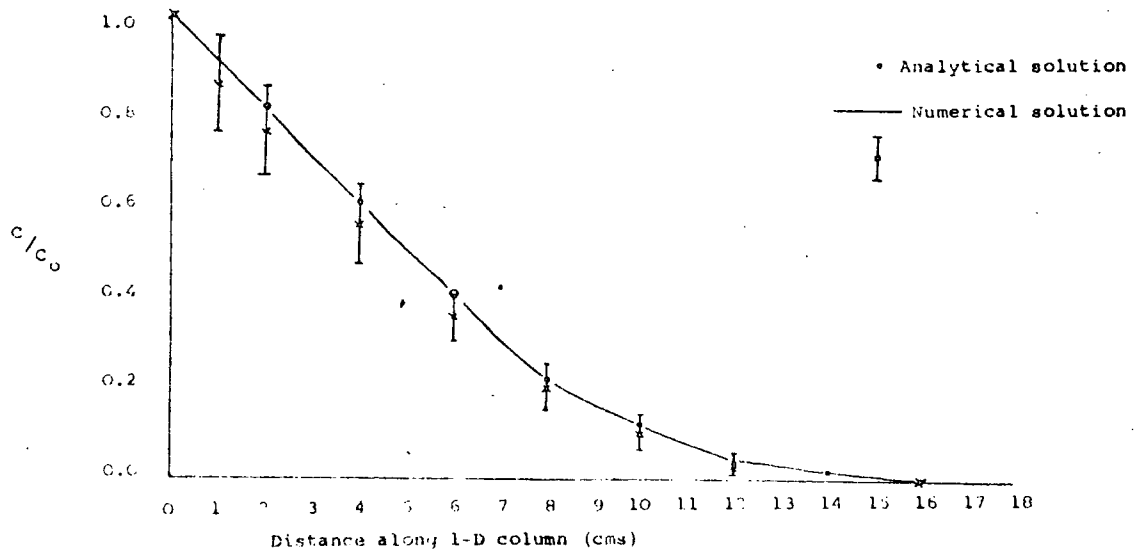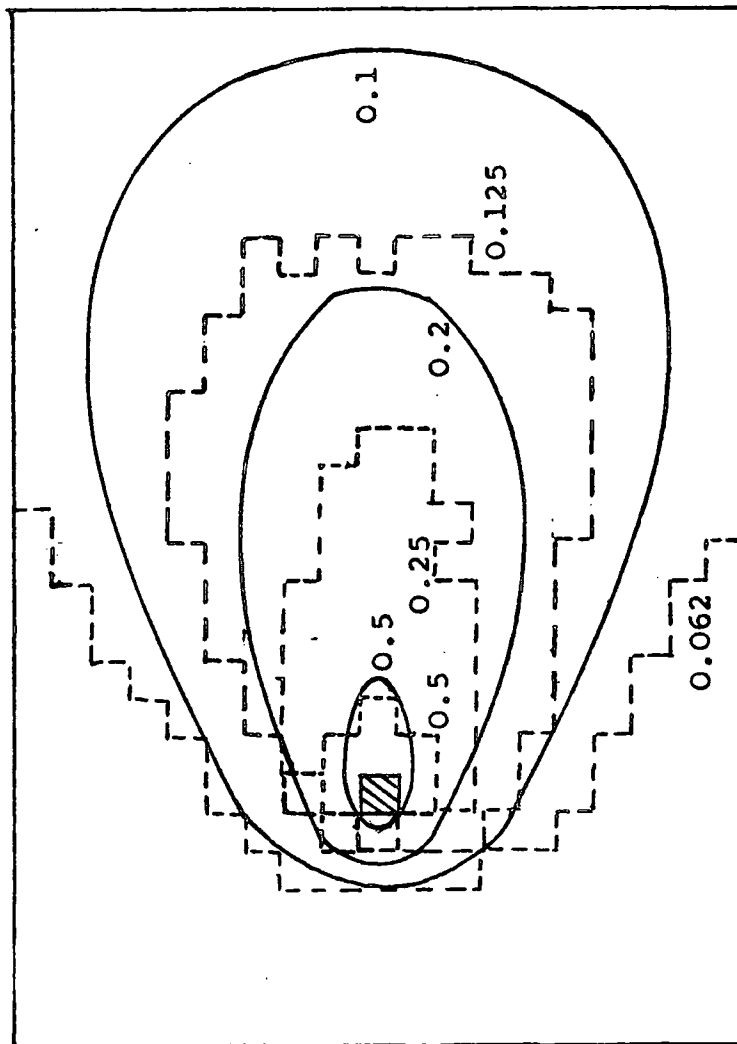
——— after Oakes (1976)
- - - run on DIFAN

(Values given are
 fractions of original
 concentration)

0.1

0.125

0.2

0.25

0.5

0.5

0.062

Fig. 11.10   Contaminated wells - plan simulation

DIFAN - animation program
Diffusion and dispersion simulation

Contaminated wells plan simulation   Step 1

Contaminated wells plan simulation   Step 2

Contaminated wells plan simulation   Step 3
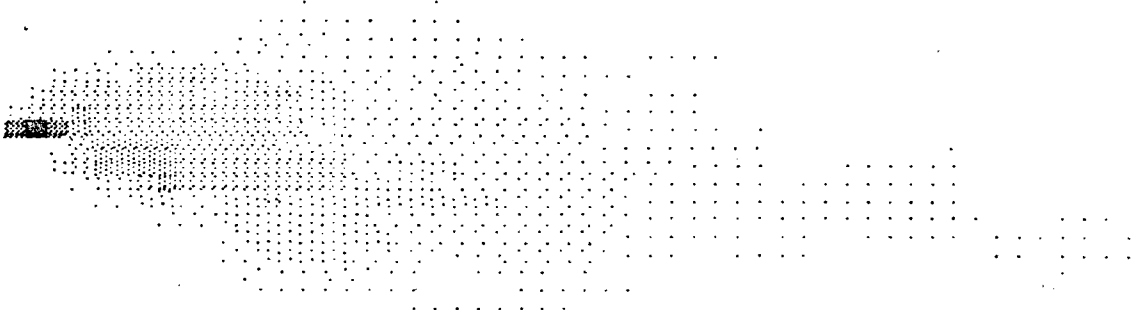
Contaminated wells plan simulation   Step 4
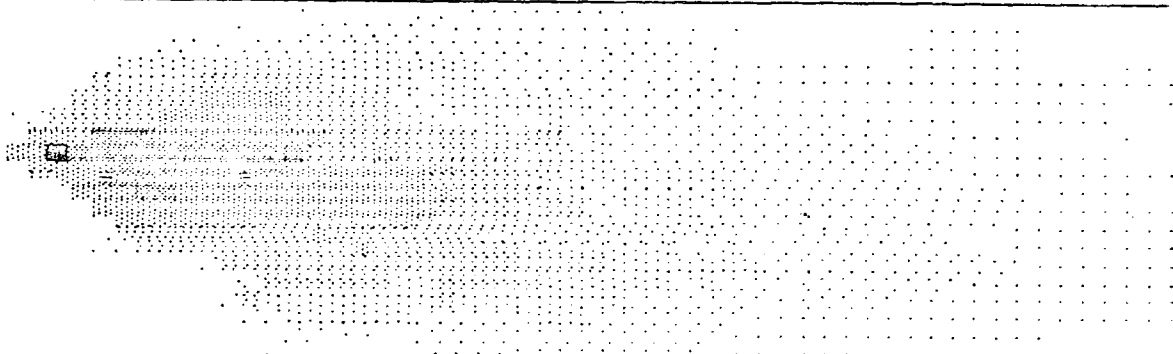
Fig. 11.11   Landfill site simulation

DIFAH - pollution animation

Landfill site simulation   Step 1
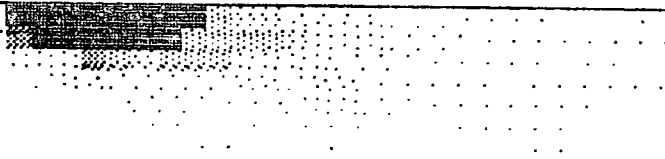
Landfill site simulation   Step 2
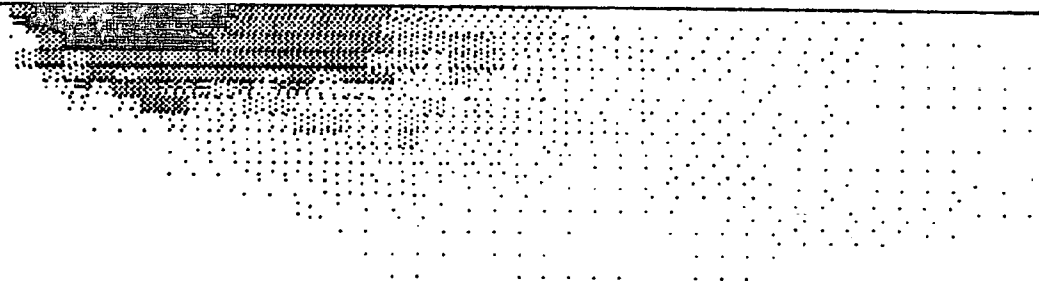
Landfill site simulation   Step 3
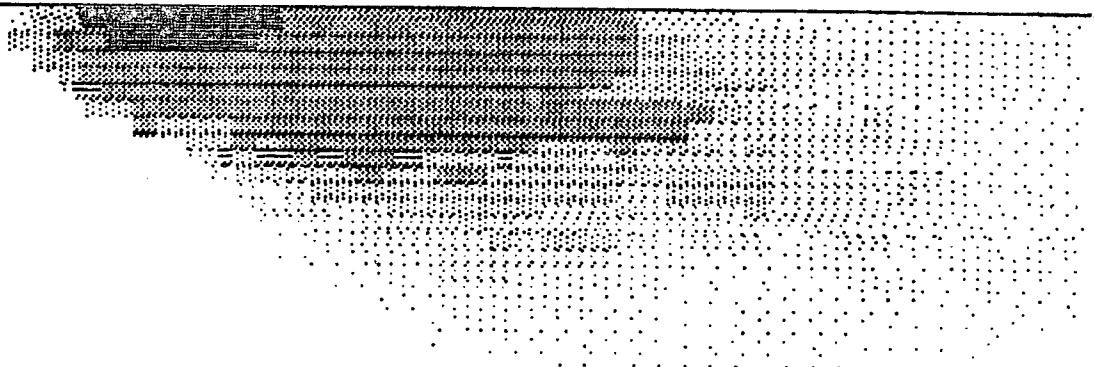
pollution plume at Snake River, Idaho reported by Robertson and Barraclough (1973). Because DIFAN was written for simple rectangular boundary configurations, only a very rough approximation could be obtained. As DIFAN was written to prove the viability of the stochastic random-walk simulation technique, the development of flexible boundary configurations was regarded as beyond the scope of this study. Development of this capability is however being undertaken at the Engineering Geology Laboratories, Durham.

The advantage DIFAN has over numerical methods is that the simulations are carried out at a speed sufficient to give the impression of animation using only a cheap desktop computer. The modelling methodology underlying DIFAN has not been described in the literature in a groundwater modelling context (so far as the author is aware) prior to Bell and Reeves (1981).

DIFAN is a prototype program written to prove the viability of the technique. It is essentially provides a very rapid means of preliminary evaluation of pollution problems, as indicated by the examples quoted, rather than a program suitable for detailed regional prediction.

Programs using the DIFAN methodology are under development at the Engineering Geology Laboratories, Durham for a variety of groundwater modelling applications :

(1) regional pollution prediction.

(2) simulation of permeability for fracture networks.

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(3) simulation of pollutant absorbtion by porous media.

CONCLUSIONS AND RECOMMENDATIONS

12.1 REVIEW:CONCLUSIONS AND RECOMMENDATIONS

Groundwater modelling problems can be subdivided into four main classes:

(1) Preliminary evaluation problems: where a quick approximate answer is required.

(2) Parameter identification problems: where parameter values are deduced by matching the observed response of a system to a known input.

(3) Response prediction problems: where models are used to predict the likely behaviour of systems to possible inputs.

(4) Sensitvity analysis problems: really response prediction problems, where the effects of potential uncertainties in data parameters on the prediction are evaluated.

The principal conclusions that can be drawn from a review of the success of models in solving practical problems are as follows:

(1) Analytical models are widely and successfully used in preliminary evaluation and parameter identification problems. There is a tendency to use such automatically without being aware of the implicit simplifying assumptions. This can sometimes lead to errors in other models since their 'data' is often derived from analytical parameter identification methods.

RECOMMENDATION: Make sure the implicit simplifying assumptions are valid before applying analytical models.

(2) Physical analogue models are often cumbersome, inflexible and expensive except as demonstrations. They are relatively rare in practical applications because of their considerable disadvantages. For problems where the porous medium skeleton and the fluid interact, physical analogues remain a valuable qualitative guide to system behaviour. Physical analogue experiments can be used to provide useful calibration data for numerical models.

RECOMMENDATION: Resort to physical analogues only for skeleton-fluid interaction problems and as a calibration data source.

(3) Electrical analogue models of the resistance capacitance type have been replaced by the much more flexible numerical methods. 'Teledeltos' paper models still provide a valuable means of rapidly evaluating 'steady-state' flow problems, particularly when the geometry of the region of interest is complex.

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RECOMMENDATION: Consider electrical analogues for preliminary evaluation of steady-state flow problems with complex boundary geometry.

(4) Distributed-parameter numerical models are the most widely used (and therefore the most widely abused) groundwater models. The abuse is to waste resources by applying a model which is too sophisticated for the available data. In parameter identification problems, numerical models should find much greater application. Sophisticated numerical models used for this purpose highlight the ambiguities in many sets of field and laboratory observation. Where data is sparse, and any regional rather than local response is to be predicted, lumped-parameter models are cost-effective alternatives.

RECOMMENDATION: Consider the alternatives and if a distributed-parameter numerical model is appropriate, choose the model to suit the application.

(5) Lumped-parameter numerical models are rarely applied, probably because of the wide availability of distributed-parameter packages. Lumped-parameter models are very powerful tools for complex system interaction problems, in planning and for preliminary evaluation of regional problems.

RECOMMENDATION: Consider the adequacy of a lumped-parameter solution and move on to distributed-parameter models only if the data and the predictions required can justify the move.

(6) Regression models were considered as a subset of

statistical models and are only briefly reviewed. They are widely and successfully used for short term prediction and data 'gap-filling' problems. They are less successful and potentially misleading when applied to long term prediction.

RECOMMENDATION: Consider regression models for short term predictions, avoid them whenever possible for long term extrapolations.

(7) Stochastic models include both models which treat aquifer and fluid characteristics as random variables and those which regard the processes of flow and dispersion as fundamentaly stochastic (random-walk models). Stochastic parameter models are valuable in sensitivity analysis and the principle can be applied to all types of analytical and numerical models. Random-walk models offer a simple, very fast and potentially flexible means of quantitative distributed-parameter simulation particularly suited to microcomputers.

RECOMMENDATIONS: Stochastic treatment of hydrogeological parameters should form an essential element in sensitivity analyses. Consider random-walk models where speed on small computers is essential.

In addition to the conclusions drawn from the review and comparative evaluation of modelling methods, the rapid spread of microcomputers has some significant implications for groundwater modelling:

(1) Models will be accesible to many more non-expert

interactive terminal users. Programs will therefore need to be much more carefully written in order to:

    (a) minimize unnecessary input/output

    (b) check validity of all input

    (c) include sensible default options

    (d) be fully self-explanatory

    (e) make extensive use of video-graphics

(2) Users require rapid response and at present microcomputers cannot provide this for FDM and FEM simulations. Random-walk models, however, seem to offer a potential alternative.

(3) Microcomputers are an ideal medium for lumped-parameter system-interaction models and for 'checklist' type decision-assisting models. Such models are neglected at present and are often regarded as 'trivial' by expert modellers.

RECOMMENDATION: Research effort be concentrated on developing simple interactive microcomputer-based models for routine use by the practical hydrogeologist and engineer rather than by the specialist modeller.

12.2 NIPREM: CONCLUSIONS AND RECOMMENDATIONS

NIPREM has been developed from an original batch-processed FORTRAN program for a mainframe computer into an interactive BASIC program for a microcomputer. The program models the soil-water-nitrogen cycle and is designed to make regional predictions for environmental planning purposes.

Considerable improvements have been made in the model over the original by Reeves (1977). NIPREM generates predictions of regional nitrate levels in run-off, the unsaturated zone, the saturated zone and total catchment discharge. It also predicts crop uptake of nitrogen and the level of nitrogen in soil organic matter. All these observations have been checked by calibration and validation runs for a variety of hydrological and agricultural systems. NIPREM remains, however, a largely empirical model since many parameters must be set during the calibration stage by matching observed data.

NIPREM is easy to run interactively as a predictive model but calibration runs are complex. Since a great deal of time must be spent on calibration, the NIPREM program could be improved by providing calibration routines permitting easy amendment of the most sensitive parameters. The output from NIPREM was designed to give final catchment outflow nitrate levels. During calibration, however, other output such as unsaturated zone nitrate profiles could be presented in graphical form. The iterative process for calculating 'equilibrium' soil nitrogen levels during calibration could be

accelerated to save time and the convergence presented graphically to minimise output volume.

NIPREM provides an alternative to the more conventional regression extrapolation models. It has been calibrated and validated on independent datasets and, within the bounds of calibration, is expected to be reliable over prediction periods of several decades.

RECOMMENDATIONS: NIPREM can be improved by modifying the input/output aspects of the calibration phase. Models of the NIPREM type can be considered as alternatives to regression extrapolation models for regional planning purposes.

12.3 MINES: CONCLUSIONS AND RECOMMENDATIONS

MINES is a very simple model using subjective probabilities based on the experience of experts to provide the user with an aid to decision-making. The simple 'menu' input prompt routine makes the user aware of the parameters relevant to the problem and should trigger the collection of further data. MINES was developed very rapidly in response to a particular problem and many other applications of similar models are possible. Incorporation of transition digraph theory into MINES-type models will allow more complex decision structures to be programmed when necessary.

RECOMMENDATION: MINES-type models to be considered for many decision-making problems using transition digraphs to formulate the decision 'trees'.

12.4 DIFAN: CONCLUSIONS AND RECOMMENDATIONS

DIFAN uses a random-walk model to simulate dispersion in 2-D. Quantitative simulations are possible and DIFAN has been validated by its ability to replicate published analytical and numerical solutions. Development of DIFAN is incomplete, in particular the theoretical relationship between field data parameters and model parameters has not been fully investigated. DIFAN is a prototype model which indicates that the method has promise.

A major advantage of the random-walk model concept exploited by DIFAN is the absence of any significant arithmetic and the very simple translation of logic operations on binary data into assembler code for a microcomputer. This leads to very fast execution and the attractive capability for animated video graphic displays.

Random-walk models are excellent for demonstration purpose but if viable on a quantitative basis can be of immense practical value.

RECOMMENDATIONS: Research effort be devoted to exploring the theoretical basis for the quantitative application of random-walk simulation of dispersion. Models based on the DIFAN prototype to be developed to demonstrate the qualitative process of dispersion through animated video displays.

Most groundwater models are created and developed by 'professional modellers' who have lost (or never had) the ability to understand the limitations and approximate nature of field data.

Most field geologists and hydrogeologists have no critical appreciation of the assumptions and limitations implicit in many groundwater models.

As a result many so-called 'prediction models' have ludicrous data requirements or are used to solve problems for which they are totally unsuited.

This study arose from such a mismatch. An excellent distributed-parameter finite element program was developed but the model data requirements were completely divorced from the real data availability. What are needed are models with data requirements that are reasonably met by field collection programs and field collection programs which concentrate on data for which model prediction sensitivity is high. A modelling exercise must answer the following questions in the following order:

1. What predictions are needed?

2. What data is available?

3. What data can reasonably be collected?

4. What models are available?

5. Which (if any) model is appropriate?

Many of the abuses and misuses of models would be avoided if these questions were considered at an early stage. Many intended exercises would be abandoned with consequent saving of resources.

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APPENDIX ONE

LIST OF SYNTHETIC DATASETS USED IN CHAPTER TWO

DATASET ONE   (Q=1E3 m3/day:T=100 m2/day:S=1E-4:R=50 m)

Pumping conditions	Time (days)	Drawdown (m)
Theis	3.47E-4	.05
	6.94E-4	.19
	1.39E-3	.47
	2.78E-3	.87
	.01	1.75
	.02	2.36
	.04	2.91
	.08	3.42
	.17	3.97
	.33	4.53
	.67	5.09
	1.00	5.41
	2.00	5.89
	4.00	6.52
	8.00	7.09

Pumping conditions	Time (days)	Drawdown (m)
Leakage	3.47E-4	.04
	6.94E-4	.19
(r/L = 1)	1.39E-3	.33
	2.78E-3	.52
	.01	.68
	.02	.67
	.04	.66
	.08	.66
	.17	.67
	.33	.67
	.67	.67
	1.00	.67
	2.00	.67
	4.00	.67
	8.00	.67

Pumping conditions	Time (days)	Drawdown (m)
Delayed Yield	3.47E-4	.03
	6.94E-4	.14
$(r/\beta = 1)$	1.39E-3	.33
	2.78E-3	.52
	.01	.67
	.02	.67
	.04	.67
	.08	.67
	.17	.66
	.33	.67
	.67	.68
	1.00	.80
	2.00	.96
	4.00	1.03
	8.00	1.12

DATASET ONE   (Q=1E3 m3/day:T=100 m2/day:S=1E-4:R=50 m)

Pumping conditions	Time (days)	Drawdown (m)
Partial Penetration	3.47E-4	.08
	6.94E-4	.20
(β = 1)	1.39E-4	.39
	2.78E-4	.64
	.01	.96
	.02	1.11
	.04	1.18
	.08	1.24
	.17	1.30
	.33	1.31
	.67	1.35
	1.00	1.36
	2.00	1.36
	4.00	1.39
	8.00	1.39

Pumping conditions	Time (days)	Drawdown (m)
Recharge boundary	3.47E-4	.17
	6.94E-4	.23
(β = 2)	1.39E-3	.43
	2.78E-3	.67
	.01	.95
	.02	1.02
	.04	1.08
	.08	1.10
	.17	1.10
	.33	1.10
	.67	1.10
	1.00	1.10
	2.00	1.10
	4.00	1.09
	8.00	1.10

Pumping conditions	Time (days)	Drawdown (m)
Barrier boundary	3.47E-4	.03
	6.94E-4	.18
(β = 10)	1.39E-3	.51
	2.78E-3	.88
	.01	1.81
	.02	2.23
	.04	2.86
	.08	3.73
	.17	4.53
	.33	5.48
	.67	6.53
	1.00	7.16
	2.00	7.96
	4.00	9.14
	8.00	10.50

DATASET TWO   (Q=1E3 m3/day:T=1E3 m2/day:S=.1:R=50 m)

Pumping conditions	Time (days)	Drawdown (m)
Theis	3.47E-4	–
	6.94E-4	–
	1.39E-3	–
	2.78E-3	–
	.01	–
	.02	–
	.04	–
	.08	.04
	.17	.07
	.33	.10
	.67	.14
	1.00	.17
	2.00	.24
	4.00	.28
	8.00	.34

Pumping condittions	Time (days)	Drawdown (m)
Leakage	3.47E-4	–
	6.94E-4	–
(r/L = 1)	1.39E-3	–
	2.78E-3	–
	.01	–
	.02	–
	.04	.01
	.08	.02
	.17	.05
	.33	.06
	.67	.06
	1.00	.07
	2.00	.07
	4.00	.06
	8.00	.07

Pumping conditions	Time (days)	Drawdown (m)
Delayed Yield	3.47E-4	–
	6.94E-4	–
(r/β = 1)	1.39E-3	–
	2.78E-3	–
	.01	–
	.02	–
	.04	–
	.08	.02
	.17	.03
	.33	.06
	.67	.07
	1.00	.06
	2.00	.07
	4.00	.08
	8.00	.06

DATASET TWO   (Q=1E3 m3/day:T=1E3 m2/day:S=.1:R=50 m)

Pumping conditions	Time (days)	Drawdown (m)
Partial Penetration	3.47E-4	–
	6.94E-4	–
(β = 1)	1.39E-3	–
	2.78E-3	–
	.01	–
	.02	–
	.04	–
	.08	.01
	.17	.05
	.33	.07
	.67	.08
	1.00	.10
	2.00	.10
	4.00	.13
	8.00	.12

Pumping conditions	Time (days)	Drawdown (m)
Recharge boundary	3.47E-4	–
	6.94E-4	–
(β = 2)	1.39E-4	–
	2.78E-4	–
	.01	–
	.02	–
	.04	–
	.08	.03
	.17	.06
	.33	.07
	.67	.09
	1.00	.10
	2.00	.11
	4.00	.11
	8.00	.11

Pumping conditions	Time (days)	Drawdown (m)
Barrier boundary	3.47E-4	–
	6.94E-4	–
(β = 10)	1.39E-3	–
	2.78E-3	–
	.01	–
	.02	–
	.04	.01
	.08	.02
	.17	.06
	.33	.10
	.67	.14
	1.00	.19
	2.00	.23
	4.00	.28
	8.00	.36

W(u,β)
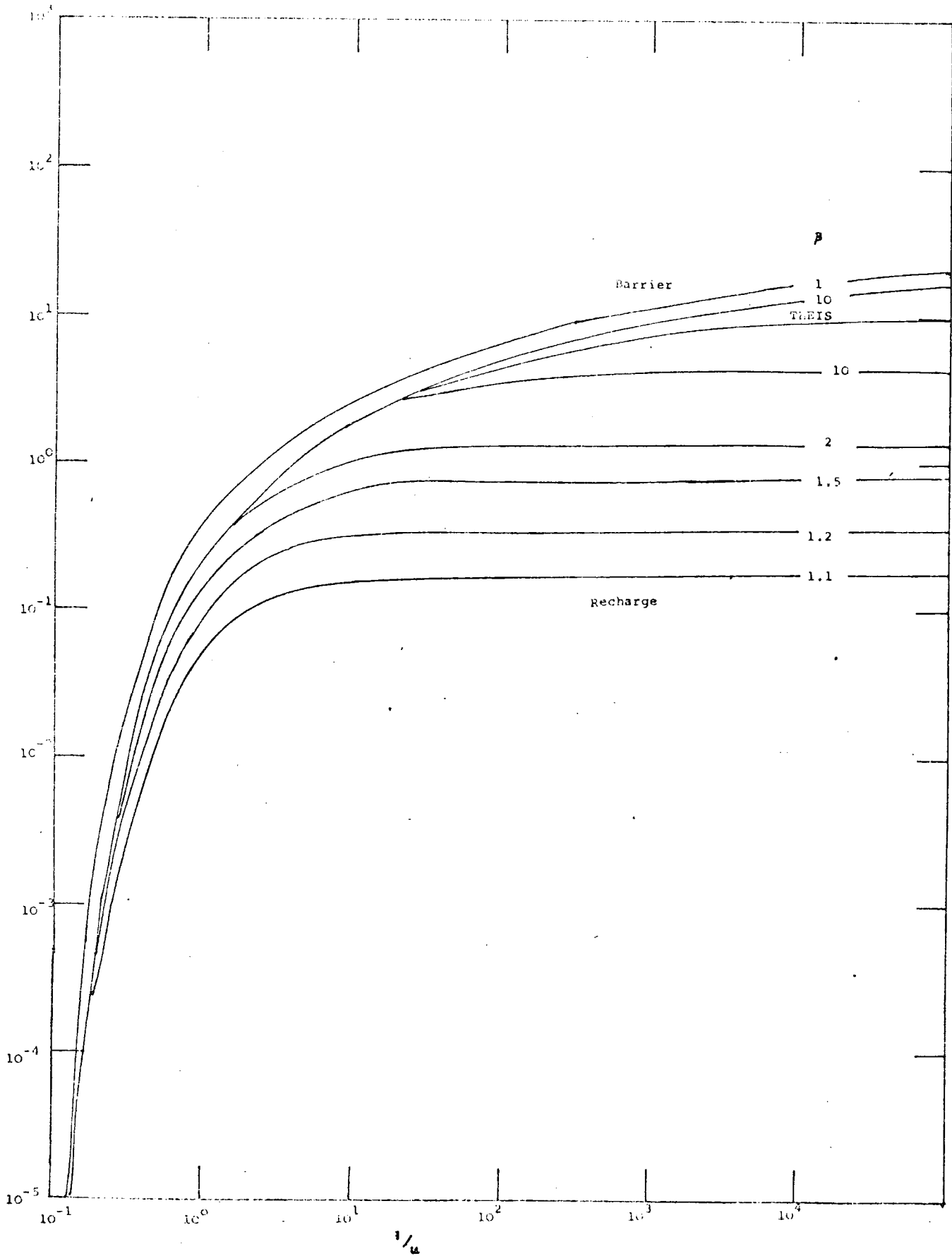
THEIS AND LEAKAGE CURVES
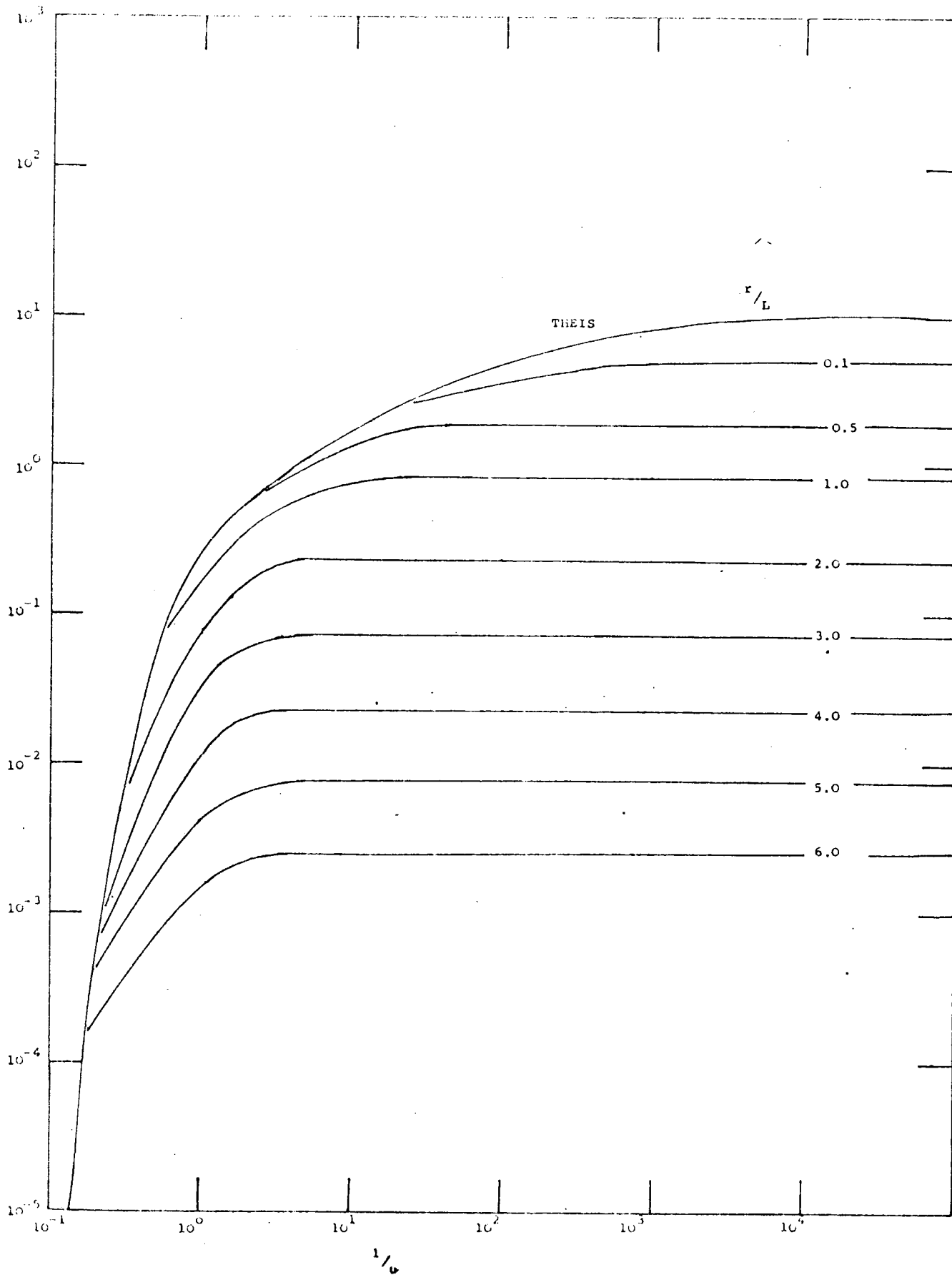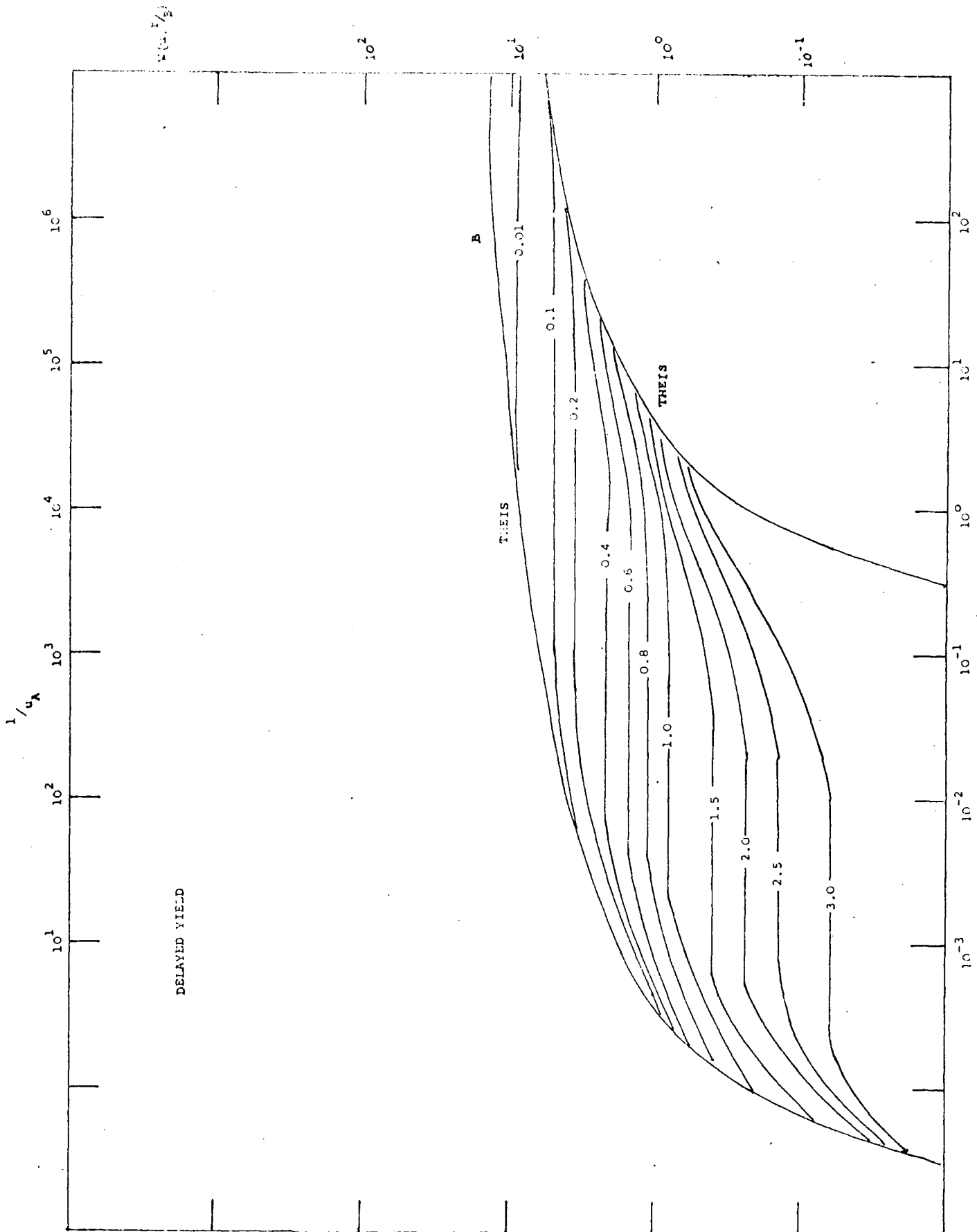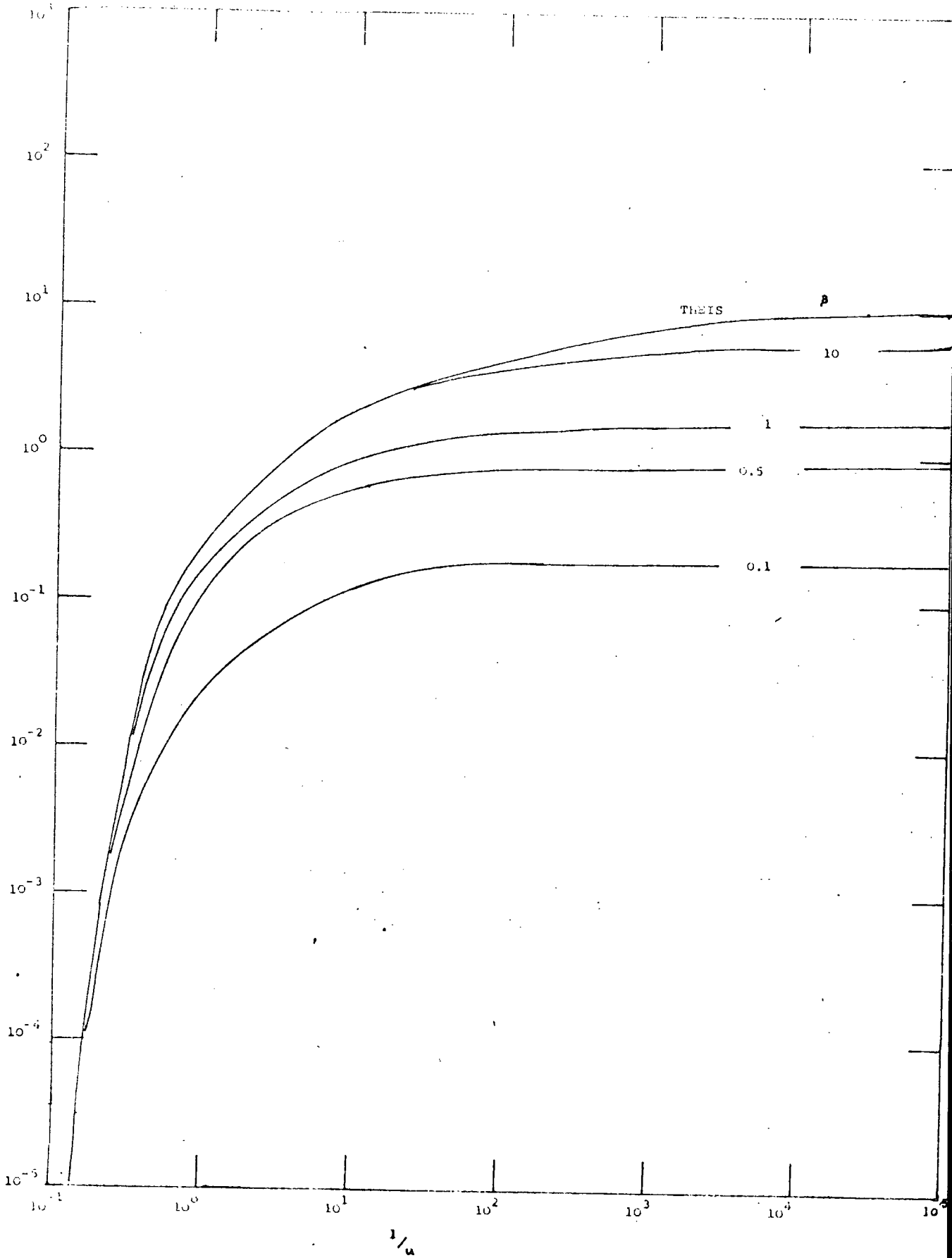
APPENDIX TWO

LISTING OF PROGRAM NIPREM

```
60 CLEAR 200

62 REM Calculate available storage

63 REM *********************************************************

64 AS=FRE(0)

68 IF AS<0 THEN AS=65536+AS

72 AS=INT((AS-8950)/1024)

74 REM Function to calculate TANTH

75 REM *********************************************************

76 DEF FNA(X)=(EXP(X)-EXP(-X))/(EXP(X)+EXP(-X))

80 REM *********************************************************

82 REM

84 REM Program to predict nitrogen content of natural waters

86 REM using climatic, land use,animal population and

88 REM fertilizer usage statistics.

90 REM

92 REM The program is self explanatory when run. The routine

94 REM that explains the model used starts at statement 1000

96 REM

98 REM *********************************************************

100 REM Main program

101 REM *********************************************************

102 NU=100

104 S$="***************":S$=S$+S$:S$=S$+S$

106 PRINT CHR$(12)

108 PRINT S$:PRINT:PRINT "Nitrate prediction model version ";

109 PRINT "3.0 written in microsoft BASIC":PRINT

112 PRINT "Program by M J Reeves / J F Bell ":PRINT:PRINT S$

116 PRINT:Q$="Do you want a full explanation of the program"
```

```
120 GOSUB 1100:ON R GOTO 124,126

124 GOSUB 1000:PRINT CHR$(12)

126 PRINT:PRINT "Main data input sequence"

127 PRINT "*************************"

128 PRINT:PRINT "How many sub-areas";:MN=1:MX=20:GOSUB 1200

132 NS=R

136 PRINT:PRINT "How many time steps";:MN=1:MX=50:GOSUB 1200

140 NT=R

143 REM Dimension minor arrays

144 GOSUB 1400

147 REM Read in basic data constants

148 GOSUB 1300

151 REM Dimension main data storage arrays

152 GOSUB 1500

155 REM Read in first time step main data

156 NI=1:PRINT:Q$="Is the data stored in data statements"

158 GOSUB 1100:ON R GOSUB 2000,1600

160 Q$="Do you want to cycle using fixed data"

162 GOSUB 1100:R=R-2:AU=-2*R

164 FOR NA=1 TO NS

167 REM Set up data for model time step

168 NP=0:GOSUB 3000

171 REM Calculate model inputs in kg/ha

172 GOSUB 3100:GOSUB 3300:GOSUB 3400:GOSUB 3200

175 REM Calculate crop recovery factors

176 IF NI=1 THEN GOSUB 3700

179 REM Calculate soil nitrogen balances

180 S1=SN

184 GOSUB 3500:GOSUB 3600

191 REM Set up unsaturated zone model for first time step
```

238

```
192 IF NI=1 THEN GOSUB 4100:GOTO 200

195 REM Operate unsaturated zone model for other time steps

196 GOSUB 4200

199 REM Operate saturated zone model

200 GOSUB 4300

203 REM Print nitrogen balance results

204 GOSUB 4700

207 REM Iterate for equilibrium SOM level

208 IF NI=1 AND ABS(SN-S1)>0.1 THEN SN=2*SN-S1:GOTO 180

209 REM Print out aquifer model data

210 REM IF NI=27 THEN GOSUB 4400

211 REM Save data for next step

212 GOSUB 4500

213 REM Repeat for next sub-area

214 NEXT NA

215 REM Display data for whole catchment

216 GOSUB 4600

219 REM Increment time step and test for end

220 NI=NI+1

224 IF NI>NT THEN 232

227 REM Read in next time step data

228 IF DR>2 THEN 164

230 ON DR GOSUB 1600,2000:GOTO 164

232 END

1000 REM Routine to explain the use of the program

1001 DATA ******************************************************

1002 DATA "NIPREM is a system dynamics program written in "

1003 DATA "BASIC for        ","implimentation on a microcompute"

1004 DATA "r with at least 32K RAM.      ","NIPREM is desig"

1005 DATA "ned to predict nitrate levels in water supplies "
```

```
1006 DATA "using climatic,land use, animal population and f"
1007 DATA "ertilizer usage ","data.",""
1008 DATA "NIPREM  is self explanatory, prompts input, and c"
1009 DATA "ontains typical","values for all data items.",""
1010 DATA "The structure of NIPREM is as follows :","","",""
1011 DATA "  1. Statements   60-74   make available and ch"
1012 DATA "eck storage.    ","  2. Statements    75-76    hyper"
1013 DATA "bolic tangent function.       ","  3. Statements"
1014 DATA "   80-232  main program with remarks.        "
1015 DATA "  4. Statements 1000-3412 data manipulation and"
1016 DATA " input.        ","  5. Statements 3500-4336 syste"
1017 DATA "m dynamics models.            ","  6. Statements"
1018 DATA " 4400-4728 data manipulation and output."
1019 DATA "Statements 60-74 are specific to the system on w"
1020 DATA "hich the program","was developed and may be replace"
1021 DATA "d or omitted.              ","The main program"
1022 DATA " from 80-232 is essentially a sequence of sub-   "
1023 DATA "routine calls anotated with appropriate remarks.",""
1024 DATA "Multiple main datasets may be incorporated by mo"
1025 DATA "difying 2896    ","to RESTORE to the start of the d"
1026 DATA "esired dataset.           ","The output routi"
1027 DATA "nes at 4400, 4600 and 4700 may be selectively   "
1028 DATA "disabled by modifying the calling statements 210"
1029 DATA ", 216 and 204.  ","The 'mobile' nitrogen model (35"
1030 DATA "00-3528) takes rainfall and     ","inorganic fertil"
1031 DATA "izer inputs plus a mineralised fraction of SOM   "
1032 DATA "and wastes input to form a mobile 'pool'. Some m"
1033 DATA "obile N is fixed","by crops, the remainder is avail"
1034 DATA "able for leaching. The leaching ","function is desc"
1035 DATA "ribed by 3516-3520. Leached N is partitioned     "
```

```
1036 DATA "between infiltration and runoff.",""
1037 DATA "The 'immobile N pool' accounts for SOM. Addition"
1038 DATA "s include a      ","fraction of wastes, non-harveste"
1039 DATA "d crop uptake and atmospheric   ","fixation. The po"
1040 DATA "ol is diminished by SOM mineralisation."
1041 DATA "Crop recovery factors are calculated as weighted"
1042 DATA " averages using","the routine at 3700.",""
1043 DATA "The unsaturated zone model is initialised by the"
1044 DATA " routine at 4100","The 'piston' displacement model "
1045 DATA "of unsaturated flow at 4200      ","allows for 'b"
1046 DATA "ypass' fissure flow and denitrification."
1047 DATA "The saturated zone model at 4300 comprises a 'fu"
1048 DATA "lly mixed pool'","allowing denitrification.",""
1049 DATA "NIPREM is a development of earlier models describ"
1050 DATA "ed by Reeves","(1975) and CWPU (1977).",""
1070 PRINT:PRINT "When you have read the text, type RETURN ";
1072 PRINT "continue or stop":PRINT
1074 RESTORE 1002
1075 DIM NL(14)
1076 NL(1)=2:NL(2)=3:NL(3)=2:NL(4)=8:NL(5)=2:NL(6)=2:NL(7)=2
1078 NL(8)=2:NL(9)=6:NL(10)=3:NL(11)=2:NL(12)=3:NL(13)=2
1080 NL(14)=2
1082 FOR I=1 TO 14
1084 NL=NL(I):GOSUB 1150
1086 IF A$="ST" OR A$="st" THEN I=14
1088 NEXT I
1090 RETURN
1100 REM Routine to handle yes/no replies
1101 REM ****************************************************
1104 PRINT Q$;:INPUT R$:R$=LEFT$(R$,1)
```

```
1108 IF R$="Y" OR R$="y" THEN R=1:PRINT:RETURN

1112 IF R$="N" OR R$="n" THEN R=2:PRINT:RETURN

1116 PRINT:PRINT "Please answer yes or no":GOTO 1104

1150 REM Routine to read explanatory strings

1151 REM ******************************************************

1152 PRINT

1154 FOR J=1 TO NL:READ A$,B$:PRINT A$+B$:NEXT J

1156 INPUT A$:A$=LEFT$(A$,2)

1158 RETURN

1200 REM Routine to handle data input

1201 REM ******************************************************

1204 INPUT R$:R=VAL(R$)

1208 IF R=0 AND R$<>"0" THEN PRINT:GOTO 1240

1212 IF R>MX OR R<MN THEN PRINT:GOTO 1244

1216 RETURN

1240 PRINT "Invalid data - try again":PRINT:GOTO 1204

1244 PRINT "Data out of range - try again":PRINT:GOTO 1204

1300 REM Routine to read in basic constants

1301 REM ******************************************************

1302 DATA 0.35,0.35

1303 DATA 55,275,85,85,0,75

1304 DATA 50,18,10,0.3,4.5

1305 DATA 0.73,0.95,0.95,0.85,0.5,0.9

1306 DATA 0.62,0.90,0.62,0.65,0.1,0.6

1309 DATA " ok",Enter new value,kg/ha,kg/yr/head

1310 DATA Fraction of animal waste N mineralised,0,0.5

1311 DATA Fraction of animal waste N volatilized,0,0.5

1312 DATA Fixation by tillage crops,25,75

1313 DATA Fixation by clover and rotation grasses,200,300

1314 DATA Fixation by permanent grass,50,100
```

```
1315 DATA Fixation by rough grass,50,100

1316 DATA Fixation by urban area,0,100

1317 DATA Fixation by woodlands,50,100

1318 DATA Cattle waste N,40,60,Sheep waste N,15,20,Pig waste N

1319 DATA 8,12,Poultry waste N,0.2,0.4,Human waste N,4,5

1320 DATA Fraction recovered tillage,0.4,0.6

1321 DATA Fraction recovered clover and rotation grass,0.8,1.0

1322 DATA Fraction recovered permanent grass,0.8,0.9

1323 DATA Fraction recovered rough grass,0.8,0.9

1324 DATA Fraction recovered urban area,0,0.5

1325 DATA Fraction recovered woodland,0.6,0.9

1326 DATA Fraction of tillage recovery harvested,0,1

1327 DATA Fraction of clover and grass recovery harvested,0,1

1328 DATA Fraction of permanent grass recovery harvested,0,1

1329 DATA Fraction of rough grazing recovery harvested,0,1

1330 DATA Fraction of urban recovery harvested,0,1

1331 DATA Fraction of woodland recovery harvested,0,1

1332 RESTORE 1302

1334 READ WM,WV

1336 FOR I=1 TO 6:READ NF(I):NEXT I

1340 FOR I=1 TO 5:READ WN(I):NEXT I

1344 FORI=1 TO 6:READ CF(I):NEXT I

1346 FOR I=1 TO 6:READ CH(I):NEXT I

1348 PRINT:Q$="Do you want to check the basic data constants"

1352 GOSUB 1100:ON R GOTO 1356,1398

1356 PRINT:READ Q$,R1$,R2$,R3$

1358 READ R$,MN,MX:PRINT R$;TAB(40);WM;:GOSUB 1100

1359 ON R GOTO 1361,1360

1360 PRINT:PRINT R1$;:GOSUB 1200:WM=R

1361 READ R$,MN,MX:PRINT R$;TAB(40);WV;:GOSUB 1100
```

```
1362 ON R GOTO 1364,1363

1363 PRINT:PRINT R1$;:GOSUB 1200:WV=R

1364 FOR I=1 TO 6:PRINT

1366 READ R$,MN,MX:PRINT R$;TAB(40);NF(I);R2$;:GOSUB 1100

1368 ON R GOTO 1372,1370

1370 PRINT:PRINT R1$;:GOSUB 1200:NF(I)=R

1372 NEXT I

1374 FOR I=1 TO 5:PRINT

1376 READ R$,MN,MX:PRINT R$;TAB(40);WN(I);R3$;:GOSUB 1100

1378 ON R GOTO 1382,1380

1380 PRINT:PRINT R1$;:GOSUB 1200:WN(I)=R

1382 NEXT I

1384 FOR I=1 TO 6:PRINT

1386 READ R$,MN,MX:PRINT R$;TAB(50);CF(I);:GOSUB 1100

1388 ON R GOTO 1392,1390

1390 PRINT:PRINT R1$;:GOSUB 1200:CF(I)=R

1392 NEXT I

1393 FOR I=1 TO 6:PRINT

1394 READ R$,MN,MX:PRINT R$;TAB(50);CH(I);:GOSUB 1100

1395 ON R GOTO 1397,1396

1396 PRINT:PRINT R1$;:GOSUB 1200:CH(I)=R

1397 NEXT I

1398 RETURN

1400 REM Routine to dimension minor arrays

1401 REM ***********************************************************

1404 DIM LA(6),NF(6),PP(5),WN(5),FA(4),CF(6),CH(6)

1408 DIM LU(NU),VU(NU),VT(NU)

1412 N2=256+48+2*NU

1416 RETURN

1500 REM Routine to dimension main data storage arrays
```

```
1501 REM ***************************************************
1503 REM Dimension aquifer and soil characteristics arrays
1504 DIM MR(NS),PH(NS),SN(NS),TU(NS),PU(NS),DU(NS),TS(NS),PS(NS)
1505 DIM DS(NS),FF(NS),FI(NS),RF(NS),EV(NS),UN(NS),RN(NS)
1507 REM Dimension land use area arrays
1508 DIM TI(NS),CG(NS),PG(NS),RG(NS),UC(NS),WD(NS),TA(NS)
1511 REM Dimension population arrays
1512 DIM CA(NS),SH(NS),PI(NS),PY(NS),HM(NS)
1515 REM Dimension fertilizer application rate arrays
1516 DIM FT(NS),FC(NS),FP(NS),FR(NS)
1519 REM Dimension climatic arrays
1520 DIM RQ(NS),ET(NS)
1521 REM Dimension unsaturated zone model arrays
1522 DIM LG(NU,NS),VG(NU,NS)
1523 REM Dimension accumulator arrays
1524 DIM GC(NS),GV(NS),RC(NS),RV(NS)
1525 REM Calculate total storage requirement
1526 N1=37
1528 PRINT "Total data storage requirement = ";
1532 PRINT INT((N2+NS*(N1+2*NU))/256);"K bytes"
1536 PRINT:PRINT "Total available data storage  = ";
1540 PRINT AS;"K bytes"
1544 RETURN
1600 REM Routine to read data in from terminal
1601 REM ***************************************************
1602 DR=1:IF NI>1 THEN DR=DR+AU
1604 FOR NA =1 TO NS
1606 IF NI>1 THEN 1712
1608 PRINT:PRINT "Sub-area";NA;"data input":PRINT
1610 PRINT "Soil mobile nitrogen level (kg/ha)";TAB(50);
```

```
1611 MN=0:MX=200:GOSUB 1200:MR(NA)=R

1612 PRINT "Soil effective grain size (mm)";TAB(50);

1616 MN=2E-3:MX=2:GOSUB 1200:PH(NA)=R

1617 PRINT "Initial SOM nitrogen level (kg/ha)";TAB(50);

1618 MN=1000:MX=10000:GOSUB 1200:SN(NA)=R

1620 PRINT "Thickness of unsaturated zone (m)";TAB(50);

1624 MN=0.01:MX=100:GOSUB 1200:TU(NA)=R

1628 PRINT "Fractional porosity of unsaturated zone";TAB(50);

1632 MN=0.001:MX=0.6:GOSUB 1200:PU(NA)=R

1636 PRINT "Unsat. zone fraction denitrified";TAB(50);

1640 MN=0:MX=0.5:GOSUB 1200:DU(NA)=R

1644 PRINT "Thickness of saturated zone (m)";TAB(50);

1648 MN=1:MX=200:GOSUB 1200:TS(NA)=R

1652 PRINT "Fractional porosity of saturated zone";TAB(50);

1656 MN=0.001:MX=0.6:GOSUB 1200:PS(NA)=R

1660 PRINT "Sat. zone fraction denitrified";TAB(50);

1664 MN=0:MX=0.5:GOSUB 1200:DS(NA)=R

1668 PRINT "Fraction of direct fissure inflow";TAB(50);

1672 MN=0:MX=0.5:GOSUB 1200:FF(NA)=R

1673 PRINT "Direct runoff as fraction of rainfall";TAB(50);

1674 MN=0.01:MX=0.99:GOSUB 1200:FI(NA)=1-R

1676 PRINT "Average annual rainfall (mm)";TAB(50);

1680 MN=500:MX=1000:GOSUB 1200:RF(NA)=R

1684 PRINT "Average annual evapotranspiration (mm)";TAB(50);

1688 MN=200:MX=1000:GOSUB 1200:EV(NA)=R

1692 PRINT "Urban rain nitrogen content (mg/l)";TAB(50);

1696 MN=0:MX=10:GOSUB 1200:UN(NA)=R

1700 PRINT "Rural area rain nitrogen content (mg/l)";TAB(50);

1704 MN=0:MX=6:GOSUB 1200:RN(NA)=R

1712 PRINT:PRINT "Time increment number";NI:PRINT
```

```
1716 PRINT "Input all requested areas in thousands of hectares"

1720 PRINT "1 hectare is 10000 square metres":PRINT

1724 MN=0:MX=1000

1728 PRINT "Tillage crop area";TAB(50);:GOSUB 1200:TI(NA)=R

1732 PRINT "Clover and rotation grass area";TAB(50);

1733 GOSUB 1200:CG(NA)=R

1736 PRINT "Permanent grass area";TAB(50);

1737 GOSUB 1200:PG(NA)=R

1740 PRINT "Rough grazing area";TAB(50);:GOSUB 1200:RG(NA)=R

1744 PRINT "Urban area";TAB(50);:GOSUB 1200:UC(NA)=R

1748 PRINT "Woodland and other rural area";TAB(50);

1749 GOSUB 1200:WD(NA)=R

1752 PRINT:PRINT "Input all population figures in thousands"

1756 PRINT:MN=0:MX=5000

1760 PRINT "Cattle population";TAB(50);:GOSUB 1200:CA(NA)=R

1764 PRINT "Sheep population";TAB(50);:GOSUB 1200:SH(NA)=R

1768 PRINT "Pig population";TAB(50);:GOSUB 1200:PI(NA)=R

1772 PRINT "Poultry population";TAB(50);:GOSUB 1200:PY(NA)=R

1776 PRINT "Human population";TAB(50);:GOSUB 1200:HM(NA)=R

1780 PRINT:PRINT "Input fertilizer application rates in kg/ha"

1784 PRINT:MN=0:MX=400

1788 PRINT "Tillage crop N application";TAB(50);

1789 GOSUB 1200:FT(NA)=R

1792 PRINT "Clover and rotation grass N application";TAB(50);

1793 GOSUB 1200:FC(NA)=R

1796 PRINT "Permanent grass N application";TAB(50);

1797 GOSUB 1200:FP(NA)=R

1800 PRINT "Rough grass N application ";TAB(50);

1801 GOSUB 1200:FR(NA)=R

1804 PRINT:PRINT "Input climatic variables in mm per time step"
```

```
1808 PRINT:MN=100:MX=2000

1812 PRINT "Rainfall in time interval";TAB(50);

1813 GOSUB 1200:RQ(NA)=R

1816 PRINT "Evapotranspiration in time interval";TAB(50);

1817 GOSUB 1200:ET(NA)=R

1820 NEXT NA

1824 RETURN

2000 REM Routine to store and read from DATA statements

2001 REM ***********************************************************

2002 REM Broadbalk wheat calibration data    0 kg/ha/a

2003 REM***********************************************************

2004 DATA 0,.2,3112

2005 DATA 5,.4,.09,95,.015,0,.15,.99,650,425,2,.9

2006 DATA 10,0,0,0,0,0,0,0,0,0,0,0,0,0,0,650,425

2007 REM Broadbalk wheat calibration data 145 kg/ha/a

2008 REM ***********************************************************

2009 DATA 1,.2,3414

2010 DATA 5,.4,.09,95,.015,0,.15,.99,650,425,2,.9

2011 DATA 10,0,0,0,0,0,0,0,0,0,0,145,0,0,0,650,425

2012 REM Park grass calibration data    0 kg/ha

2013 REM ***********************************************************

2014 DATA 0,.2,5557

2015 DATA 5,.4,.09,95,.015,0,.15,.99,650,425,2,.9

2016 DATA 0,0,10,0,0,0,0,0,0,0,0,0,0,0,0,650,425

2017 REM Park grass calibration data 145 kg/ha

2018 REM ***********************************************************

2019 DATA 0,.2,5822

2020 DATA 5,.4,.09,95,.015,0,.15,.99,650,425,2,.9

2021 DATA 0,0,10,0,0,0,0,0,0,0,0,0,145,0,650,425

2022 REM Park grass calibration data 290 kg/ha
```

```
2023 REM ***************************************************
2024 DATA 0,.2,7400
2025 DATA 5,.4,.09,95,.015,0,.15,.99,650,425,2,.9
2026 DATA 0,0,10,0,0,0,0,0,0,0,0,0,0,290,0,650,425
2027 REM Park grass calibration data 435 kg/ha
2028 REM ***************************************************
2029 DATA 0,.2,9075
2030 DATA 5,.4,.09,95,.015,0,.15,.99,650,425,2,.9
2031 DATA 0,0,10,0,0,0,0,0,0,0,0,0,0,435,0,650,425
2032 REM Hoosfield calibration data 0 kg/ha
2033 REM ***************************************************
2034 REM Change recovery from .58 for wheat to .73 for barley
2035 REM Change harvested from .56 for wheat to .62 for barley
2036 DATA 0,.5,2472
2037 DATA 5,.4,.1,95,.015,0,.15,.99,625,425,4,1.75
2038 DATA 10,0,0,0,0,0,0,0,0,0,0,0,0,0,0,625,425
2039 REM Hoosfield calibration data 48 kg/ha
2040 REM ***************************************************
2041 DATA 0,.5,2700
2042 DATA 5,.4,.1,95,.015,0,.15,.99,625,425,4,1.75
2043 DATA 10,0,0,0,0,0,0,0,0,0,48,0,0,0,625,425
2044 REM Hoosfield calibration data 96 kg/ha
2045 REM ***************************************************
2046 DATA 0,.5,3050
2047 DATA 5,.4,.1,95,.015,0,.15,.99,625,425,4,1.75
2048 DATA 10,0,0,0,0,0,0,0,0,0,96,0,0,0,625,425
2049 REM Hoosfield calibration data 144 kg/ha
2050 REM ***************************************************
2051 DATA 0,.5,3422
2052 DATA 5,.4,.1,95,.015,0,.15,.99,625,425,4,1.75
```

```
2053 DATA 10,0,0,0,0,0,0,0,0,0,144,0,0,0,625,425

2054 REM Whitehead calibration data example one-mixed grasses

2055 REM Have changed CF(.95 to .90),CH(.62 to .80)NF(85 to 91)

2056 REM ***************************************************

2057 REM ** To calibrate Whitehead data,remove REM from 3606 **

2058 REM ** and insert the value of SM in the data set ********

2060 DATA 0,.5,484

2061 DATA 1,.4,.6,95,.015,0,.15,.99,625,425,4,1.75

2062 DATA 0,0,10,0,0,0,0,0,0,0,0,0,0,340,0,625,425

2063 REM Whitehead calibration data example two-mixed grasses

2064 REM ***************************************************

2065 DATA 0,.5,484

2066 DATA 5,.4,.6,95,.015,0,.15,.99,625,425,4,1.75

2067 DATA 0,0,10,0,0,0,44,0,0,0,0,0,0,340,0,625,425

2069 REM ******Remove REM from 3522 if leaching = 0 *********

2070 REM Whitehead calibration data example three-clover/grass

2071 REM ***************************************************

2072 DATA 28,.20,7734

2073 DATA 5,.4,0,95,.015,0,.15,.99,625,425,4,1.75

2074 DATA 0,10,0,0,0,0,0,0,0,0,0,0,0,0,0,625,425

2075 REM Whitehead calibration data example four-clover/grass

2076 REM ***************************************************

2077 REM ************ NF changed from 284 to 275 *************

2079 DATA 33,.20,7734

2080 DATA 5,.4,0,95,.015,0,.15,.99,625,425,4,1.75

2081 DATA 0,10,0,0,0,0,36,0,0,0,0,0,0,0,0,625,425

2089 REM Unsat zone-New Hampshire North Field  1948 - 1974

2090 REM ***************************************************

2091 DATA 0,.2,3112

2092 DATA 20,.30,.05,95,.015,0,.10,.99,825,425,4,1.75
```

```
2093 DATA 10,0,0,0,0,0,0,0,0,0,0,75,0,0,0,825,425

2094 DATA 0,10,0,0,0,0,0,0,0,0,0,0,75,0,0,645,425

2095 DATA 10,0,0,0,0,0,0,0,0,0,0,140,0,0,0,885,425

2096 DATA 10,0,0,0,0,0,0,0,0,0,0,60,0,0,0,1000,425

2097 DATA 10,0,0,0,0,0,0,0,0,0,0,60,0,0,0,775,425

2098 DATA 10,0,0,0,0,0,0,0,0,0,0,45,0,0,0,650,425

2099 DATA 0,10,0,0,0,0,0,0,0,0,0,0,70,0,0,625,425

2100 DATA 0,10,0,0,0,0,0,0,0,0,0,0,225,0,0,825,425

2101 DATA 10,0,0,0,0,0,0,0,0,0,0,175,0,0,0,800,425

2102 DATA 0,10,0,0,0,0,0,0,0,0,0,0,150,0,0,825,425

2103 DATA 0,10,0,0,0,0,0,0,0,0,0,0,140,0,0,725,425

2104 DATA 10,0,0,0,0,0,0,0,0,0,0,170,0,0,0,730,425

2105 DATA 0,0,10,0,0,0,0,0,0,0,0,0,0,85,0,900,425

2106 DATA 0,0,0,10,0,0,0,0,0,0,0,0,0,0,200,1075,425

2107 DATA 10,0,0,0,0,0,0,0,0,0,0,60,0,0,0,765,425

2108 DATA 0,10,0,0,0,0,0,0,0,0,0,0,140,0,0,635,425

2109 DATA 0,10,0,0,0,0,0,0,0,0,0,0,150,0,0,535,425

2110 DATA 0,10,0,0,0,0,0,0,0,0,0,0,140,0,0,615,425

2111 DATA 10,0,0,0,0,0,0,0,0,0,0,0,0,0,965,425

2112 DATA 10,0,0,0,0,0,0,0,0,0,0,0,0,0,875,425

2113 DATA 10,0,0,0,0,0,0,0,0,0,0,0,0,0,0,800,425

2114 DATA 10,0,0,0,0,0,0,0,0,0,0,80,0,0,0,965,425

2115 DATA 10,0,0,0,0,0,0,0,0,0,0,110,0,0,0,715,425

2116 DATA 10,0,0,0,0,0,0,0,0,0,0,0,0,0,0,875,425

2117 DATA 10,0,0,0,0,0,0,0,0,0,0,150,0,0,0,725,425

2118 DATA 10,0,0,0,0,0,0,0,0,0,0,150,0,0,0,655,425

2119 DATA 10,0,0,0,0,0,0,0,0,0,0,120,0,0,0,745,425

2121 REM River water data calibration/verification- R.Stour

2122 REM ************************************************************

2123 DATA 0,.20,4650
```

```
2124 DATA 4,.25,.45,10,.30,0,.10,.95,560,300,4.5,2.5
2125 DATA 45,6,26,14,4,4,26,42,50,453,76,14,0,4,0,560,300
2126 DATA 47,7,24,12,4,5,28,39,42,466,77,15,0,4,0,560,300
2127 DATA 53,6,21,11,4,6,28,29,24,334,78,17,0,5,0,560,300
2128 DATA 52,8,19,11,4,7,29,27,17,297,79,18,2,5,0,560,300
2129 DATA 54,8,18,10,5,9,31,23,13,231,80,19,4,5,0,432,300
2130 DATA 55,8,17,10,5,9,30,19,14,256,82,20,5,5,0,560,300
2131 DATA 54,10,17,10,5,8,29,17,18,304,83,21,9,6,0,483,300
2132 DATA 54,10,17,10,5,8,29,16,18,335,84,22,12,7,0,560,300
2133 DATA 54,10,17,10,5,9,28,13,12,362,85,23,14,8,0,560,300
2134 DATA 55,10,16,10,5,7,28,12,17,457,86,24,17,9,0,508,300
2135 DATA 54,10,16,10,5,7,30,11,24,549,87,25,19,9,0,457,300
2136 DATA 56,8,16,10,5,8,33,11,27,580,88,26,22,10,0,533,300
2137 DATA 55,9,16,10,5,7,33,11,37,592,89,28,25,11,0,686,300
2138 DATA 56,9,16,9,5,8,31,12,45,600,92,29,26,12,0,622,300
2139 DATA 58,8,16,8,5,11,33,13,44,586,95,30,27,13,0,496,300
2140 DATA 57,8,15,8,6,10,30,13,53,543,97,32,27,13,0,610,300
2141 DATA 57,9,15,9,6,9,31,16,54,580,100,33,28,14,0,508,300
2142 DATA 57,8,15,8,6,9,33,17,52,618,103,34,29,15,0,533,300
2143 DATA 55,9,15,11,5,6,32,19,56,653,105,35,29,16,0,585,300
2144 DATA 56,8,15,11,6,6,31,21,59,706,108,44,35,18,1,788,300
2145 DATA 56,9,15,10,6,6,32,24,57,788,111,48,38,22,1,430,300
2146 DATA 57,7,14,10,6,6,34,23,55,824,113,54,42,24,2,737,300
2147 DATA 56,9,14,10,6,5,34,24,58,899,116,58,45,26,2,559,300
2148 DATA 57,8,14,10,6,7,32,23,66,831,118,65,50,29,2,483,300
2149 DATA 58,8,14,9,6,7,31,22,68,861,121,68,56,32,3,533,300
2150 DATA 59,8,13,9,6,7,30,22,77,886,124,72,59,34,3,450,300
2151 DATA 61,7,12,9,7,8,30,21,86,963,126,75,64,35,3,640,300
2152 DATA 63,5,12,8,7,8,29,20,86,965,129,79,70,38,3,560,300
2153 DATA 63,5,12,9,7,7,28,17,88,1070,132,82,77,45,3,570,300
```

```
2896 IF NI=1 THEN RESTORE 2121

2898 DR=2:IF NI>1 THEN DR=DR+AU

2900 FOR NA=1 TO NS

2902 IF NI>1 THEN 2920

2903 READ MR(NA)

2904 READ PH(NA),SN(NA),TU(NA),PU(NA),DU(NA),TS(NA),PS(NA)

2908 READ DS(NA),FF(NA),FI(NA),RF(NA),EV(NA),UN(NA),RN(NA)

2920 READ TI(NA),CG(NA),PG(NA),RG(NA),UC(NA),WD(NA)

2924 READ CA(NA),SH(NA),PI(NA),PY(NA),HM(NA)

2928 READ FT(NA),FC(NA),FP(NA),FR(NA)

2932 READ RQ(NA),ET(NA)

2936 NEXT NA

2940 RETURN

3000 REM Routine to set up model data

3001 REM ****************************************************

3004 LA(1)=TI(NA):LA(2)=CG(NA):LA(3)=PG(NA):LA(4)=RG(NA)

3005 LA(5)=UC(NA):LA(6)=WD(NA)

3008 PP(1)=CA(NA):PP(2)=SH(NA):PP(3)=PI(NA):PP(4)=PY(NA)

3009 PP(5)=HM(NA)

3012 FA(1)=FT(NA):FA(2)=FC(NA):FA(3)=FP(NA):FA(4)=FR(NA)

3013 RQ=FI(NA)*RQ(NA)/1000:RR=(FI(NA)*RQ(NA)-ET(NA))/1000

3015 FOR I=1 TO N:LU(I)=LG(I,NA):VU(I)=VG(I,NA):NEXT I

3016 MR=MR(NA):SN=SN(NA):DU=DU(NA):DS=DS(NA):FF=FF(NA):TU=TU(NA)

3020 TS=TS(NA):PU=PU(NA):PS=PS(NA):PH=PH(NA):UN=UN(NA):RN=RN(NA)

3022 RO=(1-FI(NA))*RQ(NA)/1000

3024 RA=(FI(NA)*RF(NA)-EV(NA))/1000

3025 IF RR<0 THEN RR=0

3028 RETURN

3100 REM Routine to calculate rainfall input

3101 REM ****************************************************
```

```
3104 TA=0:FOR I=1 TO 6:TA=TA+LA(I):NEXT I

3108 UA=LA(5):RU=TA-UA

3112 RI=10*(RQ+RO)*(RN*RU+UN*UA)/TA

3116 RETURN

3200 REM Routine to calculate atmospheric fixation input

3201 REM ***********************************************************

3204 AF=0:FOR I=1 TO 6:AF=AF+NF(I)*LA(I):NEXT I

3206 AF=AF/TA

3207 K4=.01:K5=3

3208 FE=((AW+AF)/(K5*RI+FI))^K4

3210 AF=FE*AF

3212 RETURN

3300 REM Routine to calculate animal wastes input

3301 REM ***********************************************************

3304 AW=0:FOR I=1 TO 5:AW=AW+WN(I)*PP(I):NEXT I

3306 AW=AW-WN(5)*PP(5)

3308 AW=AW/TA:VL=WV*AW

3312 RETURN

3400 REM Routine to calculate inorganic fertilizer input

3401 REM ***********************************************************

3404 FI=0:FOR I=1 TO 4:FI=FI+FA(I)*LA(I):NEXT I

3408 FI=FI/TA

3412 RETURN

3500 REM Routine to calculate mobile nitrogen balance

3501 REM ***********************************************************

3502 K1=-.52

3503 K2=25

3504 K3=-.02:K6=0.04

3505 FS=K6*EXP(-(K5*RI+FI)^K1/SQR(PH))*RR/RA

3506 SM=FS*SN
```

254

```
3508 MR=MR+SM+RI+WM*(AW-VL)+FI

3512 CR=CF*MR*(K5*RI+FI)^K3:MR=MR-CR

3516 FM=K2*RR*SQR(PH)*(RR/RA)

3518 IF FM>20 THEN FM=20

3520 FM=FNA(FM)

3521 REM ******Remove REM from 3522 if leaching = 0 *********

3522 REM FM=0

3524 LN=FM*MR:MR=MR-LN

3526 LR=RO*LN/(RO+RR):LN=LN-LR

3528 RETURN

3600 REM Routine to calculate immobile nitrogen balance

3601 REM ***********************************************************

3604 SN=SN+AF+(1-WM)*(AW-VL)+(1-CH)*CR-SM

3605 REM ** To calibrate Whitehead data,remove REM from 3606 **

3606 REM SN=7734

3608 RETURN

3700 REM Routine to calculate crop recovery factors

3701 REM ***********************************************************

3704 CF=0:FOR I=1 TO 6:CF=CF+CF(I)*LA(I):NEXT I

3708 CH=0:FOR I=1 TO 6:CH=CH+CH(I)*LA(I):NEXT I

3712 CF=CF/TA:CH=CH/TA

3716 RETURN

4100 REM Routine to set up unsaturated zone model

4101 REM ***********************************************************

4104 X1=1-DU:X2=1-FF:X3=1-DS

4108 UT=RA*X2/PU:N=INT(TU/UT)

4112 IF N>NU THEN 4146

4116 LU=0:VI=UT

4120 FOR I=1 TO N:Y=I-1:VU(I)=UT:LU(I)=LN*(X1^Y)

4124 LU=LU+LU(I):NEXT I
```

```
4128 VU(N+1)=TU-N*UT:LU(N+1)=LU(N)*X1*VU(N+1)/VU(N)

4132 LU=LU+LU(N+1):LI=LU(N)+LU(N+1)-LU(N)*VU(N+1)/VU(N)

4136 VI=VI*PU/PS:LI=X1*LI:CU=0.1*LU/(TU*PU)

4138 LF=LN*FF:VF=VI*FF:LP=LI:VP=VI

4140 Y=TS/(VP+VF)

4142 LS=(LF+LP)*Y*(X3^(Y-1))

4144 RETURN

4146 PRINT:PRINT "Unsaturated zone array dimensioned too small"

4148 STOP:RETURN

4200 REM Routine to drain unsaturated zone

4201 REM ******************************************************

4202 X1=1-DU:X2=1-FF:X3=1-DS

4204 UT=RR*X2/PU

4208 LU=0:FOR I=1 TO N+1:II=N+3-I:VU(II)=VU(II-1)

4212 LU(II)=X1*LU(II-1):LU=LU+LU(II):NEXT I

4216 VU(1)=UT:LU(1)=LN:LU=LU+LU(1):VI=UT

4220 LI=0:FOR I=1 TO N+1:II=N+3-I

4224 LI=LI+LU(II):UT=UT-VU(II)

4228 IF UT>0 THEN 4234

4230 LU(II)=-UT*LU(II)/VU(II):VU(II)=-UT

4232 LI=LI-LU(II):I=N+1

4234 NEXT I:N=II-1

4236 VI=VI*PU/PS:LU=LU-LI

4240 RETURN

4300 REM Routine to set up saturated zone model

4301 REM ******************************************************

4302 DT=DS*LS+DU*LU

4304 LS=LS*X3:VS=TS

4308 LF=LN*FF:VF=VI*FF

4312 LP=LI:VP=VI
```

```
4316 LS=VS*(LS+LF+LP)/(VS+VF+VP)

4324 LN=LN-DT

4328 AC=0.1*(LS*RA/(VS*PS)+LR)/(RA+RO)

4332 RETURN

4400 REM Routine to print aquifer model output

4401 REM *********************************************************

4404 PRINT:PRINT:PRINT "Sub-area model output"

4406 PRINT "*********************":PRINT

4408 PRINT "Depth (m)      N load (kg/ha)  N conc (mg/l)"

4412 PRINT:FOR I=1 TO N+1

4414 VT(0)=0:VT(I)=VU(I)+VT(I-1)

4416 PRINT TAB(2);VT(I);TAB(16);LU(I);

4418 PRINT TAB(32);0.1*LU(I)/(VU(I)*PU):NEXT I

4420 PRINT:PRINT "Unsaturated zone overall"

4424 PRINT:PRINT TAB(2);TU;TAB(16);LU;TAB(32);0.1*LU/(TU*PU)

4426 PRINT:PRINT "Saturated zone overall"

4428 PRINT:PRINT TAB(2);TS;TAB(16);LS;TAB(32);0.1*LS/(TS*PS)

4432 PRINT:PRINT "Runoff overall"

4436 PRINT:PRINT TAB(16);LR;TAB(32);0.1*LR/RO

4440 PRINT "River water nitrogen"

4444 PRINT:PRINT TAB(16);LR+LS*RA/(VS*PS);TAB(32);AC:PRINT

4448 PRINT:RETURN

4500 REM Routine to save data for subsequent calculations

4501 REM *********************************************************

4504 MR(NA)=MR:SN(NA)=SN:TA(NA)=TA

4508 FOR I=1 TO N:VG(I,NA)=VU(I):LG(I,NA)=LU(I):NEXT I

4512 GV(NA)=100*RA/(RA+RO):RV(NA)=100-GV(NA)

4516 GC(NA)=0.1*LS/(VS*PS):RC(NA)=0.1*LR/RO

4520 RETURN

4600 REM Routine to print output for all sub-areas
```

```
4601 REM ***********************************************************

4604 PRINT:PRINT:PRINT "Catchment model output"

4606 PRINT "*********************":PRINT

4608 PRINT "Sub-area";TAB(16);"Groundwater";TAB(35);"Runoff";

4609 PRINT TAB(51);"Overall"

4612 A$="Conc     Vol"

4616 PRINT TAB(16);A$;TAB(32);A$;TAB(48);A$

4620 A$="mg/l      %"

4624 PRINT TAB(16);A$;TAB(32);A$;TAB(48);A$

4625 PRINT

4626 GC=0:GV=0:RC=0:RV=0

4628 FOR NA=1 TO NS

4632 PRINT TAB(3);NA;TAB(15);0.1*INT(10*GC(NA));TAB(23);

4633 PRINT 0.1*INT(10*GV(NA));TAB(31);0.1*INT(10*RC(NA));

4634 PRINT TAB(39);0.1*INT(10*RV(NA));TAB(47);

4635 PRINT 0.1*INT((GV(NA)*GC(NA)+RV(NA)*RC(NA))/10);TAB(55);100

4636 GC=GC+GC(NA)*GV(NA)*TA(NA):GV=GV+GV(NA)*TA(NA)

4640 RC=RC+RC(NA)*RV(NA)*TA(NA):RV=RV+RV(NA)*TA(NA)

4644 NEXT NA:PRINT

4652 PRINT "Overall";TAB(15);0.1*INT(10*GC/GV);TAB(23);

4653 PRINT 0.1*INT(1000*GV/(GV+RV));TAB(31);0.1*INT(10*RC/RV);

4654 PRINT TAB(39);0.1*INT(1000*RV/(GV+RV));TAB(47);

4655 PRINT 0.1*INT(10*(GC+RC)/(GV+RV));TAB(55);100

4656 PRINT

4660 RETURN

4700 REM Nitrogen balance print routine

4701 REM ***********************************************************

4704 IF NP>0 THEN 4716

4706 PRINT:PRINT:PRINT "Nitrogen balance model"

4707 PRINT "*********************":PRINT
```

```
4708 PRINT "Soil N levels";TAB(23);"Inputs";TAB(48);"Outputs"
4709 PRINT TAB(3);"kg/ha";TAB(23);"kg/ha";TAB(49);"kg/ha"
4710 PRINT "Immob";TAB(9);"Mob";TAB(14);"Atmos";TAB(20);"Waste";
4711 PRINT TAB(26);"Rain";TAB(32);"Fert";TAB(40);"Crop";TAB(46);
4712 PRINT "Volat";TAB(52);"Denit";TAB(58);"Leach"
4713 PRINT
4716 PRINT INT(SN);TAB(8);INT(MR);TAB(14);INT(AF);TAB(20);
4717 PRINT INT(AW);TAB(26);INT(RI);TAB(32);INT(FI);TAB(40);
4718 PRINT INT(CH*CR);TAB(46);INT(VL);TAB(52);INT(DT);TAB(58);
4719 PRINT INT(LN+LR)
4720 NP=NP+1
4724 IF NP=25 THEN NP=0
4728 RETURN
```

APPENDIX THREE

LISTING OF PROGRAM MINES, PLUS TYPICAL RUNTIME DIALOGUE

```
10 PRINT CHR$(12)

20 PRINT" PROG  MINE  -A SYSTEM FOR DETERMINING"

30 PRINT" THE LIKELY COMPOSITION OF WASTEWATER"

40 PRINT" FROM MINE WORKINGS AND TIPS."

50 PRINT"          Program by J.F.Bell"

60 PRINT

70 PRINT"Do you want a brief explanation of the program";

80 INPUT ZZ$

90 ZZ$=LEFT$(ZZ$,1):IF ZZ$="Y"ORZZ$="y"THEN GOSUB 1530

91 REM ************************************************

92 REM Datasets for question/answer routines

93 REM ************************************************

100 DATA GRAIN SIZE,Large brassy crystals

110 DATA Small visible crystals,Finely disseminated,.5,1,3

120 DATA HUMIDITY,100%,Moist/unknown,Dry,3,1,.01

130 DATA TEMPERATURE (CENTIGRADE),Much greater than 20

140 DATA Greater than 20,Less than 20,3,2,1

150 DATA DEPTH OF BURIAL OF PYRITE/COVER ON PYRITE

160 DATA Little/no cover,Cover more than one metre (clay)

170 DATA Deliberately covered in clay,3,.1,.01

180 DATA AMOUNT OF COMPACTION OF TIP/TIP FORMATION

190 DATA Loose tipping,Some compaction/grading,B.S.Compacted

200 DATA 3,1,.5,AMOUNT OF CARBONATE IN COUNTRY ROCK

210 DATA Lst/Dolomite present in excess,Lst/Dolomite absent

220 DATA Some carbonate present,.5,2,1,PERMEABILITY OF SOIL

230 DATA Heavily fissured/jointed,Impermeable (clay covering)

240 DATA Not significant,2,.1,1,CONCENTRATION OF OXYGEN PRESENT

250 DATA Fully aerated,Partially aerated,Anaerobic,3,1,.01
```

```
260 DATA BACTERIAL ACTIVITY,Obviously present

270 DATA Possibly present,Absent,3,1,.5

280 DATA SOURCE OF POLLUTION,Mainly spoil heaps,Mainly mines

285 DATA 2,1,1,.5,.5,.1,1,1,2,1.5

290 DATA DEPTH OF MINE WORKINGS,Shallow <100m,Deep >1000m

295 DATA 2,1,1,.5,1,.1,1,1,2,1

300 DATA VENTILATION OF MINES OR SPOIL,Good,Bad

305 DATA 2,1,1.5,1,2,.1,1,.5,1,.5

310 DATA SULPHUR CONTENT OF ORE/COAL,More than 3%,Less than 3%

315 DATA 1,2,1,1,1,1,.1,1,1,1

320 DATA pH OF GROUNDWATER,Less than 3.5,Greater than 3.5

330 DATA 1,2,2,.5,1,1,.5,.5,2,1

340 DATA CLAY/CARBONATE OBVIOUSLY PRESENT IN MINED ROCK,Yes,No

345 DATA 1,.5,.5,2,1,1,2,2,.5,1

350 DATA STATE OF MINING,Active,Ceased

355 DATA 1,1,1,1,2,1,1,1,1,.5

360 DATA SITE OF MINING,USA,UK,1.5,1,2,.25,1,.1,1,.5,1.5,1

361 REM **************************************************

362 REM Calculate probability of pollution occuring

363 REM **************************************************

370 FY=.5:NF=.5

380 FOR X1=1 TO 9:READ D1$

390 PRINT:PRINT D1$:PRINT

400 GOSUB 530

410 NEXT X1

411 REM **************************************************

412 REM Calculate probabilities of polluting waters

413 REM **************************************************

420 FOR JK=1 TO 5:P(JK)=.2:NEXT JK

430 FOR X3=1 TO 8:READ D3$
```

```
440 PRINT:PRINT D3$:PRINT

450 GOSUB 760

460 NEXT X3

465 GOSUB 1160

470 REM Prog nearly finished

480 PRINT:PRINT"Do you wish to begin again";:INPUT ZZ$

490 ZZ$=LEFT$(ZZ$,1):IF ZZ$="Y"ORZZ$="y"THEN 510

500 GOTO 520

510 RESTORE:GOTO 10

520 PRINT:PRINT "RUN COMPLETE":PRINT:END

525 REM ********************************************************

530 REM Subr to select answers to "factors" questions

535 REM ********************************************************

540 FOR II=1 TO 3:READ D2$:PRINT II;":";D2$:NEXT II

550 PRINT" 4: Don't know/Not applicable"

560 PRINT:PRINT"ENTER (1/2/3/4):";:INPUT X2$:X2=VAL(X2$)

570 IF X2$="/" THEN 520

580 IF X2>4 OR X2<1 THEN 560

585 FOR II=4 TO 6:READ D2$:D2=VAL(D2$)

586 IF (II-3)=X2 THEN F=D2

587 IF X2=4 THEN F=1

588 NEXT II

589 GOSUB 1085:RETURN

755 REM ********************************************************

760 REM Subr to assess the type of waste expected

765 REM ********************************************************

770 FOR JJ=1 TO 2:READ D4$:PRINT JJ;":";D4$:NEXT JJ

780 PRINT" 3: Don't know/Not applicable"

790 PRINT:PRINT"ENTER (1/2/3):";:INPUT X4$:X4=VAL(X4$)

800 IF X4$="/" THEN 520
```

263

```
810 IF X4<1 OR X4>3 THEN 790

815 FOR JJ=3 TO 12:READ D4$:F(JJ-2)=VAL(D4$):NEXT JJ

816 FOR MM=1 TO 5

817 IF X4=2 THEN F(MM)=F(MM+5)

818 IF X4=3 THEN F(MM)=1

819 NEXT MM

820 GOSUB 1115:RETURN

1085 REM ***********************************************

1090 REM Subroutine to establish FY + NF

1095 REM ***********************************************

1100 FY=F*FY:FZ=FY+NF:FY=FY/FZ:NF=NF/FZ

1110 RETURN

1115 REM ***********************************************

1120 REM Subroutine to re-calculate probabilities

1125 REM ***********************************************

1126 SU=0

1130 FOR KK=1 TO 5

1140 P(KK)=P(KK)*F(KK):SU=SU+P(KK):NEXT KK

1150 FOR KL=1 TO 5:P(KL)=P(KL)/SU:NEXT KL:RETURN

1155 REM ***********************************************

1160 REM Subr to print out results

1165 REM ***********************************************

1170 P1=INT(P(1)*100):P2=INT(P(2)*100):P3=INT(P(3)*100)

1180 P4=INT(P(4)*100):P5=INT(P(5)*100)

1190 PRINT:PRINT"FY=";FY:PRINT

1200 IF FY>.5 THEN 1230

1210 IF FY<.5 THEN 1370

1220 IF FY=.5 THEN 1400

1230 AJ$=" FAIRLY "

1240 IF FY>.6 THEN AJ$=" MODERATELY "
```

```
1250 IF FY>.7 THEN AJ$=" "

1260 IF FY>.8 THEN AJ$=" HIGHLY "

1270 IF FY>.9 THEN AJ$=" EXTREMELY "

1280 PRINT:PRINT"POLLUTED MINEWATER IS";AJ$;

1290 PRINT"LIKELY IN THIS CASE":PRINT

1300 PRINT"PROBABILITIES (EXPRESSED AS %)......."

1310 PRINT"     FREE ACID (SULPHURIC)       ";P1;"%"

1320 PRINT"     ACIDIC CONTAINING FE(2+)    ";P2;"%"

1330 PRINT"     ACIDIC CONTAINING FE(3+)    ";P3;"%"

1340 PRINT"     NEUTRAL CONTAINING FE(2+)   ";P4;"%"

1350 PRINT"     EXCESS FE(3+) IN SUSPENSION ";P5;"%"

1360 PRINT:GOTO 470

1370 PRINT:PRINT"MINEWATER QUALITY IS UNLIKELY TO BE A POLL";

1380 PRINT"UTION PROBLEM GIVEN":PRINT"THESE CONDITIONS":PRINT

1390 GOTO 470

1400 IF P(1)>P(2) THEN PC=P(1)

1410 IF P(1)<P(2) THEN PC=P(2)

1420 IF PC<P(3) THEN PC=P(3)

1430 IF PC<P(4) THEN PC=P(4)

1440 IF PC<P(5) THEN PC=P(5)

1450 PRINT"POLLUTED MINE WATER IS A POSSIBILITY"

1460 PRINT"----MOST LIKELY TYPE IS........."

1470 IF PC=P(1) THEN PRINT"FREE ACID"

1480 IF PC=P(2) THEN PRINT"ACIDIC PLUS FE(2+)"

1490 IF PC=P(3) THEN PRINT"ACIDIC PLUS FE(3+)"

1500 IF PC=P(4) THEN PRINT"NEUTRAL PLUS FE(2+)"

1510 IF PC=P(5) THEN PRINT"EXCESS FE(3+) IN SUSPENSION"

1520 RETURN

1525 REM ********************************************************

1530 REM Subr giving explanation of program
```

```
1535 REM ****************************************************
1540 PRINT CHR$(12)
1550 PRINT"This program predicts the likely";
1560 PRINT" type of wastewater from coal"
1570 PRINT" mines and tips based on a serie";
1580 PRINT"s of multiple choice questions"
1590 PRINT"and answers.":PRINT
1600 PRINT"     The different minewaters li";
1610 PRINT"kely to be encountered are"
1620 PRINT"listed (in terms of acidity and ";
1630 PRINT"iron content), in a paper"
1640 PRINT"presented by Glover(1976) at a s";
1650 PRINT"ymposium in Katowice on mine"
1660 PRINT"drainage pollution.":PRINT
1670 PRINT"     The program consists of two";
1680 PRINT" sections:"
1690 PRINT"     (1) The probability of brea";
1700 PRINT"kdown of pyritic material giving"
1710 PRINT"rise to mine drainage pollution ";
1720 PRINT"problems."
1730 PRINT"     (2) The probability of any ";
1740 PRINT"given type of drainage, given"
1750 PRINT"the state of the workings.":PRINT
1760 PRINT"     A number, F, is printed wit";
1770 PRINT"h the final prediction. If this"
1780 PRINT"number approaches unity then the";
1790 PRINT" probability of pollution is"
1800 PRINT"high.":PRINT
1810 PRINT "TYPE RETURN TO START RUN";:INPUT Z$
1820 PRINT CHR$(12):RETURN
```

PROG   MINE   -A SYSTEM FOR DETERMINING
THE LIKELY COMPOSITION OF WASTEWATER
FROM MINE WORKINGS AND TIPS.
                    Program by J.F.Bell

Do you want a brief explanation of the program? Y

This program predicts the likely type of wastewater from coal
 mines and tips based on a series of multiple choice questions
and answers.

        The different minewaters likely to be encountered are
listed (in terms of acidity and iron content), in a paper
presented by Glover(1976) at a symposium in Katowice on mine
drainage pollution.

        The program consists of two sections:
        (1) The probability of breakdown of pyritic material giving
rise to mine drainage pollution problems.
        (2) The probability of any given type of drainage, given
the state of the workings.

        A number, F, is printed with the final prediction. If this
number approaches unity then the probability of pollution is
high.

GRAIN SIZE

    1 :Large brassy crystals
    2 :Small visible crystals
    3 :Finely disseminated
    4: Don't know/Not applicable

ENTER (1/2/3/4):? 4

HUMIDITY

    1 :100%
    2 :Moist/unknown
    3 :Dry
    4: Don't know/Not applicable

ENTER (1/2/3/4):? 1

TEMPERATURE (CENTIGRADE)

    1 :Much greater than 20
    2 :Greater than 20
    3 :Less than 20
    4: Don't know/Not applicable

ENTER (1/2/3/4):? 2

DEPTH OF BURIAL OF PYRITE/COVER ON PYRITE

    1 :Little/no cover
    2 :Cover more than one metre (clay)
    3 :Deliberately covered in clay
    4: Don't know/Not applicable

ENTER (1/2/3/4):? 1

AMOUNT OF COMPACTION OF TIP/TIP FORMATION

    1 :Loose tipping
    2 :Some compaction/grading
    3 :B.S.Compacted
    4: Don't know/Not applicable

ENTER (1/2/3/4):? 4

AMOUNT OF CARBONATE IN COUNTRY ROCK

    1 :Lst/Dolomite present in excess
    2 :Lst/Dolomite absent
    3 :Some carbonate present
    4: Don't know/Not applicable

ENTER (1/2/3/4):? 3

PERMEABILITY OF SOIL

```
1 :Heavily fissured/jointed
2 :Impermeable (clay covering)
3 :Not significant
4: Don't know/Not applicable
```

ENTER (1/2/3/4):? 1

CONCENTRATION OF OXYGEN PRESENT

```
1 :Fully aerated
2 :Partially aerated
3 :Anaerobic
4: Don't know/Not applicable
```

ENTER (1/2/3/4):? 1

BACTERIAL ACTIVITY

```
1 :Obviously present
2 :Possibly present
3 :Absent
4: Don't know/Not applicable
```

ENTER (1/2/3/4):? 2

SOURCE OF POLLUTION

```
1 :Mainly spoil heaps
2 :Mainly mines
3: Don't know/Not applicable
```

ENTER (1/2/3):? 2

DEPTH OF MINE WORKINGS

```
1 :Shallow <100m
2 :Deep >1000m
3: Don't know/Not applicable
```

ENTER (1/2/3):? 1

VENTILATION OF MINES OR SPOIL

```
1 :Good
2 :Bad
3: Don't know/Not applicable
```

ENTER (1/2/3):? 1

SULPHUR CONTENT OF ORE/COAL

  1 :More than 3%
  2 :Less than 3%
  3: Don't know/Not applicable

ENTER (1/2/3):? 3

pH OF GROUNDWATER

  1 :Less than 3.5
  2 :Greater than 3.5
  3: Don't know/Not applicable

ENTER (1/2/3):? 3

CLAY/CARBONATE OBVIOUSLY PRESENT IN MINED ROCK

  1 :Yes
  2 :No
  3: Don't know/Not applicable

ENTER (1/2/3):? 2

STATE OF MINING

  1 :Active
  2 :Ceased
  3: Don't know/Not applicable

ENTER (1/2/3):? 2

SITE OF MINING

  1 :USA
  2 :UK
  3: Don't know/Not applicable

ENTER (1/2/3):? 2

FY= .990826

POLLUTED MINEWATER IS EXTREMELY LIKELY IN THIS CASE

PROBABILITIES (EXPRESSED AS %).......
        FREE ACID (SULPHURIC)   0 %
        ACIDIC CONTAINING FE(2+)   34 %
        ACIDIC CONTAINING FE(3+)   25 %
        NEUTRAL CONTAINING FE(2+)   12 %
        EXCESS FE(3+) IN SUSPENSION   25 %

Do you wish to begin again? N

RUN COMPLETE

READY

APPENDIX FOUR

LISTING OF PROGRAM DIFAN, PLUS Z80 ASSEMBLER ROUTINES

```
100 REM Main program DIFAN (C) M.J.Reeves/J.F.Bell 1981

110 REM ------------------------------------------------

120 REM GOSUB 1630:END

130 RESTORE 1070:GOSUB 1070

140 GOSUB 310

150 PRINT "The following simulations are available :":PRINT

160 PRINT TAB(5);"1. Landfill site with regional gradient"

170 PRINT TAB(5);"2. Injection well section"

180 PRINT TAB(5);"3. Contaminated wells plan"

190 PRINT TAB(5);"4. Saline wedge"

200 PRINT TAB(5);"5. Terminate program"

210 PRINT:PRINT "Enter choice (1-5)";:INPUT A$:A=VAL(A$)

220 IF A>5 OR A<1 THEN 210

230 ON A GOTO 240,250,260,270,280

240 GOSUB 350:GOSUB 310:GOSUB 610:GOSUB 440:GOSUB 490:GOTO 140

250 GOSUB 350:GOSUB 310:GOSUB 700:GOSUB 440:GOSUB 490:GOTO 140

260 GOSUB 350:GOSUB 310:GOSUB 780:GOSUB 440:GOSUB 490:GOTO 140

270 GOSUB 350:GOSUB 310:GOSUB 840:GOSUB 440:GOSUB 490:GOTO 140

280 PRINT:END

290 REM Header routine

300 REM --------------

310 PRINT CHR$(12)

320 PRINT "DIFAN - diffusion/dispersion animation program"

330 PRINT "(C) M.J.Reeves/J.F.Bell 1981":PRINT

340 RETURN

350 REM Set limits routine

360 REM ------------------

370 POKE 8192,0:POKE 8193,242     :REM Part screen  F200H
```

```
380 POKE 8194,128:POKE 8195,247   :REM End of video F780H

390 POKE 8196,64:POKE 8197,0      :REM Video row length 40H

400 POKE 8198,7                   :REM Number plot chars

410 AD=8199:RETURN

420 REM Read routine

430 REM ------------

440 FOR I=0 TO 3:READ DB:POKE AD+I,DB:NEXT I:READ N:POKE AD+4,N

450 FOR I=1 TO 2*N:READ A:POKE AD+4+I,A:NEXT I

460 RETURN

470 REM Simulation routine

480 REM ------------------

490 FOR I=1 TO 1:PRINT:NEXT I

500 ST=0:POKE 260,0:POKE 261,33:U=USR(0)

510 ST=ST+1:PRINT CHR$(23);T$;TAB(45);"Step";ST;"          "

520 POKE 260,232:POKE 261,233:U=USR(0)

530 POKE 260,67:POKE 261,33

540 FOR I=1 TO 15:U=USR(0):NEXT I

550 REM POKE 260,0:POKE 261,128:U=USR(0)

560 PRINT CHR$(23);T$;TAB(45);"Continue";:INPUT A$

570 A$=LEFT$(A$,1):IF A$="y" OR A$="Y" THEN 510

580 RETURN

590 REM Landfill site data

600 REM ------------------

610 T$="Landfill site simulation"

620 DATA 1,255,170,170,14

630 DATA 92,242,93,242,94,242,95,242

640 DATA 96,242,97,242,98,242,99,242

650 DATA 157,242,158,242,159,242,160,242

660 DATA 161,242,162,242

670 RESTORE 620:RETURN
```

```
680 REM Borehole section data

690 REM --------------------

700 T$="Contaminated well section simulation"

710 DATA 255,255,255,255,12

720 DATA 96,242,160,242,224,242,32,243

730 DATA 96,243,160,243,224,243,32,244

740 DATA 96,244,160,244,224,244,32,245

750 RESTORE 710:RETURN

760 REM Borehole plan data

770 REM ------------------

780 T$="Contaminated wells plan simulation"

790 DATA 255,1,68,68,1

800 DATA 136,244

810 RESTORE 790:RETURN

820 REM Saline wedge data

830 REM ------------------

840 T$="Saline intrusion simulation"

850 DATA 170,255,255,255,81

860 DATA 64,242,128,242,192,242,0,243

870 DATA 1,243,64,243,65,243,128,243

880 DATA 129,243,192,243,193,243,194,243

890 DATA 0,244,1,244,2,244,64,244

900 DATA 65,244,66,244,67,244,128,244

910 DATA 129,244,130,244,131,244,192,244

920 DATA 193,244,194,244,195,244,0,245

930 DATA 1,245,2,245,3,245,4,245

940 DATA 64,245,65,245,66,245,67,245

950 DATA 68,245,128,245,129,245,130,245

960 DATA 131,245,132,245,192,245,193,245

970 DATA 194,245,195,245,196,245,197,245
```

```
980 DATA 0,246,1,246,2,246,3,246

990 DATA 4,246,5,246,64,246,65,246

1000 DATA 66,246,67,246,68,246,69,246

1010 DATA 128,246,129,246,130,246,131,246

1020 DATA 132,246,133,246,134,246,192,246

1030 DATA 193,246,194,246,195,246,196,246

1032 DATA 197,246,198,246,0,247,1,247

1034 DATA 2,247,3,247,4,247,5,247

1036 DATA 6,247

1040 RESTORE 850:RETURN

1050 REM Machine code animation routine in DATA

1060 REM --------------------------------------

1070 DATA 0,0,0,0,0,0,0,0

1080 DATA 0,0,0,1,0,0,0,0

1090 DATA 0,2,0,0,0,0,64,0

1100 DATA 0,32,2,0,0,32,2,0

1110 DATA 34,0,68,0,34,0,68,0

1120 DATA 17,68,17,68,17,68,17,68

1130 DATA 85,170,85,170,85,170,85,170

1140 DATA 255,255,255,255,255,255,255,255

1150 DATA 0,0,0,0,0,0,0,255

1160 DATA 255,0,0,0,0,0,0,0

1170 DATA 33,176,32,17,0,252,1,80

1180 DATA 0,237,176,42,0,32,237,91

1190 DATA 2,32,237,75,4,32,229,54

1200 DATA 128,35,124,186,32,249,125,187

1210 DATA 32,245,235,237,66,17,2,32

1220 DATA 235,115,35,114,225,65,58,6

1230 DATA 32,198,129,119,60,18,61,35

1240 DATA 19,16,248,17,0,32,235,115
```

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```
1250 DATA 35,114,201,237,95,50,60,1
1260 DATA 42,4,32,229,42,0,32,229
1270 DATA 229,205,126,33,225,126,254,128
1280 DATA 40,7,229,205,148,33,205,232
1290 DATA 33,209,193,35,235,9,237,82
1300 DATA 40,9,25,237,66,235,197,213
1310 DATA 229,24,222,42,2,32,237,82
1320 DATA 200,197,213,213,24,211,58,6
1330 DATA 32,198,128,79,58,11,32,71
1340 DATA 121,33,12,32,94,35,86,35
1350 DATA 18,16,249,201,205,153,217,241
1360 DATA 225,209,193,197,213,229,245,58
1370 DATA 60,1,203,71,40,15,58,7
1380 DATA 32,7,50,7,32,48,19,35
1390 DATA 205,34,34,24,13,58,8,32
1400 DATA 7,50,8,32,48,4,43,205
1410 DATA 22,34,58,60,1,203,79,65
1420 DATA 40,15,58,9,32,7,50,9
1430 DATA 32,208,35,16,253,205,61,34
1440 DATA 201,58,10,32,7,50,10,32
1450 DATA 208,43,16,253,205,47,34,201
1460 DATA 126,71,241,209,245,26,184,40
1470 DATA 33,56,9,61,4,184,40,26
1480 DATA 56,2,24,247,60,5,184,40
1490 DATA 17,56,249,0,0,0,0,0
1500 DATA 0,0,0,0,0,254,135,32
1510 DATA 1,61,119,18,235,201,229,213
1520 DATA 55,63,237,82,209,225,208,35
1530 DATA 35,201,229,213,235,9,43,237
1540 DATA 82,209,225,208,43,43,201,229
```

```
1550 DATA 237,91,0,32,55,63,237,82

1560 DATA 225,208,9,9,201,229,237,91

1570 DATA 2,32,27,235,55,63,237,82

1580 DATA 225,208,63,237,66,237,66,201

1590 AD=8368:FOR I=0 TO 415:READ A:POKE AD+I,A:NEXT I

1600 RETURN

1610 REM Temporary machine code store routine

1620 REM -----------------------------------

1630 LS=8448:LN=25

1640 FOR I=12 TO 20:PRINT LN;" DATA ";:LN=LN+1

1650 FOR J=0 TO 7:A$=STR$(PEEK(LS+16*I+J)):N=LEN(A$)

1660 A$=RIGHT$(A$,N-1):IF J<>7 THEN A$=A$+","

1670 PRINT A$;:NEXT J:PRINT:PRINT LN;" DATA ";:LN=LN+1

1680 FOR J=8 TO 15:A$=STR$(PEEK(LS+16*I+J)):N=LEN(A$)

1690 A$=RIGHT$(A$,N-1):IF J<>15 THEN A$=A$+","

1700 PRINT A$;:NEXT J:PRINT:NEXT I

1710 RETURN
```

```
          GLOBAL   RAND      ;BASIC rand no store addr

RAND      EQU      013CH

          GLOBAL   RANDOM    ;BASIC rand no generator

RANDOM    EQU      0D999H

          ORG      02000H    ;Set origin

LIMS      DEFW     0F080H,0F780H,00040H

PKEY      DEFB     007H

RIGHT     DEFB     0FFH

LEFT      DEFB     0FFH

DOWN      DEFB     0FFH

UP        DEFB     0FFH

POLS      DEFS     000A5H

CHARS     DEFB     <8,000H,>

          DEFB     <3,000H,>,001H,<4,000H,>

          DEFB     000H,002H,<4,000H,>,040H,000H

          DEFB     <2,000H,020H,002H,000H,>

          DEFB     <2,022H,000H,044H,000H,>

          DEFB     <4,011H,044H,>

          DEFB     <4,055H,0AAH,>

          DEFB     <8,0FFH,>

          DEFB     <7,000H,>,0FFH

          DEFB     0FFH,<7,000H,>

;SETUP  - clear screen and set up graphics

;-----------------------------------------------

SETUP     LD HL,CHARS        ;Get storage addr

          LD DE,0FC00H        ;Get user graphics addr

          LD BC,00050H        ;Get size of storage area

          LDIR                ;Copy storage to graphics
```

```
                LD HL,(LIMS)        ;Get video top addr

                LD DE,(LIMS+02H)    ;Get video base addr

                LD BC,(LIMS+04H)    ;Get video row len

                PUSH HL             ;Save video top addr
J0              LD (HL),080H        ;Insert blank char

                INC HL              ;Update video addr

                LD A,H              ;Test high byte

                CP D
J1              JR NZ,J0-J1

                LD A,L              ;Test low byte

                CP E
J2              JR NZ,J0-J2

                EX DE,HL            ;Save video base addr

                SBC HL,BC           ;Reduce by one row

                LD DE,LIMS+02H      ;Get video base limit addr

                EX DE,HL            ;Save new video base addr

                LD (HL),E           ;Save low byte

                INC HL              ;Next byte

                LD (HL),D           ;Save high byte

                POP HL              ;Get video top addr

                LD B,C              ;Set up col counter

                LD A,(PKEY)         ;Get no scale pixs

                ADD A,081H          ;Set ASCII char
J3              LD (HL),A           ;Draw upper bdry

                INC A               ;Next ASCII char

                LD (DE),A           ;Draw lower bdry

                DEC A               ;Reset ASCII char

                INC HL              ;Next upper col

                INC DE              ;Next lower col
J4              DJNZ J3-J4          ;Next col
```

```
        LD DE,LIMS

        EX DE,HL        ;Save new video top addr

        LD (HL),E       ;Save low byte

        INC HL          ;Next byte

        LD (HL),D       ;Save high byte

        RET

;DIFUSE - animated video simulation of diffusion

;--------------------------------------------------

DIFUSE  LD A,R          ;Get refresh reg

        LD (RAND),A     ;Seed rand no generator

        LD HL,(LIMS+04H);Get video row len

        PUSH HL         ;Save it

        LD HL,(LIMS)    ;Get init row start addr

        PUSH HL         ;Save it

        PUSH HL         ;Init current pix addr

K0      CALL PIXREF     ;Refresh source

        POP HL          ;Get current pix addr

        LD A,(HL)       ;Find curr pix ASCII char

        CP 080H         ;Test for blank

KJ      JR Z,KS-KJ      ;Skip

        PUSH HL         ;Save curr pix addr

        CALL PIXDIS     ;Displace current pix

        CALL PIXALT     ;Update curr and disp pixs

KS      POP DE          ;Get curr row start addr

        POP BC          ;Get video row len

        INC HL          ;Update current pix addr

        EX DE,HL

        ADD HL,BC       ;Find next row start addr

        SBC HL,DE       ;Test for new row

K1      JR Z,K3-K1
```

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```
            ADD HL,DE          ;Restore old row addr

            SBC HL,BC

            EX DE,HL

            PUSH BC            ;Save video row len

            PUSH DE            ;Save curr row start addr

            PUSH HL            ;Save current pix addr

K2          JR K0-K2           ;Next pix

K3          LD HL,(LIMS+02H)   ;Get video base addr

            SBC HL,DE          ;Test for complete pass

            RET Z              ;END

            PUSH BC            ;Save video row len

            PUSH DE            ;Save curr row start addr

            PUSH DE            ;Save current pix addr

K4          JR K0-K4           ;Next row

;PIXREF - a routine to refresh pollution source

;------------------------------------------------

PIXREF      LD A,(PKEY)        ;Get no scale pix

            ADD A,080H         ;Find high pix ASCII char

            LD C,A             ;Save it

            LD A,(POLS)        ;Get no source pix

            LD B,A             ;Save it

            LD A,C             ;Get high scale pix

            LD HL,POLS+01H     ;Get source addr location

N0          LD E,(HL)          ;Get low addr byte

            INC HL             ;Next byte

            LD D,(HL)          ;Get high addr byte

            INC HL             ;Next byte

            LD (DE),A          ;Refresh source

N1          DJNZ N0-N1         ;Next source addr

            RET
```

```
;PIXDIS - a routine to displace video pixels
;---------------------------------------------
PIXDIS     CALL RANDOM        ;Call random disp routine

           POP AF             ;Get sub ret addr

           POP HL             ;Get current pix addr

           POP DE             ;Get curr row start addr

           POP BC             ;Get video row len

           PUSH BC            ;Save video row len

           PUSH DE            ;Save curr row start addr

           PUSH HL            ;Save current pix addr

           PUSH AF            ;Save sub ret addr

           LD A,(RAND)        ;Get random number

           BIT 0,A            ;Test bit 0
L0         JR Z,L2-L0         ;Left or right?

           LD A,(RIGHT)       ;Get right data byte

           RLCA               ;Rotate data left

           LD (RIGHT),A       ;Save new data byte
LR         JR NC,L3-LR        ;Displace?

           INC HL             ;Right

           CALL BDRYR         ;Apply bdry cond
L1         JR L3-L1           ;Now check row
L2         LD A,(LEFT)        ;Get left data byte

           RLCA               ;Rotate data left

           LD (LEFT),A        ;Save new data byte
LL         JR NC,L3-LL        ;Displace?

           DEC HL             ;Left

           CALL BDRYL         ;Apply bdry cond
L3         LD A,(RAND)        ;Get random number

           BIT 1,A            ;Test bit 1

           LD B,C             ;Init row count
```

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```
L4        JR Z,L7-L4        ;Up or down?

          LD A,(DOWN)        ;Get down data byte

          RLCA               ;Rotate data left

          LD (DOWN),A        ;Save new data byte

          RET NC             ;Displace?

L5        INC HL             ;Down

L6        DJNZ L5-L6         ;Row count complete?

          CALL BDRYD         ;Apply bdry cond

          RET

L7        LD A,(UP)          ;Get up data byte

          RLCA               ;Rotate data left

          LD (UP),A          ;Save new data byte

          RET NC             ;Displace?

L8        DEC HL             ;Up

L9        DJNZ L8-L9         ;Row count complete?

          CALL BDRYU         ;Apply bdry cond

          RET

;PIXALT - a routine to update video pixels

;-------------------------------------------

PIXALT    LD A,(HL)          ;Get disp pix ASCII char

          LD B,A             ;Save it

          POP AF             ;Get sub ret addr

          POP DE             ;Get current pix addr

          PUSH AF            ;Save sub ret addr

          LD A,(DE)          ;Get curr pix ASCII char

          CP B               ;Compare curr & disp chars

M0        JR Z,MB-M0         ;current = disp

M1        JR C,M6-M1         ;current < disp

M2        DEC A              ;current > disp

          INC B
```

```
                CP B            ;Test for equalisation

M3              JR Z,MB-M3      ;current = disp

M4              JR C,M6-M4      ;current < disp

M5              JR M2-M5        ;current > disp

M6              INC A           ;current < disp

                DEC B

                CP B            ;Test for equalisation

M7              JR Z,MB-M7      ;current = disp

M8              JR C,M6-M8      ;current < disp

                LD C,A          ;current > disp

                LD A,(RAND)     ;Get random number

                BIT 2,A         ;Test bit 2

                LD A,C          ;Get current char back

M9              JR Z,MA-M9

                DEC A           ;Degrade ASCII char

MA              CP 087H         ;Check for source char

MC              JR NZ,MB-MC     ;No

                DEC A           ;Yes

MB              LD (HL),A       ;Display modified disp pix

                LD (DE),A       ;Display modified curr pix

                EX DE,HL        ;Save current pix addr

                RET

;BDRYL - a routine for LHS boundary condition

;----------------------------------------------

BDRYL           PUSH HL         ;Save current disp addr

                PUSH DE         ;Save curr row start addr

                SCF             ;Ensure carry off

                CCF

                SBC HL,DE       ;Test

                POP DE          ;Get them back
```

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```
            POP HL

            RET NC          ;In

            INC HL          ;Out

            INC HL

            RET
```

;BDRYR - a routine for RHS boundary condition

;---

```
BDRYR       PUSH HL         ;Save current disp addr

            PUSH DE         ;Save curr row start addr

            EX DE,HL

            ADD HL,BC       ;Find current row end addr

            DEC HL

            SBC HL,DE       ;Test

            POP DE          ;Get them back

            POP HL

            RET NC          ;In

            DEC HL          ;Out

            DEC HL

            RET
```

;BDRYU - a routine for upper boundary condition

;---

```
BDRYU       PUSH HL         ;Save current disp addr

            LD DE,(LIMS)    ;Get up bdry addr

            SCF             ;Ensure carry off

            CCF

            SBC HL,DE       ;Test

            POP HL          ;Get it back

            RET NC          ;In

            ADD HL,BC       ;Out

            ADD HL,BC
```

```
        RET

;BDRYD - a routine for lower boundary condition

;------------------------------------------------

BDRYD   PUSH HL          ;Save current disp addr

        LD DE,(LIMS+02H);Get down bdry addr

        DEC DE           ;Test

        EX DE,HL

        SCF              ;Ensure carry off

        CCF

        SBC HL,DE

        POP HL           ;Get it back

        RET NC           ;In

        CCF              ;Ensure carry off

        SBC HL,BC        ;Out

        SBC HL,BC

        RET
```