A COMPUTER PROGRAMME FOR THE SIMULATION OF WATER RETICULATION SYSTEMS IN GOLD MINES

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ABSTRACT

This report investigates the application of digital computer simulation models to the analysis and optimization of complex mine water reticulation systems. A simulation program is developed and documented. Guidelines in the construction and use of mine water models are applied in a case study of water quality and quantity aspects of Unisel Gold Mine.

DECLARATION

I declare that this dissertation is my own unaided work. It is being submitted for the degree of Master of Science in the University of the Witwatersrand, Johannesburg. It has not been submitted before for any degree or examination in any other University, nor has it been prepared under the aegis or with the assistance of any other body or organization or person outside the University of the Witwatersrand, Johannesburg.

MARK COLLINS HOLTON

28th day of May, 1982.

To my wife Elna.

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PREFACE

Mine water reticulation systems are complex and solutions to water quality and quantity problems require an understanding of both the system and the environment of the system. A systems approach is therefore advocated herein. The implications for the gold mining industry of increasing demand and pollution of the water resources of the Vaal basin are examined. Mine water reticulation systems are discussed in detail together with a brief look at the causes and effects of poor quality mine service water. The different options open for solving water quality and quantity related problems are discussed. This report investigates the use of simulation models as a means of studying relationships between components of a mine water system and its environment and finding ways to make them work together in the best possible way.

Mathematical relationships common to all mine water reticulation systems are identified and discussed together with different numerical solution techniques. A general computer program incorporating a variety of solution techniques is then developed. The program can be used for simulating mine water models and has many useful facilities for input, simulation and output. The user must have a knowledge of the programming language, BASIC.

Guidelines, based on experience and the literature, are suggested for developing and using simulation models. A case study of Unisel Gold Mine illustrates suggested procedure. The models developed of Unisel G.M. are essentially complete and only require certain data to callibrate and validate them. Methods

are also discussed for using simulation in optimisation.

Considerable effort has been expended in making the simulation program as independent of computer facilities and programmer as possible. The program was written in BASIC language for use on a Hewlett Packard HP-85 desk top computer. Modern modular/structured programming techniques were used to write the program. The program and models are well documented and should be easy to read, maintain or transfer to another computer. Steps for running the simulation program are flow charted and explained in the appendices.

This report is one of a series on mine water service water quality, including causes, effects and alternative remedies by a research group working in conjunction with the Mining Technology Laboratory of the Chamber of Mines Research Organisation.

The author wishes to express his sincere thanks to the following organisations and individuals for their assistance: The Chamber of Mines of South Africa for their financial support and the opportunity to work with the Water Systems Research Programme at the University ; the officials of Unisel Gold Mine who assisted in data collection in order to make this study meaningful.

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CHAPTER ONE

1. INTRODUCTION

1.1 WATER REQUIREMENTS OF SOUTH AFRICAN GOLD MINES

It is now nearly a century since the discovery of gold on the Witwatersrand in 1886. For a long time gold mining was confined to the 121km long belt known simply as, 'The Reef'. This consisted of three gold-fields; the Central Rand, the West Rand and the East Rand. Today there are some thirty operating mines on the Witwatersrand stretching from Carltonville in the west to Nigel and Kinross in the east. Another twenty mines are situated in the Western Transvaal and also near Welkom in the Orange Free State. These fifty odd mines produce seventy percent of the free world's gold and provide the South African economy with nearly one fifth of its income.

The pace of development in these areas, particularly the Witwatersrand, has been one of the most rapid in the world. The present population of the Vaal Basin is nine million and can be expected to be 15 million by the year 2000. The increase in the demand for water in the area has averaged six percent per annum over the last seventy-five years (Stephenson, 1980). The original sources of water on The Reef were the springs flowing on the ridge which gave the area its name, 'Witwatersrand'. These original sources were rapidly developed to their limit and sources were sought further and further away as mining activity increased. In 1923 the Vaal Barrage was constructed on the Vaal River and water was pumped to The Reef. The water supplied from

the Vaal Barrage also became inadequate by 1938 when the construction of the Vaal Dam was completed. In 1972 the Vaal Dam was drawn to its limit when it was necessary to import raw water from the Tugela River, 300 kilometers further away. Schemes that will be completed this decade include the raising of the Vaal Dam wall, the building of numerous new dams within the Vaal catchment area and the inter basin transfer of water through the Tugela-Vaal Scheme. The present water consumption along the Vaal River is approximately 5200 megalitres per day and is expected to nearly double by the end of the century.

Most great civilizations have developed on the shores of rivers and lakes, whereas the major growth centres in South Africa are away from the largest water resources. This is because our economic development is largely based on mining activities rather than agriculture. The present water supply network radiates outwards from the purification works at Vereeniging to supply mining areas as far afield as Carltonville on the West Rand. The cost of water supplied by the Rand Water Board is likely to rise steeply in the future due to additional water having to be obtained from further away or from more expensive sources.

Up to 80 percent of the water supplied by the Rand Water Board is not consumed but is returned to water sources which return most of the flow to the Vaal. The gold mines currently use about 2000 megalitres per day of which 90 percent is recycled within the mine. Although the present mine water consumption of 10 percent, or 200 megalitres per day seems minor in relation to that of other consumers (5200 Mℓ/d total), saline mine pumpage accounted for approximately 25 percent of the total salt load originating from the Southern PWV catchment in 1977/78 (Herold 1981). Water consumption in the gold

mines could, furthermore, rise dramatically if water cooling is adopted for future deep level mines and may be responsible for up to seventy percent of total water consumption from the Vaal Basin by the end of the century.

Pollution in the form of various dissolved salts is present in increasing concentrations in the return flows to the Vaal and because of the 80% recirculation of water, salts accumulate in the water system. The Rand Water Board is continuously updating its water purification system to cater for the decreasing water quality. A greater environmental awareness of the effects of pollution are also bringing about stricter discharge regulations. The increasing cost of purchasing raw water and stricter discharge regulations have resulted in the mines being the most intensive recyclers of water. The water quality or recycled mine service water is generally poor, which limits surface discharges, which, in turn, causes recycling and higher build-ups of dissolved salts within the mine water systems.

1.2 MINE SERVICE WATER IN GOLD MINES

Gold mines require between 1 and 3 cubic metres of water per ton of ore mined. The water used is recycled within the mine and obtained from external sources such as regional water boards, surface supply dams, groundwater infiltration and neighbouring mines. Mine service water (MSW) is used for cooling, drilling, water jetting of excavated material, dust suppression and in hydraulic emulsions. Make-up water from external sources is used to replace water losses such as evaporation, water removed with ore hoisted to the surface or water deliberately discharged because of poor quality.

The gold bearing ore (the Reef) has an average thickness

of 1m and dips at between 20° and 45° depending on the location. The reef is excavated from the top downwards. Mining is currently being carried on at depths up to 3500 metres below surface where the rock temperature is in excess of 65 degrees centigrade. Mining operations are taking place at greater and greater depths. Since the rock temperature increases with depth at the rate of 2°C per 100m, considerable quantities of water may be used for the extensive cooling operations required in future deep level mines. Current mechanisation programmes are promoting the use of stoping machinery which use large quantities of oil-in-water emulsions.

Mine service water is generally supplied from the surface to each working level via a system of break pressure dams or via pipes with pressure reducing valves. Sufficient water is supplied to satisfy the demand at each level. The used MSW gravitates down inclined shafts and stopes and then along drains or pipes in the haulage-ways of each level to a vertical drain which conveys the water from all levels towards the lowest level. All groundwater infiltration present in the mine is mixed with the used MSW by the time the lowest level is reached. A flocculant is added and the water is passed through settlers so that suspended particles can be removed as mud from the bottom of the settlers. The effluent is pumped to the surface for chilling or to the top of the distribution system for recycling. Any excess water due to infiltration is removed from the system. Alternatively any water losses are replaced with make-up water from external sources.

1.3 MINE SERVICE WATER QUALITY AND ITS EFFECTS

The quality of mine service water (MSW) is of prime importance, since poor quality water can have a detri-

mental effect on the performance and life of all equipment exposed to it. The high chloride concentration in MSW in the Orange Free State is suspected of being one of the causes of corrosion of metal pipework and equipment. Sulphates and carbonates in the waters closer to the Witwatersrand give rise to scaling and blockages. Scaling is common in heat exchange equipment found in refreigeration plants used for chilling the MSW. Hydraulic roof supports and new mechanised mining equipment is designed to operate hydraulically using oil-in-water emulsions. Water hardness, due to sufficiently high concentrations of calcium carbonate causes a breakdown of the emulsions. There is also the problem of potability to be considered. Corrosion, scaling, blocking and fouling are problem phenomena which manifest themselves in different ways. Stephenson et al (1981) and Stephenson (1981a) discuss the causes and effects of poor quality water in reports to the Chamber of Mines.

The cost of water pumping equipment and water piping on a typical mine is of the order of R10 million. The annual electricity supply to pumping installations is frequently in excess of a million Rand (Stephenson 1981a). Poor water quality and the associated problems of corrosion, scaling, etc., can markedly affect the life of equipment and pipes. Because of the large heads and flows involved in pumping, power costs are very sensitive to corrosion and wear of pumps (which reduces efficiency) and to scaling of pipework (which increases pumping heads). The extent of such problems and the cost implications are largely unknown at present.

The quality of make-up water obtained from external sources such as regional water boards, surface supply dams and groundwater infiltration is often acceptable. Once used underground the water quality deteriorates

rapidly. The deterioration can be attributed to a number of factors. The primary source of contamination is chemicals such as sulphates which are leached from the mined ore. Another source is poor quality make-up water which contains high salt concentration, e.g. saline surface pans. The groundwater infiltration in the OFS is very saline whereas groundwater from the dolomites in the West Rand is very good. A secondary effect which increases total dissolved solids concentrations (TDS) is evaporation from within the mine and from surface cooling towers. The release of soluble chemicals by explosives or even chemical dosing for settling, pH control or disinfection, should be considered too. All these effects are magnified by the process of recycling MSW.

1.4 SOLUTIONS TO PROBLEMS RELATING TO POOR QUALITY SERVICE WATER

A major part of the operating costs of the gold mining industry depends both directly and indirectly on the quality and quantity of the MSW used in the mines. Since the South African economy is highly dependent on the gold mining industry, any improvements in this sector constitute an improvement to the economy as a whole. The problems discussed so far can be summarised as follows:

1) The quality of existing MSW is inadequate for some existing mine useage and for new mechanical mining equipment being introduced.

2) Various degrees of corrosion, scaling, fouling and blocking are being experienced.

3) The extent of such problems and the cost implications are largely unknown at present.

The South African economy and the water resources of the country are part of a wider system within which gold mines operate. The objectives set for solving problems in mine water reticulation systems must, therefore, be formulated to maximise the utility for the wider system as a whole. A reductionist approach of considering only the problems associated with mine water systems may lead to a worse situation when viewed in the light of the wider system and its objectives.

Water quality problems and water quantity are closely related. If an unlimited source of cheap, good quality water were available, then the obvious solution would be to use the water once and discharge it from the mine. This is generally not possible because of the already high and increasing cost of raw water supplied and because of stricter discharge regulations in effect. There are a number of ways of dealing with pollution in general:

1) Dilution of the polluted water by the addition of better quality water.

2 Concentration of the pollutant through the use of a desalination plant. A highly concentrated, or polluted, stream of water from the mine would have to be disposed of.

3) Prevention of the pollution or problem by somehow removing the causes.

4) Acceptance of the pollution and modifying the system to cope with the problems.

5) Some combination of the above.

Dilution is carried out in most mines in the form of good quality make-up water which replaces water losses from the system. Some mines have an excess of groundwater infiltration which has a diluting effect provided the quality is better than that of the water in the system. Generally the quantity of good quality make-up water from regional boards, surface dams etc., is limited for economical reasons or because of restrictions on the quantity available.

Desalination methods of possible interest to the gold mining industry include, Electrodialysis, Reverse Osmosis, Multi-stage Flash Evaporation, Freezing Processes and Solar Distillation. These methods result in a highly concentrated brine which must be disposed of somehow. Regulations for surface discharges generally limit the quality and not the quantity of the discharge. This favours dilution and not the concentration of pollutants which results from desalination methods.

The cost of desalination is a function of the method, the capacity of the plant and the feed salinity. The concentrations of total dissolved solids (TDS) in circulated mine service water varies between 1000 and 20 000 milligrams per litre. Flow rates can be up to 100 megalitres per day. The capital, power, labour, materials and running costs of all these methods applied to the full flow is prohibitively expensive when compared with alternative sources of water. It may be economical to desalinate a slip stream for a specific requirement such as hydraulic machinery. Binnie & Partners (1981) and Stephenson (1981b) discuss different methods, costs and applicability to different fields and requirements in reports to The Chamber of Mines.

The quality of the mine water deteriorates when the water

comes in contact with ore and dust. It is suspected that a considerable amount of leaching of salts occurs in the drains due to contact with the silt deposited at the bottom of the drains and with suspended solids transported in the water. There may be a few hundred kilometres of drains in a mine with up to 50 percent of the cross sectional area occupied by silt. The removal of the bulk of suspended solids at the head of the drains with settlers or silt traps may be a means of preventing a significant amount of pollution further down stream. It may also reduce the work involved in continuously desilting the drains. Stewart, Sviridov & Oliver (1981) discuss various settling and filtration methods and costs for the removal of suspended solids in MSW. Neutralising or protective chemicals (e.g. scale and corrosion inhibitors) can also be used to prevent problems (Stephenson 1981b).

The objective of most mines operating at present is to minimise the cost of water purchased and the cost of water treatment. The quality of water is considered acceptable provided no serious short term problems result which can be linked to the water quality. Details on the life of pipes, corrosion and scaling rates, types of corrosion active, scale composition etc. are not available. Very little information is, in fact, available for a long term economic assessment of the cost of pollution to the mining industry.

It is most probable that no single method discussed will provide the complete solution to the water quality problems of any particular mine. The probable solution lies in some combination of these techniques. The objective used in arriving at solutions to mine water quality and quantity problems should be the maximisation of benefit or utility for the wider system as a whole. The wider system includes such systems as the regional

water resources, the economy of the country and the gold mining industry itself.

1.5 SYSTEMS ANALYSIS TECHNIQUES AND THE USE OF SIMULATION MODELS

Developments in Operation Research have led to numerous extremely powerful Systems Analysis techniques. These techniques can be broadly classified into two main categories:

1) Direct optimization techniques

2) Simulation techniques

Direct optimization techniques can be used to find the optimum solution to certain problems. Grosman (1981) describes the application of transportation programming, extended transportation programming, linear programming and separable programming in a case study of Doornfontein Gold Mine. Costs are estimated for raw water, conveyancing and desalination. The techniques are used to calculate the average flows from each source to each demand point. The flows satisfy minimum water quality and quantity constraints and result in the minimum total cost solution.

The techniques used in the Doornfontein Gold Mine study unfortunately assume steady state conditions in the analysis. Average flows and constant water quality are assumed at all the sources and demand points. The average flows are calculated which result in the minimum cost. Real mine water systems are never in a steady state. Water required at demand points generally varies between zero and several megalitres a day. During peak demand periods it may not be possible to draw water from the different sources in the optimum ratio deter-

mined. The concentration of salts in used MSW collected at the bottom of the mine varies throughout the day and week depending on what the MSW was used for and the proportion of groundwater blended with it. This water is often pumped to a surface dam where make-up water of a different quality is added sporadically depending on the dam level. The water in such a surface dam therefore represents a source with a water quality which is not steady. It can be concluded that optimum solutions derived from deterministic models which assume steady flows and constant water quality may not be realistic. The 'optimum solution' cannot guarantee that the constraints will be satisfied at all times, that the solution is practical or, indeed, that the solution is an optimal one at all.

Simulation provides a means of observing the behaviour of the components of a system under varying conditions. No 'solution' in the mathematical sense is sought. The objective is to gain an understanding of the relationships among components of the system and to find ways to make them work together in the best possible way. Simulation does not yield an optimal solution directly and it is thus necessary to simulate iteratively in order to achieve an optimum. Even when combined with efficient techniques for selecting the values of each decision variable, an enormous computational effort may lead to a solution which is still far from the best possible.

To its credit, simulation can be used to solve models with highly non-linear relationships and constraints. The direct optimization techniques used in Grosman's study of Doornfontein Gold Mine are seldom able to deal with all the complexities and non-linearities which are easily incorporated into a simulation model. Simulation can be used to experiment with alternative

'optimum solutions' and together with direct optimization techniques it may be possible to narrow the search for a real global optimum. Little or no cost, time or risk is involved with simulation. The time scale can be controlled and long and short term effects of quantity and quality can be determined and used as an aid to decision making and planning. More important variables and parameters can be identified by changing their values and studying the effects. Certain parameters and relationships can be determined from simulations. A simulation model can be visualised by most people and the results are generally more convincing than those obtained from deterministic approaches.

It was observed in early studies of mine water systems that the rate of change of water quantity and quality, with respect to time, could always be described by a set of first order ordinary differential equations. These equations can be solved simultaneously at each iteration in a simulation using powerful numerical methods. The solution to the set of equations yields the volume of water and the mass of salts in each storage component of the system at the end of each simulation time-step. These values can be used in conjunction with the operating rules and various relationships to determine pump on/off settings, make-up flows, demands, salt concentrations, leaching rates, overflow, etc. The degree to which the model represents the real system and the accuracy of the results depends on the validity of the model and the accuracy of the solution of the set of equations.

A general simulation program has been written which can be used to simulate mine water models. The model must be described by a system of first-order ordinary differential equations. Such a model, consisting of j

equations and involving q variables, can be written in the general form:

$$\frac{dx_i}{dt} = \phi(t, x_1, x_2, \text{---} x_q, \frac{dx_1}{dt}, \frac{dx_2}{dt}, \text{---} \frac{dx_q}{dt})$$

where i = 1,2 --- j

The simulation program has been successfully applied to models other than mine water systems. Surge problems, gradually varied flow, reservoir routing, elastic beam analysis and vibrating systems are examples of systems which can be modelled using the program.

According to James (1978), the orderly procedure for constructing of simulation models is:

1) Systems Analysis: the salient components, interactions, relationships, and dynamic mechanism of a system are identified.

2) System Synthesis: the model is constructed and coded in accordance with Step 1).

3) Verification: the model's responses are compared with those which would be expected if the model's structure was prepared as intended.

4) Validation: the responses from the verified model are compared to corresponding observations of, and measurements from the actual system.

5) Inference: experiments with, and comparisons of responses from, the verified and validated model - this is the design stage.

A systems analysis has been carried out on Unisel Gold Mine. Two models have been developed (or synthesized); one model is a very simplified representation of the real system and the other is a detailed model. The simple model consists of a single component or element and assumes steady average flows and a constant volume of water in the system. This model is used to simulate the change of the average salt mass and concentration in the system. An analytical solution is used to verify and validate the model. The detailed model is used to simulate the change of salt mass and water volume in each of the eight storage elements of the system. Other useful information is calculated from these values. The model is considered to be verified because it responds in the situations tested as one would expect. The model can only be considered partially validated because insufficient in situ data is available at present for calibrating the model and for comparison with the real system.

CHAPTER TWO

2. MINE WATER RETICULATION: A SYSTEMS APPROACH

2.1 INTRODUCTION

Water is continually recycled in gold mines because of the high cost of procuring surface water resources, the limited sources of groundwater infiltration, and the environmental problems of disposing of poor quality mine service water. Poor quality mine service water (MSW) can lead to problems in mines which means that the objective of mine water systems, which is to supply water of adequate quantity and quality for the different mining activitties, is sometimes not satisfied. MSW is used underground largely for cooling but also for drilling, dust suppression and, in some mines water jetting to move ore.

Solutions to mine water problems require an understanding of the system and the method proposed here is the use of simulation models. Steps used in the construction of simulation models are outlined in chapter 5. One of the steps in model construction is Systems Analysis which requires the analyst or model builder to identify; the salient components of the system, interaction between components, operating relationships and the dynamic mechanisms of the system. Examples of the components of the system are the reticulation pipework, dams, pumps, purification and refrigeration plants, sources of water supply and pollution, and sinks for the discharge of polluted water.

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The water reticulation system of Unisel Gold Mine is

described in this chapter. The basic components, interactions, relationships and dynamic mechanisms are identified. The mine has been selected for study because its water reticulation system is relatively simple compared to those of other mines visited (Doornfontein and Elandsrand Gold Mines). Mathematical relationships are derived which describe the dynamic behaviour of some of the system components. These relationships are examined further in chapter 3 and are used to develop a general simulation program and two models of Unisel Gold Mine. Examples are given in chapters 6 and 7 to show how the simulation program is used to run the models of Unisel Gold Mine.

2.2 THE WATER RETICULATION SYSTEM OF UNISEL GOLD MINE

A schematic representation of the mine water system analysed herein is given in Fig.2.1. The boundary of the system only includes the components shown. Water volume and salt mass flows between components and in and out of the system as a whole are the only interactions considered. Other interactions such as information flows, power requirements, decisions, money etc. are not relevant to the system being modelled.

2.2.1 Water Flows

MSW is used extensively in Unisel for cooling. Water chilled to approximately 10°C leaves the coldwell on the surface and enters an underground storage dam approximately 1000m below the surface. Water is then fed to a series of smaller cascade dams, one at each working level in the mine. The cascade dams act as pressure breaks and each dam supplies water to a level two levels below (i.e. approximately 200m lower). When the water surface in any of the dams drops below a certain level a valve is actuated at the storage dam and water is released to feed the top cascade dam. Water then overflows to the dam below and so on until

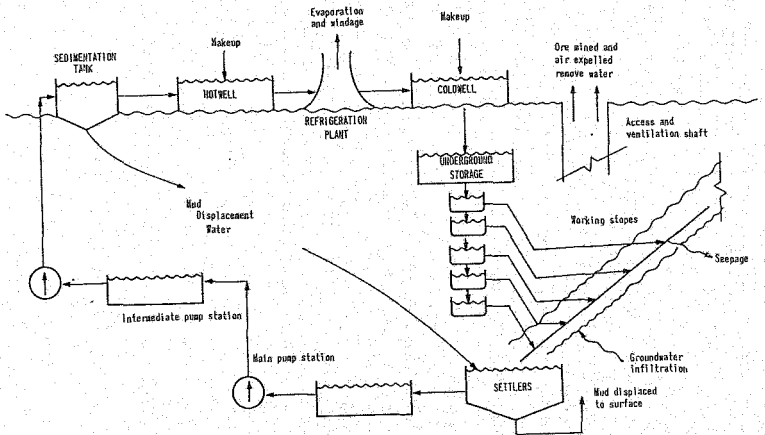

FIG. 2.1 UNISEL GOLD MINE WATER RETICULATION SYSTEM

the empty dam(s) fill and the valve is again closed. MSW at each working level is used for cooling, dust suppression, drilling and water jet cleaning. Some of the water used is removed from the mine with the ore mined and some is evaporated and removed with the probably saturated or supersaturated ventilation air expelled from the mine. The remainder of the used MSW and any groundwater infiltration, gravitates to the bottom of the mine via a network of drains and pipes.

The water enters settlers at the bottom of the mine after a flocculant has been added to promote the settlement of suspended matter. The settled mud is removed from the bottom of the settlers and taken to the surface reduction works where it is processed for gold. Cleaner water from the surface sedimentation tank is used to displace the mud at the bottom of the mine. The displacement water and the clarified water from the settlers enters the main pump station dams from where it is pumped to the intermediate pump station and then to the sedimentation tank on surface. The water is pumped in two vertical stages of approximately 1000m each. Associated with each pump station are large storage dams. These are used for emergencies such as pump failures and for periods when outflow from the settlers exceeds the pumping capacity of the pumps. The pumps are operated manually to start pumping at a certain dam level and to stop when the level drops to some other predefined level.

From the sedimentation tank the water from underground enters the hotwell at a temperature of approximately 30°C. This water is pumped at a constant flow rate to the top of a cooling tower. The temperature is lowered approximately 7°C after passing through the tower. The water is then pumped through the refrigeration plant to the coldwell from where it re-enters the mine as MSW at approximately 10°C to complete the cycle.

Make-up water is added to the hotwell and coldwell from a local surface dam and the regional water board. The make-up water replaces water removed from the system; with ore mined, evaporation in the workings, evaporation at cooling towers and windage, mud removed from the settlers and periodic overflow from the hotwell. Overflow from the hotwell occurs particularly on weekends when there is little or no demand for MSW from the mine and water pumped up, to maximise safe storage underground, fills all surface dams and overflows from the hotwell. Some mines require no make-up as the groundwater infiltration results in a surplus which must be pumped out of the mine.

Mining operations take place over 24 hours per day in three 8-hour shifts during weekdays. The basic mining operations include drilling, charging holes, blasting, extraction and cleaning. The activities described generally occur simultaneously on all working levels and this results in a distinctive pattern in the flow rate for water leaving the cascade dams at different times of the day and different days of the week. There is also a distinctive pattern in the flow rate for water entering the settlers at the bottom of the mine. The instantaneous flowrates for the water leaving the cascade dams and entering the settlers are not the same because of the different travel times from each of the levels and constant groundwater infiltration which mixes with used MSW in the different levels. Weekday flow patterns differ from those on weekends because no work is done on Sundays and only two shifts are worked on Saturdays. The flow patterns discussed are determined from in situ measurements.

2.2.2 Dissolved Salts in the Mine Water

The quality of make-up water obtained from external sources such as regional water boards, surface supply

dams and groundwater infiltration is often acceptable. Once used underground the water quality deteriorates rapidly. (i.e. the concentration of dissolved salts increases). The deterioration is attributable to a number of factors which are discussed separately in this section. The causes and effects of poor quality water are discussed in detail in Stephenson (1981a) and summarised in section 1.3 above.

Salt concentration is defined as the mass of salt(s) per unit volume of water. Concentrations are usually expressed in units of milligrams per litre (mg/ℓ) or or kilograms per megalitre (kg/Mℓ). Total dissolved solids (TDS) is a commonly used term and equals the total mass of all salts present in a sample divided by the volume of the sample. High salt concentrations in mine water are undesirable and water with a high concentration of salts is referred to as a poor quality or a highly contaminated or polluted water. Conversely, good quality water has a low salt concentration.

2.2.2.. Processes affecting the Salt Concentrations

If the total mass of salts and the total volume of water in all the components of the water system is known at a particular instant in time, then the average concentration of salts can be calculated. The effects on the salt mass and average concentration for each process is discussed below. In order to simplify the explanation, the effects discussed are those which would occur if they were the only ones taking place in the system. The combined effects of the processes, as they accur in an actual system, are discussed subsequently. Some of the main processes are:

1) Water is constantly being removed from the system by evaporation from within the mine and from sur-

face cooling towers (see fig 2.1 The water evaporated has a negligible salt concentration and does not affect the mass of salts in the system. Evaporation therefore has a concentrating effect as the volume of water is reduced while the salt mass remains unchanged.

2) A primary source of contamination is iron sulphides (pyrites) which are leached from the ore to form sulphates. Leaching of salts causes an increase in the total mass of salts in solution while the water volume remains constant. Leaching therefore has a concentrating effect.

3) The release of soluble chemicals by explosives or chemical dosing increases the concentration in a similar manner.

4) Contaminated groundwater infiltration into the mine adds both to the total mass of salts and to the volume of water in the system. If the salt concentration of the infiltration is greater than the average salt concentration of the system water then the infiltration has a concentrating effect. Conversely, an infiltration with a low concentration has a diluting effect. The total salt mass in the system is increased in both cases.

5) Make-up water replenishes any volume losses from the system due to evaporation and water removed with mud and ore mined. Make-up has the same concentrating or diluting effect as infiltration.

6) Water is periodically removed from the system with the ore mined and with mud removed from the settlers. Seepage of water out of the system is another possible loss in dry mines. If, for some reason, the water removed has a greater salt con-

centration than the average system concentration then the system concentration would be reduced, and vice versa. If water, with the same concentration as the system, is removed in the manner described, it will not affect the system concentration.

7) A contaminated stream in the system could be diverted to a desalination plant. A desalination process produces two new streams; one more contaminated than before and one less contaminated. The less contaminated stream would be re-introduced into the system at a suitable point and would have a diluting effect. The more concentrated stream would have to be disposed of outside the system.

In the real system, many processes occur simultaneously and the net effect is to either increase or decrease the total salt mass with time, or maintain it at some equilibrium level. The total salt mass of the system will increase with time when the mass flow rate of all inflows exceeds that of all the outflows. At equilibrium the mass flow rate of all the inflow equals that of the outflows. An equilibrium total salt mass does not imply a constant concentration in the system. Also, an increase in the total salt mass does not imply that there is a corresponding increase or decrease in the water volume of the system. Salt concentration depends on the mass of salts and the volume of water in the system, both of which may be either increasing or decreasing at any time.

2.3 GENERAL MATHEMATICAL RELATIONSHIPS DESCRIBING THE DYNAMIC BEHAVIOUR OF THE SYSTEM COMPONENTS

2.3.1 Water Quantity

The quantity of water in most storage components is not constant over time but varies according to the law of continuity. The state of the system, the time of day or week and the operating relationships determine the inflows and outflows of a component. Designate V as the volume or quantity of water in a component such as the hotwell shown in fig.2.1 The inflow and outflow rates to and from the component are designated Q_1 and Q_2 respectively. If the inflow does not equal the outflow, then the rate of change of volume of stored water is:

$$\frac{dv}{dt} = Q_1 - Q_2 \qquad (2\text{-}1)$$

If, for example, the inflow exceeds the outflow there will be an increase in the volume of water stored in the component. If the inflow equals the outflow the volume will remain constant.

2.3.2 Water Quality

Let Q_1 and Q_2 be defined as inflows and outflows to a component and C_1 and C_2 as the corresponding salt concentrations. M is the mass of salts dissolved in the water stored in the component. At a particular instant the mass of salts entering and leaving the component per unit time is Q_1C_1 and Q_2C_2 respectively. If Q_1C_1 does not equal Q_2C_2 then the mass of salts in the component, M, is changing. The rate of change of salt mass stored is given by

$$\frac{dM}{dt} = Q_1C_1 - Q_2C_2 \qquad (2\text{-}2)$$

If for example the mass inflow rate Q_1C_1 exceeds the outflow Q_2C_2 then there will be an increase in the mass of salts stored in the component over a period of time. If the concentration of the inflow C_1 were sufficiently high, the element could experience a simultaneous increase in the mass of salts stored and a decrease in the quantity of water stored, i.e., dM/dt is positive and dV/dt is negative. Under such conditions there would be an increase in the salt concentration of the water stored in the component.

2.4 MATHEMATICAL MINE WATER MODELS OF UNISEL GOLD MINE

The dynamic mathematical equations, (2-1) and (2-2), have been used to construct two simulation models of Unisel Gold Mine. The use of the two basic equations in the construction of the models is discussed. The problem of solving the differential equations present in the models is introduced and the need for a general simulation program to do this is motivated. Of the two Unisel models, one is a simple one which can be solved analytically and the other is more detailed and has to be solved numerically (simulated).

2.4.1 Simplified Model of Steady Flow and Unsteady Salt Balance

The model in chapter 6 crudely describes the change of salt concentration with time in the system depicted in fig.2.1. The system is represented by a model which consists of a single component with constant water volume and flows. Due to the simplicity of the system an analytical solution is available for the single differential equation describing the system. The differential equation is similar to equation (2-2) derived above. The analytical solution and the simulation of

the model is described in detail in chapter 6

2.4.2 Detailed Model of Unsteady Flow and Salt Balance

The water reticulation system of Unisel Gold Mine has several water storage components. In each of these components the salt mass and concentration of the stored water varies with time. The mass and volume inflow and outflow rates vary with time in most components. The volume of water stored in these components therefore varies as well. The mass of salts and the volume of water in the system as a whole is also changing due to interactions with the wider system (evaporation, make-up, leaching, seepage, infiltration, mud and ore loss).

The system can be described by a differential equation of the type (2-1) for each storage component where the water volume changes and by an equation (2-2) for each component where the salt concentration changes. The model in chapter 7 describes the system in considerably more detail than the simple model in chapter 6 Fifteen differential equations describe dynamic behaviour of the eight components shown in fig.2.1; settlers, main pump station, intermediate pump station sedimentation tank, hotwell, coldwell, underground storage and cascade dams. Two differential equations describe the rate of change of each component's volume and salt mass. The settler volume is effectively constant and only one equation is required for salt mass changes.

2.5 SIMULATION OF MATHEMATICAL MINE WATER MODELS

Equations (2-1) and (2-2) are first order ordinary differential equations. An analytical solution to the detailed model of Unisel Gold Mine would be the equiva-

lent of solving 15 differential equations simultaneously. The result would be 15 functions describing the salt masses and volumes of the components as a function of time. Such a result is infeasible when the component inter-relationships and mathematical discontinuities introduced by the operating relationships are considered. Typical operating relationships which make an analytical solution unpractical are: pumps switching on and off when storage volumes are high or low respectively; adding make-up water when volumes are low enough; drawing water out of the cascade dams to satisfy varying demand throughout the day.

The differential equations are best solved using numerical methods. The differential equations are 'solved' at different times. Calculation can only start at some initial time when the initial values (volumes and salt masses) are 'known'. Although the differential equations are solved numerically at each step the procedure is referred to as a simulation wherein the model is run.

The numerical solution of the equations, describing quality and quantity and other theoretical considerations is discussed with examples in chapter three. The incorporation of these methods into a general simulation program for running mine water models is described in chapter four.

CHAPTER THREE

3. THEORETICAL ANALYSIS OF MINE WATER SYSTEMS

3.1 INTRODUCTION

It was shown in chapter 2 that the basic functions of each component of the system could be described by equations (2-1) and (2-2). Gerald (1980) describes these as first-order ordinary differential equations of the form:

$$\frac{dy}{dt} = f(y,t)$$

The variable y is a dependent variable such as the volume or mass of salts in a component and t is the independent time variable. Ogata (1978) distinguishes between linear and non-linear, time-invariant and time-varving differential equations and between linaar and non-linear systems. An equation is linear if the dependent variable y and its derivatives appear as linear combinations. An equation is time invariant if the coefficients of all the terms are constants. The order of the equations refers to the highest order derivative present.

Examples

$\frac{dy}{dt} + 5y = 0$. (linear, time invariant, 1st order)

$\frac{d^2y}{dt^2} + 4ty = 0$ (linear, time variant, 2nd order)

$\frac{d^2y}{dt^2} + (y^2-)\frac{dy}{dt} = 0$ (non-linear, time invariant, 2nd order)

The equations that characterise mine water systems

investigated so far are 1st order, linear time variant and time invariant. The model equations are linear and therefore constitute a linear system. The most important property of linear systems is that the principle of superposition applies. This principle states that the response to several inputs can be calculated by dealing with one input at a time and then adding the results. By application of the principle of superposition, complicated solutions to a system of linear differential equations of any order can be expressed as the sum of simple solutions.

In all differential equations, one or more values must be known in order to evaluate the function. These several values are generally specified at the same value of the independent time variable, generally at the start time. They are referred to as initial values. When the function values are known at different times, generally the end-points, then the values are referred to as boundary-values. Boundary-value problems are extremely difficult to solve for systems of equations, because the technique usually involves a trial-and-error process of guessing different initial values and simulating until the correct boundary-values are obtained at the correct time. The shooting method and others are described in Gerald (1980) for the solution of boundary-value problems. Fortunately mine water system models can be classed as initial-value problems because the state of the system and the initial values are generally known or can be estimated at the beginning of a simulation.

Numerical solution techniques for single, linear 1st-order differential equations are discussed initially and then it is shown how they are applied to a general system of equations describing a model. It is not the intention of this chapter to verify the theory involv-

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ed. The reader is referred to Stummel and Hainer (1980) Gerald (1980), Ogata (1972) and Kreyshig (1972) for the development of the theory. A knowledge of basic principles and theory behind the solution of single equations and systems of equations is required for the construction of models (discussed in chapter 5) and to understand and modify the simulation program (discussed in chapter 4).

3.2 NUMERICAL METHODS FOR THE SOLUTION OF SINGLE DIFFERENTIAL EQUATIONS.

Numerical solutions appear in the form of a tabulation of the values of the functions at various values of the independent time variable and not as a functional relationship. Numerical methods have the ability to solve practically any equation but they have the disadvantage that the entire table must be recomputed if the initial conditions are changed.

If a function f(t) can be represented by a power series in a certain interval then it can be represented by the Taylor series expanded about a point $t = t_0$, i.e. about the initial value:

$$y(t)=y(t_0)+y^{I}(t_0)(t-t_0)+\frac{y^{II}(t_0)}{2!}(t-t_0)^2+\frac{y^{II}(t_0)}{3!}(t-t_0)^3 + \ldots$$

Letting n represent the previous step at time t_0 and n+1 represent the next step at t_0+h, the series can be written as:

$$y_{n+1}=y_n+hy_n^{I}+\frac{h^2y_n^{II}}{2}+\frac{h^3y_n^{III}}{6}+\ldots\ldots \qquad (3\text{-}1)$$

Consider the example problem

$$y' = \frac{dy}{dt} = y+t \qquad (3\text{-}2)$$

with initial conditions

$y(0) = 1$

This is a linear time variant 1st order differential equation. The analytical solution to the problem, $y = 2e^{t}-t-1$ will be used to compare the numerical results of some of the methods and to show exactly the error at any step.

3.2.- The Simple Euler Method

The Euler method is the simplest but least accurate of all the methods discussed. To obtain an exact numerical solution to the example problem (3-2), all the derivatives y^{II}, y^{III}, y^{IV} ... must be evaluated and substituted into the Taylor series (3-1). Knowing the initial values of y_n, y_n, y_n^{II}..., y_{n+1} could be evaluated after a time increment h. The values of all the derivatives could then be calculated at n+1, and y_{n+2} could be evaluated after the next time increment and so on. Derivatives of arbitrary functions cannot easily be formulated in computer programs. The derivatives y^{II}, y^{III}, etc. are easy to evaluate for the example (3-2) but this is not generally the case. The Euler method truncates the Taylor series by excluding the terms after the first derivative and eliminates the problem of having to evaluate the second and subsequent derivatives. Then

$$y_{n+1}=y_n+hy_n^{I}+0(h^2)\text{error} \qquad (3-3)$$

Neglecting $h^2y_n^{II}/2$ and the subsequent terms in (3-1) results in a truncation error of order h^2 which is denoted $0(h^2)$. This is the local error and results from

one step only, i.e. from n to n+1. It can be shown that the global error accumulated over many steps becomes O(h), i.e. an error of order h.

Substituting the example (3-2) into the Euler algorithm (3-3) gives :

$$y_{n+1} = y_n + h.(y_n + t_n) \qquad (3\text{-}4)$$

The initial condition y(0)=1 means that y=0 at t=0. Choosing the time increment h=0,02 and letting the step number n=0 at t=0, the values for y can be evaluated at successive time increments as follows:

$y_1 = y_0 + h.(y_0 + t_0) = 1 + 0,02.(1+0) = 1,0200$

$y_2 = y_1 + h.(y_1 + t_1) = 1,0200 + 0,02(1,0200 + 0,02) = 1,0408$

$y_3 = y_2 + h.(y_2 + t_2) = 1,0408 + 0,02(1,0408 + 0,04) = 1,0624$

$= 1,0848$

$= 1,1081$

etc.

The numerical solution after 5 steps is y(0,10)=1,1081 whereas $y=2e^{t}-t-1$ gives the exact analytical solution as y(0,10)=1,1103. Hence the absolute global error is 0,0022, i.e. two-decimal-place accuracy. Since the global error of the Euler method is proportional to h, i.e. O(h), the step size h must be reduced at least 22-fold to gain four-decimal accuracy, i.e. h<0,004. This would increase the computational effort 22-fold. Fig.3.1 shows how the slope at the beginning of the interval y_n^I is used to determine the function value at the end of the iteration in the Euler Method.

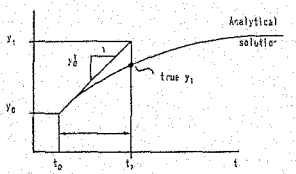

Fig. 3.1 The Euler Method.

The slope at the beginning of the interval is always wrong unless the solution is a straight line. Thus the simple Euler method suffers from the disadvantage of lack of accuracy, requiring an extremely small step size.

3.2.2 The Modified Euler Method

Fig. 3.1 and the subsequent discussion suggest how the Euler method can be improved with little additional computational effort. The arithmetic average of the slopes at the beginning and the end of the interval is used (only the slope at the beginning is used in the Euler method).

$$y_{n+1}=y_n+h\frac{y_n^I+y_{n+1}^I}{2} \qquad (3\text{-}5)$$

The Euler algorithm must first be used to predict y_{n+1} so that y_{n+1}^I can be estimated. Applying the same example (3-2) as before and substituting $y^I=x+t$ into (3-5) gives

$$y_{n+1}=y_n+h\frac{(y_n+t_n)+(y_{n+1}+t_{n+1})}{2}.$$

Substituting the Euler equation (3-4) for y_{n+1} gives

$$y_{n+1}=y_n+h\frac{(y_n+t_n)+(y_n+h(y_n+t_n)+t_{n+1})}{2}.$$

Using h=0,02 and the initial conditions; $y_0=1, t_0=0$

$$y_1=y_0+h\frac{(y_0+t_0)+(y_0+h(y_0+t_0)+t_1)}{2}$$

$$=1+0,02\ \frac{(1+0)+(1+0,02(1+0)+0,02)}{2}$$

$$=1,0204$$

$$y_2=1,0204+0,02\frac{(1,0204+0,02)+(1,0204+0,02(1,0204+0,02)+0,04)}{2}$$

$$=1,0416$$

.

.

.

$y_5=1,1104$ cf. analytical solution 1,1103

The answer agrees to within 1 in the fourth decimal place. Nearly twice as much work was done as in the Euler method but certainly not the 22 times more that would have been needed with that method to attain four-decimal-place-accuracy. It can be shown that the local and global errors of the Modified Euler method are $0(h^3)$ and $0(h^2)$ respectively. The Modified Euler and the simple Euler methods are often referred to as second and first order methods respectively.

3.2.3 Runge-Kutta Methods

The Fourth-Order Runge-Kutta methods are amongst those which provide the greatest accuracy per unit of computational effort. The development of the method is algebraically complicated and is given completely in Stummal & Hainer (1978) whil[illegible]ald (1980) derives the Second-Order Runge-Kutta *algorithm and explains the* principles behind the methods. All the Runge-Kutta methods use the simple Euler method as a first estimate. Improved estimates are then made using previous estimates and different time-values within the time interval h. A weighted average of all the estimates is used to calculate y_{n+1}. The Fourth-Order Runge-Kutta methods are the most widely used because of their power and simplicity. The following is a particular Fourth-Order method which is commonly used and which is included in the simulation program:

$$y_{n+1}=y_n+\frac{1}{6}(k_1+2k_2+2k_3+k_4)$$

$$k_1 = hf(t_n, y_n)$$

$$k_2 = hf(t_n+\tfrac{1}{2}h, y_n+\tfrac{1}{2}k_1)$$

$$k_3 = hf(t_n+\tfrac{1}{2}h, y_n+\tfrac{1}{2}k_2)$$

$$k_4 = hf(t_{n+1}, y_n+k_3) \qquad (3\text{-}6)$$

Again the problem given in (3-2) above is solved as an example: $dy/dt=f(t,y)=t+y, y(0)=1$. This time y(0,1) is calculated in one step (h=0,1) whereas y(0,1) was calculated in *five time increments* (h=0,02) using the simple and modified Euler methods above.

$k_1 = h.(x_n + y_n)$

$= 0,1(0+1)$ $= 0,10000$

$k_2 = 0,1(0,05+1,05)$ $= 0,11000$

$k_3 = 0,1(0,05+1,055)$ $= 0,11050$

$k_4 = 0,1(0,10+1,1105)$ $= 0,12105$

$y(0,1) = 1,0000 + \frac{1}{6}(0,10000 + 2.0,11000 + 2.0,11050 + 0,12105)$

$= 1,11034$

This agrees to five decimals with the analytical result and illustrates a further gain in accuracy with less effort than required by the previous Euler methods. It is computationally more efficient than the modified Euler method because, while four evaluations of the function are required for each step rather than two, the steps can be many-fold larger for the same accuracy. The simple Euler method would have required of the order of 220 steps to achieve five-decimal accuracy in $y(0,1)$ but each step involves only one evaluation of the function. The efficiency of the Euler and Runge-Kutta methods can be roughly compared by calculating the number of function evaluations required for the same order of accuracy. In this particular example the Runge-Kutta method is approximately 50 times more efficient than the simple Euler method (220/4). The local error term for the Fourth-Order Runge-Kutta algorithm (3-6) is $0(h^5)$ and the global error would be about $0(h^4)$.

3.2.4 Multistep Methods

The simple Euler, Modified Euler and Runge-Kutta me-

$k_1 = h.(t_n + y_n)$

$= 0,1(0+1)$ $= 0,10000$

$k_2 = 0,1(0,05+1,05)$ $= 0,11000$

$k_3 = 0,1(0,05+1,055)$ $= 0,11050$

$k_4 = 0,1(0,10+1,1105)$ $= 0,12105$

$y(0,1) = 1,0000 + \frac{1}{6}(0,10000+2.0,11000+2.0,11050+0,12105)$

$= 1,11034$

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3.2.4 Multistep Methods

The simple Euler, Modified Euler and Runge-Kutta me-

thods are called single step methods because they use only the information from the last step computed. In this they have the ability to perform the next step with a different step size and are ideal for beginning the solution where only the initial conditions are available. The principle behind a multistep method is to utilise the past values of y and/or y^I to construct a polynomial that approximates the derivative function and to extrapolate this into the next time interval. Most multistep methods have the disadvantage that they use a constant step size h to make the construction of the polynomial easier. Another disadvantage of multistep methods is that several past points are required whereas only the initial conditions are available at the start. The starting values are generally calculated from the initial conditions using a single-step method such as a Runge-Kutta method.

The Milne and Adams-Moulton Methods are multistep methods having a global error one more than the degree of the polynomial used. The algorithms consist of a predictor and a corrector equation. The two equations can be compared and relationships in Gerald (1980), allow one to estimate the error and the maximum step size for the next iteration so that the desired accuracy can be maintained with the least computational effort. Milne's method is rarely used because it sometimes becomes unstable. Both the Milne and Adams-Moulton methods are about twice as efficient as the Fourth-Order Runge-Kutta methods.

3.3 CONVERGENCE CRITERIA

Stummel and Hainer (1978) derive consistency conditions for the Runge-Kutta methods. The consistency of the approximation equations with the differential equation,

and the consistency of the initial conditions are essential pre-requisites for the convergence of solutions of a one step method to the required solution of the initial-value problem. Gerald (1980) derives convergence criteria for the Milne and Adams-Moulton multistep method. These criteria are applicable to single first-order equations only. A similar analysis for systems of equations such as those describing the mine water models is practically impossible. During a simulation of a complex model it is simple to detect when the solution is not converging; variables become unrealistically large and sign reversals occur. It is felt that reducing the step size with successive simulations until the results appear realistic is possibly the most practical means of ensuring convergence.

3.4 ERRORS AND ERROR PROPAGATION.

The local and global truncation errors have been mentioned while discussing the different numerical methods. There are several sources of error in numerical calculations in addition to the truncation error.

1) Original data errors will affect the solution

to a greater or lesser extent depending on the solution of the equations. Highly sensitive equations are said to be subject to inherent instability.

2) Round-off errors result when a number is rounded or chopped off. Carrying more decimal places in the intermediate calculations than is required in the final answer is the normal practice to minimise this. The simulation program written for the Hewlett Packard HP85 minicomputer uses double precision to store twelve significant figures for the model variables. In lengthy calcula-

tions this source of error is difficult to analyse and control.

Stummel and Hainer (1980) have developed a general expression for the total error due to truncation and rounding. The expression is difficult to use, but does illustrate the oppositely acting effects of the two types of errors. Fig. 3.2 shows this qualitatively.

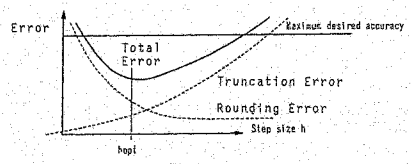


Fig. 3.2 Step Size Selection and Errors.

3.5 TIME-STEP-SIZE SELECTION

The choice of the time-step h is an important consideration in applying any of the numerical methods discussed so far. If the step size h is too small the computational effort and simulation time increases and rounding error may become large. Large truncation errors and instability may result if the step size is too large. In addition, an error caused by the fact that dy/dt is evaluated at the estimated point (tn,yn) and not at the exact point (tn,y(xn)) of the function being calculated. The latter error would be nil if dy/dt were independent of y and it will become more significant the faster dy/dt varies as y varies. An optimum step size therefore exists for each iteration of a simulation as shown in fig.3.2 above. Depending on the desired accuracy, a larger time-step can generally be selected which will result in acceptable errors

greater than the minimum possible error shown in the figure. Kreyszig (1972) derives the following criterion for controlling the step size h for the Fourth-Order Runge-Kutta algorithm:

$$kn = h\left|\frac{\partial f(t,y_i)}{\partial t}\right| = 2\left|\frac{k_3-k_2}{k_2-k_1}\right| \qquad (3\text{-}7)$$

k_1, k_2 and k_3 are defined above in (3-6). By evaluating kn, the step size can be controlled so that at each iteration a relationship, for example, such as $0,5 \leq Kn \leq 0,2$ holds. If the relationship does not hold then h is either halved or doubled, (if doubling is possible without increasing he beyond a suitably chosen number H, which depends on the desired accuracy). This criterion is not included in the simulation program as it is derived for a single differential equation and it is not clear how it will perform with a system of equations. A future modification could be made to the simulation program so that an important, or the most sensitive, variable in a model could be monitored and step size adjustments made accordingly.

The criterion derived below could possibly be used as another control of h, by using the results from performing the same simulation with two different step sizes, h_1 and h_2. This results in different answers, A_1 and A_2, at a particular simulation time, with unknown errors E_1 and E_2. Since the global truncation errors are proportional to the order O(h) of the numerical method,

$$E_1/E_2=(h_2/h_1)^{O(h)} \qquad (3\text{-}8)$$

To obtain a new step size h_3 which will produce a desired error E_3

$$E_3/E_1=(h_3/h_1)^{O(h)}$$

so that

$$h_3=h_1(E_3/E_1)^{1/O(h)} \qquad (3-9)$$

Substituting $E_1-E_2=A_2-A_1$ into (3-8) gives the error associated with step size h_1 as

$$E_1=(A_2-A_1)/(1-(h_2/h_1)^{O(h)}) \qquad (3-10)$$

Substituting (3-10) into (3-9):

$$h_3=h_1\left|E_3(1-h_2/h_1)^{O(h)}/(A_2\right. \qquad (3-11)$$

The expression can be used to estimate a new step size h_3 which will result in an error E_3 for a particular variable. The error varies with time for a particular variable during the simulation and using (3-11) will only ensure that the E_3 will be acceptable at the time when A_1 and A_2 were calculated. Calculating h_3 by using A_1 and A_2 values at the time in the simulation when the absolute value of A_2-A_1 is a maximum, should ensure that all errors for the particular variable are less than or equal to E_3. No experience has been gained regarding the effectiveness of (3-11) with models using more than one differential equation.

Example:-

Two simulations with step sizes h_1 and h_2 equalling 0,0005 and 0,005 respectively, resulted in the following answers: A_1=1,23456 and A_2=1,23450. (3-11) is used to estimate a new step size h_3 which will ensure an answer approximately correct to one decimal place, that is, E_3=0,05. A fourth-order method is used.

$$h_3=0,005\left|0,05(1-0,005/0,0005)^4/(1,23450-1,23456)\right|^{\frac{1}{4}}$$

$$=0,0242 \text{ say } 0,02$$

More sophisticated methods such as Runge-Kutta-Merson and Runge-Kutta-Fehlberg are discussed in Gerald (1980) Extra functional evaluations are required, but the advantage is that an estimate of the error is available and the step size can be adjusted accordingly at each step to minimise computational effort. These are single step methods, generally applied to solve single first-order equations.

3.6 METHODS USED IN THE SIMULATION PROGRAM

Three numerical methods are included in the simulation program as options; the simple Euler, the modified Euler and the Fourth-Order Runge-Kutta methods. The reasons for the choice of methods is discussed.

The least efficient simple Euler algorithm, and the Modified Euler algorithm are included as options in the simulation program because it has been found necessary at times to use a small time-step for reasons other than accuracy. Small time-steps are sometimes required when, for example, a large inflow is being pumped to a dam which is nearly full at the beginning of the time interval and which will be unrealistically surcharged at the end of a too-long time interval. The operating relationships, such as stopping the pump, can only be performed at the end of time intervals. If small time-steps are required for reasons other than accuracy, then the use of a more efficient algorithm only results in longer execution time and unwanted additional accuracy. The Euler, Modified Euler and Fourth-Order Runge-Kutta algorithms are included as options in the simulation program so that the correct one may be selected for the model being simulated and for the accuracy desired.

The more powerful multistep methods have been excluded

because of the more complex programming required. The multistep methods require the application of single step methods to obtain sufficient starting values from the initial conditions. Important objectives in writing the simulation program were simplicity, readability and ease of maintenance. The Fourth-Order Runge-Kutta method is one of the most powerful and simple single step methods to program, and it is felt that the more efficient Adams-Moulton multistep method does not justify the complexity of the program.

Time-step size variation during simulation is performed easily by the three methods chosen. None of the criteria discussed for selecting the optimum step size have been included in the simulation program because they have been derived for single equations and not for systems of equations. The program does have the facility that the time-step size can be changed by the user at any stage of the simulation.

It was discovered that the simple Euler and Modified Euler algorithms could be presented in a similar format to the Runge-Kutta method, that is, using k values as in (3-6). Compare the following with (3-3) and (3-5):

Simple Euler $y_{n+1}=y_n+k_1$

$$k_1=hf(t_n,y_n) \qquad (3\text{-}12)$$

Modified Euler $y_{n+1}=y_n+\frac{1}{2}(k_1+k_2)$

$$k_1=hf(t_n,y_n)$$

$$k_2=hf(t_{n+1},y_n+k_1) \qquad (3\text{-}13)$$

where $dy/dt=f(t,y)$. The same format allows the same

subroutine (MODEL), containing the differential equations of the model, to be simply used by all the algorithms.

3.7 SYSTEMS OF FIRST-ORDER AND HIGHER-ORDER DIFFERENTIAL EQUATIONS

Only the case of a single first-order differential equation has been treated so far. The mine water systems described in chapter 2 can generally be described by a set of differential equations. Although the systems discussed so far and the examples in appendices E and F, involve only first-order equations, some higher-order linear equations may be included in other models. It is first shown how higher-order differential equations can be reduced to first-order differential equations. It is then shown how a system of firstorder equations can be solved by applying the methods previously discussed. Only initial-value problems are considered.

3.7.1 *Higher-Order Equations*

Consider the linear second-order equation

$$\frac{d^2x}{dt^2} = -\frac{1}{M}\left(c\frac{dx}{dt}+kx\right) \qquad (3\text{-}14)$$

representing a vibrating system in which a spring with spring constant k restores a mass m, displaced by x, against a damping force equal to c times the mass velocity dx/dt. (A diagram of the system is shown in section 4.3 where this example is discussed further). The equation is simply converted into a pair of first-order equations by creating another variable y, then

$$\frac{dx}{dt} = y$$

$$\frac{dy}{dt} = \frac{-1}{M}(cy+kx) \qquad (3\text{-}15)$$

A simultaneous solution of the two equations would yield values of x and y, (displacement and velocity), at successive values of t(time). Therefore any system of linear equations of varying-order, can simply be converted to a larger set of first-order linear equations.

3.7.2 Solution of Systems of Equations

Consider the application of the modified Euler method (3-13) to a pair of first-order equations. The method of solution is explained in general terms together with the solution of two actual equations.

$$\frac{dx}{dt} = f(t,x,y) \qquad \frac{dy}{dt} = F(t,x,y)$$

$$= xy+t,\ x(0)=1 \qquad = ty+x,\ y(0)=-1$$

Letting h=0,1 the k_1 and K_1 values are first calculated *for both equations:*

$k_1 = h.f(t_n,x_n,y_n)$, and $K_1 = h.F(t_n,x_n,y_n)$.

$=0,1(1(-1)+0)$ $\qquad = 0,1(0(-1)+1)$

$= -0,1$ $\qquad = 0,1$

The k_2 values are calculated next:

$k_2 = h.f(t_n+h,x_n+k_1,y_n+K_1)$

$= 0,1((1-0,1).(-1+0,1)+(0+0,1)) = 0,071$

and

$k_2 = h.F(t_{n+1}, x_n+k_1, y_n+K_1)$

$= 0,1((0+0,1)(-1+0,1)+(1-0,1)) = 0,081$

Finally, the x and y values are calculated at the end of the time-step

$x_{n+1} = x_n+\frac{1}{2}(k_1+k_2)$

$x(0,1)=1+\frac{1}{2}(-0,1-0,071)$

$=0,9145$

$y_{n+1} = y_n+\frac{1}{2}(K_1+K_2)$

$y(0,1)= -1+\frac{1}{2}(0,1+0,081)$

$= -0,9095$

The above example can be extended to include any number of equations and can be solved in similar fashion using the simple Euler (3-12) and the Runge-Kutta (3-6) methods. The program statements of the three methods are listed and discussed in appendices B and C.

The simulation program, discussed in chapter 4, solves any number of linear first-order differential equations used in the formulation of a model. The simple Euler, Modified Euler and Fourth-Order Runge-Kutta methods are available as options. The program user enters the differential equations into a single subroutine along with the rest of the statements required to describe the model. In the above example, two equations are

solved for the two dependent variables x and y. In mine water system models, the differential equations are generally functions of far more variables than there are differential equations (or state variables). The extra variables may be functions of operating relationships and they may or may not be generated by the system. These extra variables present in the differential equation are therefore not determined directly from the solution of the differential equations. The different types of relationships and variables are discussed in chapter 5.

CHAPTER FOUR

4. A GENERAL PROGRAM FOR SIMULATING MODELS

4.1 INTRODUCTION

One of the basic requirements of a simulation program is to permit the systems analyst to concentrate his efforts on the modelling of the system and not on the process of programming the model in computer language. The systems analyst constructs the mathematical model and translates it into simple program statements understandable to the simulation program. The model is then entered into the simulation program as a single subroutine and can then be simulated. The program takes care of the data input, the simultaneous solution of the differential equation describing the system being modelled and the output of the results. The program presented herein therefore provides a general framework for solving any mathematical model which can be described by a system of first-order linear differential equations.

4.2 ADVANTAGES OF SIMULATION

It can be concluded from the discussion of mine water systems in chapter 2 that simulation by mathematical models is often the only practical means of studying the behaviour of such systems. James (1978), however, questions whether the simulation study is to have a *long-term pay-off any more tangible than a mere clear* explanation of the dominant processes and interactions involved. He questions the need for a simulation model by enquiring what analysis would be performed if the model were available for experiment. Cox (1968) lists some advantages of simulation, which are included in

the following list of reasons why it was decided to simulate mine water systems.

1) Models of existing and proposed complex mine water systems can be experimented with without the cost, risk and expenditure or time involved in experimenting with the real system. Examples of possible experiments are: a desalination plant introduced at some point in the system; an optimum allocation strategy (Grosman 1981) to supply mine service water from available sources to demand points having different quantity and quality requirements; a pump operation policy to reduce the total power-peak-demand for the mine as a whole. Changes are brought about by modifications to the model and/or by controlling pertinent parameters and variables. A change in one part of a system often has far-reaching interactions with many other parts and would be extremely difficult to trace manually.

2) Forecasting and projecting into the future may be accomplished as an aid to decision making and planning. The increasing cost of surface water resources, the environmental problems of disposing of used mine service water and the improved water quality requirements for mechanisation programs are some of the factors which will markedly affect mine water systems in the near future.

3) The more important variables can be identified in terms of their interactions and effects on the system performance. Parametric or sensitivity analyses may be performed, that is, measuring the effects of changing certain parameters. It is often useful to know the relative effects of evaporation, leaching, makeup water and infiltration

on water quality. It may be possible to produce simple, practical and approximate models by eliminating unimportant variables.

4) The time scale can be controlled; that is, expanded or compressed so that long-term or detailed short-term effects may be simulated.

5) The communication of findings to others is generally easier because a simulation may be visualised as representing the real system. A statistical analysis or a complex mathematical equation is not nearly as convincing, especially to a non technical person or to someone not familiar with the details of the problem.

6) Certain parameters that cannot easily be written as an equation, may be represented as a table of values or via a stochastic process having parameters or distribution functions that satisfy the relationship, such as Monte Carlo simulation. Many input parameters such as the variation of flows with time are determined from in situ measurements and are best used in tabular form - the model in chapter 7 uses tables of average flows. A further degree of sophistication in the example may be to use random numbers to choose values from probability distributions instead of average values. Various probability distributions may be constructed using sampling techniques to obtain the data required (Cox 1968).

7) Certain parameters and relationships are not known and simulation may be useful in helping to find them. Some of the mine water systems observed are extremely complicated and little is known about the quantity and quality of flows in many parts of

the system. The rate of leaching of salts from the ore into the mine service water is a particular example where simulation may be used to estimate parameters. It is felt that the rate of leaching (R) by the mine service water may be a first-or-second-order-reaction (n) and that it may be a function of the concentration (C) and equilibrium salt concentrations (E) of the service water, i.e.

$$R = \text{constant } X(E-C)^n. \qquad (4\text{-}1)$$

The constant and n in the above equation are unknown parameters. By observing the state of the system at various times, it should be possible to estimate unknown parameters by repeatedly simulating and changing the parameters until the simulation approximates the real system. The simulation program has been written in such a way that the simulation can take place with positive or negative time steps. The advantage of being able to simulate forwards or backwards through time is that the state of the system at the beginning of, or at the end of an observation time period, may be used as the initial values.

8) Operational control of systems or subsystems is often done via a properly contructed simulation model. In such applications the simulation model is made an integral part of the system. A monitoring system updates records so that parameters can be recomputed and 'optimal' control is carried out, based on the results of the simulation. Such a monitor and control system could simply consist of a programmed desk-top computer on site, which is periodically updated with observed data and used to make better decisions by being able to predict the consequences of certain actions.

4.3 SIMULATION PROGRAM OBJECTIVES

In the initial stages of development of the simulation program some of the following questions were unanswered: which mine water system(s) would be simulated; can a general model be constructed to represent any system; who would be responsible for constructing models and maintaining them and the simulation program; which computer and which language. Most of these questions, which are still valid today, are the reasons why an attempt has been made to meet the objectives discussed below.

4.3.1 General Framework for Simulating Mine Water System Models.

The simulation program provides the following facilities:

a) A simple format for entering any model into the simulation program when the system being modelled may essentially be described by a single or a system of linear first-order differential equations. Examples of such systems are mine water, vibrations, backwater, water-hammer and surge. The construction of simulation models is discussed in chapter 5.

b) Entry of input data (initial values, parameters, plotting requirements, function tables, data for variables stored in queues etc.) is simply done using data statements and/or interactive conversation through the keyboard. Data statements provide a means whereby input data may be stored on tape with the model and may be repeatedly used whenever the program and model are loaded onto the machine. Input data, entered via interactive conversation (respond-

ing to prompts on the screen), is destroyed whenever a change is made to the program, or when the computer is switched off.

c) Different relationships may be presented in convenient tables. Many model relationships are determined from measurements on site. Certain relationships, for example, water demand versus time, can be represented only as a table of data pairs and not as a convenient mathematical relationship.

d) Past variable values may be stored in queues. It is often necessary to know the value of certain variables at a time earlier than the current time in the simulation. For example, water being conveyed in a long pipe from one dam to another may have a long travel time. If the salt concentration of the water discharged into the downstream dam is required, then the salt concentration of the upstream dam must be known at the time when the water entered the pipe. i.e. at the current time, less the travel time. During a simulation only the latest values of all variables are stored and when the previous value of a variable is required then sufficient values are entered in a queue so that the value at the time of interest can be interpolated from the stored values. As the simulation proceeds by one time increment, the last value in the queue is discarded and the queue displaced by one position to make space for the latest value.

e) One of three different solution algorithms may

be chosen to solve the system of differential equations of the model. How the computational effort may be minimised by choosing the best algorithm for the time-step size and the accuracy required are explained in section 3.6 and in appendix E.

f) The flexibility of the program during simulation is illustrated by discussing some of the options available. Simulation is carried out over a specified time interval using a specified time-step size. At the end of the interval any or all of the following changes can be made before simulation continues: change the time-step size and sign, i.e. simulate backwards or forwards in time; change the input, table and queue data (b,c,d, above); change the solution algorith (e above); change the output specifications (g below). During simulation the initial variable values are retained so that simulation may repeatedly be started from the initial conditions, perhaps for stability, sensitivity analysis or accuracy estimations, (sections 3.3, 3.4 and 3.5). If the simulation appears to be going unstable (large numbers, unrealistic signs), then a 'panic button' may be pressed, which will halt execution and transfer control to the input mode where changes may be made before another simulation is attempted.

g) Output may be requested in various forms. Output consists of variable values at different times in the simulation and the user can specify whether the output is to be in tabular or graphi-

cal form, or both. Both outputs are displayed on the screen and can be printed on paper as well. The user specifies which variables, how frequently and during what time intervals the various outputs must be given. Tabular output is listed as it is generated during simulation, while the larger amount of output requiring graphical presentation is stored on tape until the end of the simulation, when all graphs are plotted.

4.3.2 Reliability, Simplicity and Maintenance.

Most programmers would rather start from scratch than make use of a program written by someone else. Experience has taught that most programs are difficult to follow and there are likely to be aspects which are not rigorously dealt with. Structured Programming embraces a collection of methods that result in programs: of sound design to ensure that the program does what is expected of it; can easily be modified or extended; can easily be adapted to different machines; can easily be shared by other users. Kelly (1980) describes how programs normally evolve until the result looks like a bowl of spaghetti. He describes the principles of structured programming as follows:

a) Programs must be clear and easy to read: by giving variables meaningful names (if the language permits); by including sufficient commentary; by confining the main logic to approximately one-page-long modules. One should be able to follow the logic by consulting more detailed modules (or routines) - doing this resulted in the modular structure and five levels of detail shown in appendix A. This top-down approach helps concentrate the reader's

attention on important aspects of the logic and is easy to follow because the modules only occupy about one page of source listing each. Detail is relegated to minor routines at a lower level where they belong.

b) The program must have a sound structure. Many programs tend to evolve and as time passes, extra portions of code are inserted until the result looks like a bowl of spaghetti. Research has been done on the subject and the findings were that any programming task can be completed with only three types of structure: sequence, choice and loop. Each structure has one entry and one exit and is executed from top to bottom. Choice is carried out using logical IF statements, and GOTO statements are avoided as they are the cause of most spaghetti. DO.... NEXT is avoided because the index is undefined on exit. Kelly discusses the reasons for this in his paper.

Kelly admits that languages such as BASIC and FORTRAN are not ideally suited to structured programming. Most of the principles discussed have nonetheless been used in the simulation program (appendix C). Because the reader can see all the essential information at a glance, structured programming has done away with the need for flowcharting and maintaining flowcharts. Each program module is discussed in Appendix B, using the idea of HIPPO diagrams (Hierarchical-Input-Processing-Output), a method developed by IBM for describing modular programs (Yourden (1975)).

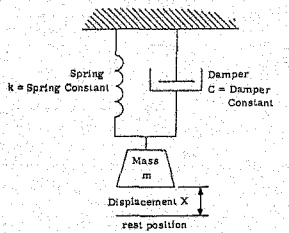
4.3.3 Available Hardware and Software Options.

The choice of hardware was restricted to the Hewlett-Packard HP-85 and 9830A desk top computers in the Department of Civil Engineering and the IBM370 mainframe facilities at the University Computer Centre. Software programs included a number of simulation packages available for use at the Computer Centre.

Simulation languages are all designed to take advantage of common features in simulation studies. These languages are intended to permit the systems analyst to concentrate his efforts in the modelling of the system and to greatly simplify the process of programming the model in computer language. Mize and Cox (1968) describe some of the older languages such as GPSS, SIMSCRIPT, GASP, DYNAMO and SIMULA. There is generally not an appreciable choice in the simulation languages available and users are forced to use the package(s) available at the nearest computing facility. The fifth editions of GPSS (1970) and CSMP (1972) are available at the Computer Centre at the University of the Witwatersrand but are currently being phased out and replaced by the second edition of ACSL (1975). Staff at the Computer Centre have considerable experience with CSMP (Continuous System Modelling Program) but practically no experience with ACSL (Advanced Continuous Simulation Language). The packages available at the Computer Centre, GPSS and CSMP are both IBM packages which require familiarity with introductory users' manuals before the users' manuals can be attempted (notoriously difficult to follow). Both languages assume some knowledge of control theory, boolean algebra and block diagram representations of systems (see Ogata (1978)).

Consider the example shown in figures 4.1 to 4.3 of a simple spring, mass damper system taken from the CSMP

(Diagrams from CSMP Users Manual)



Model Equation: $\ddot{X} = \frac{-1}{m}(c\dot{X} + kX)$

Fig. 4.1 Model of spring mass damper system

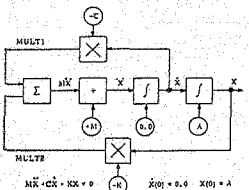


Fig. 4.2 Block diagram for the solution

```
MX2DOT=MULT1+MULT2
X2DOT=MX2DOT/M
XDOT=INTGRL(0.0,X2DOT)
MULT1=-C*XDOT
X=INTGRL(A,XDOT)
MULT2=-K*X
```

Fig. 4.3 Structure statement development from the block diagram

Users Manual. The second-order linear equation of the above model,

$$\frac{d^2x}{dt^2} = -\frac{1}{m}\left(c\frac{dy}{dt} + kx\right),$$

can be converted to two first-order equations

$$\frac{dx}{dt} = y$$

and

$$\frac{dy}{dt} = -\frac{1}{m}(cy + kx), \qquad (4\text{-}1)$$

as shown in section 3.7.1. In the mine water simulation program the first order differential equations are entered as F(1)=dA(1)/dt,F(2)= dA(2)/dt,---etc., and the simultaneous solution of the equations (section 3.7.2) yields values of A(1), A(2) ---- etc., at successive intervals of time. Applying this notation to the spring model by letting A(1) = X and A(2) = y, the above two equations (4-1), written in BASIC, would be

```
F(1) = A(2)
```

and

```
F(2) = -(C*A(2)+K*A(1))/M                    (4-2)
```

The above procedure and resulting program statements (4-2) are considerably simpler than the use of block diagrams and the statements as shown in figures 4.2 and 4.3 respectively. The programming and running of models is discussed in greater detail in chapter 5 and appendix E.

ACSL, the latest simulation package in the 'Wits System', allows model preparation from block diagram interconnection, conventional FORTRAN statements or a mixture of both. Solution is via a remote terminal or keypunched cards. The user manual is clear and easy to understand with useful examples.

The majority of package simulation languages can only be used on large mainframe computer installations. The use of packages on mainframes lacks many of the advantages of personal computing with a desk top computer. Following are some of the reasons why it was decided to develop the simulation program on a desk top computer instead of using a simulation package on the mainframe computer:

1) The Wits System (and large systems in general) operates only during certain hours and difficulty is often experienced in gaining access to terminals. The system experiences regular breakdowns (several per week) which often results in long down-times and loss of programs not stored. Difficulty is also experienced when files allocated to the department are fully utilised and storage is limited. Printed output is available at the computer only after a time delay and is sometimes lost or accidentally taken by others.

2) The Hewlett-Packard HP-85 computer is one of the most popular and up-to-date desk top computers being used in South Africa for engineering and scientific work. Desktops (micros, minis etc.) are continually becoming cheaper, more powerful and compact and will always be preferred to the less friendly, less personal

mainframe where the problem size permits. BASIC is a simpler language than FORTRAN and it is standard with most scientific desk top computers, while FORTRAN is not.

3) The simulation program was developed from basics for use on the HP-85 to avoid dependence on a single computer facility. The program developed (and the computer) can easily be transported to another site or translated for use on another computer. The program has many of the powerful features of the mainframe packages (section 4.3.1), yet it is small enough to be completely understood by someone in a relatively short time. The development of the simulation program led to a good understanding of the basic principles and limitations involved, something which is not normally possible when using large package programs. The limited experience of computer staff with the package program ACSL, and the package mounting time of several hours (ACSL is presently under-utilised) are also factors which contributed towards the decision to develop a simulation program.

If a very large and detailed mine water system has to be modelled at some stage, then the use of a simulation package program like ACSL may become necessary.

4.4 PROGRAM AND COMPUTER RESTRICTIONS

The simulation program is written in BASIC language for the Hewlett-Packard HP-85 and includes certain statements peculiar to the HP-85. Conversion of the program to fit another computer using BASIC language would not involve much work as variations in BASIC

between different computer manufacturers are generally not significant.

The simulation program and the complete detailed model in chapter 7 occupy close to 32 kilobytes of computer capacity (the upper limit of the HP-85 computer). If the program should be converted for use on another computer, then a computer with a capacity greater than 32 kilobytes should be considered. A larger capacity would then be required if larger models are needed, if the simulation program is extended or if arrays and matrices are expanded.

CHAPTER FIVE

5. DEVELOPING AND USING MINE WATER SIMULATION MODELS

5.1 INTRODUCTION

Simulation models are often difficult and time-consuming to code. In addition, many data must be collected for digestion by the computer and for validation of the model. It must be decided whether the study is to have a long-term payoff, i.e. what analysis would be performed if the model were available for experimentation. In other words the purpose of the simulation must be identified and also whether the purpose can be met. These are some of the questions which must be answered first if the possibility of a trivial answer is to be avoided.

The success or failure of many past water resource studies is in a large part attributable to the efforts expended or not expended on ensuring adequate and meaningful communication amongst analysts, engineers responsible for systems operation and design, and policy makers (Loucks et. al. 1981). Those who will use the models and present the information derived from the models, as well as those responsible for making decisions must be intimately involved with model development, solution and analysis. Only then can they appreciate the assumptions on which any model is based, and hence adequately evaluate the reliability of the results. Any water resource systems study that involves only outside consultants and internal communication between consultants and planners within a responsible management agency, is unlikely to have a significant impact on the planning process. Models that are useful are alive, constantly being modified and applied by those who are

responsible for plan preparation, evaluation and implementation.

The chapter is intended to give some guidelines on the construction and use of models. Reference is made to two models constructed of Unisel Gold Mine in appendices E and F. Meta Systems Inc. (1978) does, however, point out that simulation is one of those activities which can be learnt well but taught only poorly. The examples in the appendix have therefore been explained and discussed in detail and features of the models which are common to all gold mine water systems can be used to construct other models. The whole process of model construction is an iterative one involving continual changes as one's understanding increases and as more information becomes available. This is illustrated in fig. 5.1 below.

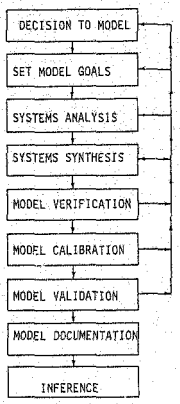


FIG. 5.1 THE MODELLING PROCESS

There is no best single model for all situations. An important decision that must be made early in the planning process is the selection of the modelling method or methods appropriate. A mine water system, for example, which uses excess groundwater infiltration without recycling may be modelled and optimised using deterministic methods without recourse to simulation (see Grosman 1981). The modelling method must also be adapted to fit within the limits of available time, money and human resources.

The objectives of the Unisel Gold Mine study and the development of simulation models were partly to understand mine water systems better and to study the process and applicability of simulation to mine water systems. Simulations on mine water systems carried out in future would probably be for the purpose of analysis or design and would therefore involve goals or some objective function. For example, it may be necessary to design a minimum volume storage dam on surface which is large enough to contain all water pumped from underground during low demand periods on weekends. The effects of a desalination plant, settlers at the head of drains or a different blend of make-up water are examples where a simulation can be used for analysis (experimental) purposes. The model must be constructed so that the goals can be achieved. Measures of performance (for example accuracy levels) must be specified to ensure that the model does achieve its goals. The whole process of model development is an iterative trial-and-error process of repeating and modifying earlier steps (shown by the arrows in fig. 5.1). Having sufficient data, for instance, is a stringent requirement and may be the decisive criterion in modifying or limiting the original goals which can be achieved with the model.

Once it has been decided to simulate and the initial model goals have been set then the steps shown in fig.5.1 may be

described as follows:

1) Systems Analysis: the salient components, interactions and dynamic mechanism of the system are identified.

2) Systems Synthesis: the system's behaviour is organised in accordance with the preceding Systems Analysis stage.

3) Verification: the model's responses are compared with those which would be expected if the model's struccure was prepared as intended.

4) Calibration: the model parameters are adjusted in order to produce an output that is close to the actual observed output. One or more sets of input and output data are used.

5) Validation: the responses from the verified and calibrated model are compared to corresponding observations of, and measurements from the actual system. Data that are independent of the calibration data are used.

6) Documentation: flow diagrams, assumptions, limitations, instructions etc. This dissertation serves as an example of documentation.

7) Inference: experiments with and comparisons of responses from, the verified and validated model; this is the design stage.

These steps are often not taken systematically, which can jeopardise the development of the model. The following typical questions should continually be asked during the modelling process:

- just how complex should the model be?
- should more data be collected to improve the model?
- is the model producing reasonable results?
- are the correct processes involved?

5.2 SYSTEMS ANALYSIS OF THE PROTOTYPE SYSTEM

Meta Systems Inc. (1975) describe Systems Analysis in the context of simulation model building as the process whereby the following items are obtained:

1) System Components: Example: cascade dams, external supply sources, discharge sinks, refrigeration plant.

2) Relationships:

   a) Operating Relationships: rules whereby the components are operated. Example: pumps are switched on when the dam level reaches a certain point and the downstream dam is not full.

   b) Internal consistency relationships: rules which specify the physical realities of the prototype. Examples: the law of continuity which states that the inflow rate minus the outflow rate (of water volume or salt mass) equals the change in storage

   c) Evaluating relationships: rules which govern the computation of response or measure the fulfilment of the objective function. Example: the object of simulation may be to determine the maximum salt concentration of water in a component when a desalination plant is incorporated in the system. The salt concentration

equals the mass of salts stored divided by the volume of water in the component.

3) Variables

a) Independent variables or parameters: values assigned to the constants of the several relationships which jointly define a particular design or analysis experiment. Examples: capacity flow rates of pumps; on/off dam levels for pumping; salt concentration of the regional water board; evaporation rates.

b) State variable: representing the condition of the components, generally time varying and dependent on the model. Examples: the mass of salts and volume of water in each storage element.

c) Internal variables: dependent variables generated by the system which affect the state of the system and may be of interest as output. Examples: make-up water inflow which may depend on the level of a dam.

d) Output variables : dependent values calculated from the state variables specifically to enable the response of the system to be evaluated and to check the results against the objective function. They do not affect the state of the system. Examples: the salt concentration of flows and of water in storage components.

e) External variables: variables given independent' which act upon the system. Example: the mine service water demand and the inflow to the settlers at various times of a weekly cycle.

4.3 SYNTHESIS OF THE MATHEMATICAL MODEL

At this stage the goals of the simulation model have been set and Systems Analysis has identified the components, variables, parameter and relationships of the physical system. These four component elements must be expressed such that a model can be constructed that realistically imitates the system being studied.

Components are usually expressed quantitatively in terms of their significant attributes. Some of the components of the mine water system models of Unisel Gold Mine are each described by one differential equation for the rate of volume change and one for the rate of change of salt mass (see chapters 2 and 3). Variables are expressed within functional relationships. Parameters are expressed as constants that can be changed only at the command of the experimenter. Relationships are expressed as mathematical and logical statements. Collectively these expressions comprise what is called a mathematical model of the system being investigated.

The model is an abstraction of the physical system it presumably represents. Mize (1968) summarises guidelines for determining the proper degree of abstraction as follows: The model must be

1) Simple enough for manipulation and understanding by those who would use it,

2) representative enough in the total range of the implications it may have, and

3) complex enough to accurately represent the system under study.

This is a matter of judgement and experience on the part of the analyst or model builder.

5.3.1 First-stage and Higher-Order Models

James (1978) recommends an orderly development from a first stage model to higher-order models. The simplified model (Unisel Gold Mine in chapter 6 is an example of a first stage model . The model treats the prototype or real system as a single entity and can be used to check the reliability of existing data. High-frequency processes such as water volume fluctuations are filtered out. Dominant processes such as the leaching rate or evaporation can be identified for elaboration in the next stage of development and the system for obtaining data can be modified at each stage. Data collection can be expensive and time consuming and a process of orderly model development will also, ensure optimum use of resources for data collection. The detailed model of Unisel Gold Mine in chapter 7 was developed from a number of simpler models which initially dealt with water quality and quantity aspects separately but considered the components of the prototype system individually.

Model development requires more-or-less continuous sensitivity analysis. The analysis proceeds by holding all parameters constant but one and varying that parameter within reasonable limits. The variation of the objective function (for example: measure of fit between observed and calculated salt concentration) is then observed. If a small variation in the parameter produces large changes in the objective function, the system is said to be sensitive to that parameter and vice versa. If a parameter is extremely insensitive then the parameter and its associated system component may be redundant and should be deleted from the next stage of development of the model. Conversely, a component represented by a very sensitive

variable may need to be described in greater detail in the model. Of course the values of other parameters held constant may affect the sensitivity and so their values should also be typical of the conditions modelled.

The greater detail that generally results from each stage of model development (disaggregation) often results in greater data requirements. In some instances there may not be sufficient resources available for data collection (time, money, people). The model goals may then have to be changed.

Due to repeated disaggregation at each stage, it may be found that insufficient computer resources limit the modelling process. For example, the detailed model of Unisel Gold Mine in chapter 7, when loaded together with the simulation program on the Hewlett Packard HP85 computer leaves only 1500 bytes of memory for any further disaggregation. Figure 5.2 below is an expansion of fig. 5.1 which includes the points discussed.

5.3.2 Deterministic and Stochastic Models

A simulation model may be deterministic or stochastic, depending on the significance of randomness among input events, outputs or relationships. If no random aspects are involved the model is deterministic. The models of Unisel Gold Mine are deterministic. Stochastic meteorological phenomena such as humidity, temperature and pressure, on the other hand, may significantly affect evaporation. The time variation in demand for mine service water could also be evaluated statistically. Mine water models can be operated in either or both types of mode.

Undoubtedly the most data-demanding model type is the stochastic or probabalistic model when compared with its deterministic counterpart. Deterministic models yield estimates of mean values of quantity

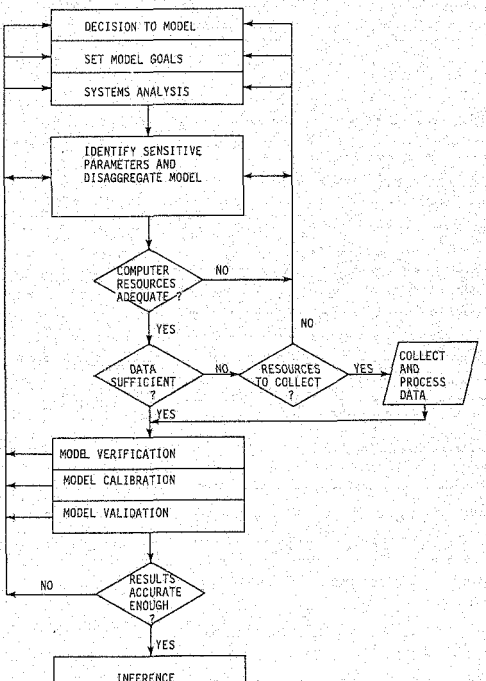


FIG. 5.2 Detailed Modelling Process

and quality constituents, whereas probablistic models explicitly take into account the randomness or uncertainty of various physical, biological or chemical processes. Validation of stochastic models is especially difficult due to the quantity of prototype data necessary to compare probability distributions of variables rather than just their expected or mean values.

Unisel Gold Mine was selected because it is a simple system compared with other gold mines investigated. The mine has a sophisticated monitor and control system from which useful data can be obtained for simulation studies. Even with such a simple system, considerable work has been done in bringing the model to its present form. Essential data is still being sought and little is known about the chemical leaching processes involved . The inclusion in the Unisel model of detailed refinements such as stochastic relationships at the present stage of development would probably not make the model any more valid or accurate.

5.3.3 Time-Sequenced and Event-Sequenced Models

A simulation model may be time-sequenced or event-sequenced. In time sequencing the computer examines the state of the system (flows, volumes, salt masses etc.) at successive time intervals. This has the disadvantage that events of interest may go unnoticed. Consider, for example, a storage dam on surface that receives make-up water during a time interval and from which the same volume flows underground to supply the mine with MSW. At the end of the interval there is no evidence of either events as the volume has not changed. A further disadvantage of time-sequencing is that pumps, for example, can only be switched on (or off) at the end of a time

interval. If the time interval is excessive then the pump sump or dam level may be unrealistically high (or low) at the end of an interval. Conversely event sequenced simulations note the time whenever an event of interest occurs.

The form in which water resource (and mine water) data is available generally makes event-sequencing too cumbersome for general use. The simulation program used to run the models is therefore time-sequenced. The disadvantage of events of interest going unnoticed is overcome in the example in chapter 7 by creating output variables for the events which can then be monitored during output. In situations where it is necessary to reduce the time-step for reasons other than accuracy, a less accurate but faster solution algorithm can be used. There is a choice of three algorithms to choose from in the program; the Euler, Modified Euler and Fourth-Order Runge-Kutta methods.

5.4 VERIFICATION, CALIBRATION AND VALIDATION

The experimenter or analyst should attempt to demonstrate that the model which has been formulated adequately represents the system that is being studied. Mize (1968) feels that this process of validation should be carried out by performing manual calculations before a computer program is constructed. The author feels that this step is best performed using the computer. It cannot be expected that the model will be an exact representation of the physical system being studied. The analyst should however satisfy himself that the more important characteristics of the system are contained in the model and that the mathematical and logical statements of the relationships in the model adequately portray the true behaviour of the system components.

5.4.1 Model Verification

In the verification of a deterministic model it is imperative that some specific condition is used from which the model response could be exactly predicted if, indeed, the model is structured as intended. Verification tests are not conducted by comparisons of model responses with those of the prototype system; rather, comparisons between model responses and theoretically anticipated results are made in as many cases as possible for which this is known (James 1978). The model should respond exactly according to the relationships used in the model. E.g. do the pumps switch on and off at the correct switch levels? Does the dam upstream of a pump start filling? Does the salt concentration of the dam increase or decrease according to the concentration of the inflows? These are some of the questions which can help to verify a model.

5.4.2 Model calibration

Model calibration is performed using one or more observed data sets of both inputs and outputs. The model parameters and, indeed, the model itself are adjusted or modified in order to produce an output that is close to the actual observed water quality and quantity as is possible. The evaluation of model parameters, usually a subjective trial-and-error procedure, can be aided by least squares, quasi-linearization and other statistical methods (Loucks et al 1981).

The time interval is important as it affects the accuracy and duration of the simulation. The intervals should be selected as large as possible but still ensuring that the state variables change so little during the time interval that the initial

values can be assumed to govern the relationships during the entire interval. This can be accomplished by reducing the time step during repeated simulations until no significant difference in the system response is detected.

5.4.3 Model Validation

Validation implies the comparison of results of field measurements to another model known to be accurate, or to some other adequate criterion to ensure that the model is producing accurate results. Model verification requires a set of input and output data which is independent of the data used to calibrate the model. A model is verified if the model's predictions for a range of conditions other than those used to calibrate the model, compares favourably with observed field data. If these comparisons indicate that the model results are not sufficiently accurate, the model is altered and the procedure is repeated. The validation procedure, as shown in fig. 5.2, generally involves several iterations of model changes and field measurements before a satisfactory confidence level is achieved. Here again the criteria for deciding whether or not model output and observed field data are essentially the same, for the same input conditions, is largely subjective. What constitutes a satisfactory comparison depends on the nature of the problem, the type of model developed and its purpose, and the extent and reliability of available input and output data.

Techniques used in the validation of an analytical model are listed in James (1978):

1) Validation of parameters and results against field observations.

2) Cross-correlation of its results with those of another proved model.

3) Some combination of field observations and modelling.

The most accurate method of validation of a model is the comparison of responses from the (now verified) model with corresponding field measurements. In some of the mine water systems examined to date, field measurements are extremely difficult because facilities do not exist for monitoring the performance of the system (level recorders, flow meters, recorded times of operations, etc.). Under conditions where proper validation tests are not feasible, the analyst then undertakes a greater risk in making inferences from the model responses. Under these conditions it may be preferable to change the model goals or not to simulate in the first place.

5.5 INFERENCE FROM THE MODEL

In the final stage experiments are conducted with the verified, calibrated and validated model. There are a number of categories into which most analytical modelling goals can be placed:

1) The dynamic behaviour of the model during a stipulated period of time, for example, the salt mass build-up in the water system.

2) The determination of the relative (or marginal) effects of changes in some of the environmental conditions on the model's expected response at the end of a specified period of time. For example, the effect on the equilibrium salt concentration of add-

ing a desalination process at some point in the mine water system.

3) The determination of the particular environmental specification at which the model's expected response is optimised, for example the minimum cost desalination plant to satisfy the water quality requirements of a demand point.

4) The determination of unknown parameters or relationships within the system by trial-and-error until the model output fits the observed output for the given input. For example it may be possible to estimate parameters required for the relationship describing the leaching of salts from ore, by observing (in the prototype) the transient changes in salt concentrations with time as the quality of make-up water is varied. The leaching parameters can be determined by varying them in the model until the model output fits the observed data.

5.5.1 Simulations Dealing With Stead-State and Transient Conditions.

A simulation may deal with steady-state (equilibrium) or transient (unsteady) conditions, or both. The study of a mine water system during a period after which the system has been purged of polluted water and replaced by good quality water from the regional water board, lies in the area of transient analysis. The mine water quality can be expected to deteriorate in the period subsequent to the purge. If the environmental conditions of the mine water system remain constant, the system will reach equilibrium or steady state after a certain period of time. During this transient period, the mass rate of

salt inflow to the system will exceed the outflow rate. A zero net inflow rate of salt mass signifies steady-state or equilibrium conditions regarding the salts present in mine water system.

Models can deal with multiple states simultaneously depending on what is being modelled. The model of Unisel Gold Mine in chapter 7 deals with water quality and quantity aspects which can both be either in a steady- or unsteady-state at the sam times. For example, there may be a zero net in of water into the system (steady-state), yet the salt concentration in the system is in a transient state. The Unisel model responds to weekday and weekend demands for mine service water, which varies throughout the day. Water entering or leaving components, and the system as a whole, is never constant. Since the water quality and quantity is constantly changing in each system component and the system as a whole, it can be concluded that the system is never in equilibrium or steady-state in the true sense of the word. If, however, the system response is compared for successive weeks it can be seen whether the internal and external cycles of water quality and quantity are being repeated or not. In this case it may be convenient to define steady-state conditions as those which produce weekly quality and/or quantity responses which are identical.

Starting conditions are important when simulating. The system, (or model) is normally allowed to attain equilibrium before the system performance is recorded, in which case two alternatives are open; ignore data generated during some intial 'warming up' period, or choose starting conditions that approximate the steady-state condition of the system. Owing to the unfortunate fact that accurate starting conditions cannot generally be specified for all variables

a combination of the alternatives is usually necessary. A practical way to approach the problem of starting conditions is to use the best estimates of starting conditions and then to simulate sufficient cycles (weeks in the Unisel example above) until equilibrium is attained. The final values obtained are then used as the starting values for subsequent simulations.

5.5.2 Sampling and Search Procedures for Model Development and Optimisation.

One of the major problems inherent in simulation modelling is the determination of the number of sets of design and operating policy values (decision variables) that need to be simulated. During model development such procedures may be employed in the verification and calibration stages to find certain parameters and relationships. Having noted that simulation is a trial-and-error technique rather than a deterministic analytic process which is used to find unknowns, it is useful to ask how the analyst proceeds from trial to trial and how reliable are the results after a given number of trials. In other words, should the work continue at all and, if so, what should the next trial be. This is the general question of sampling and search procedures.

Simulation is often employed in design problems to optimise the performance of a system. For example, finding the minimum cost of supplying water from different sources to demand points in a mine, subject to quality and quantity constraints. An optimisation would involve simulations with different combinations of the decision variables. Each simulation will result in a description of the system's performance as measured by the objective function

(a cost value in the example). Many such performance pictures (or cost values), each one corresponding to a set of decision variables, define an imaginary response surface. The optimisation problem is analogous to finding the highest (maximisation) or lowest (minimisation) point on the earth's surface. The highest point on the surface in a maximisation problem corresponds to the global optimum and any other peak corresponds to a local optimum.

The uniform grid sampling approach consists of an examination of specific uniformly spaced values of the decision variables. In large problems with many decision variables, an evaluation of the response surface on even a coarse grid requires a very large number of simulations. A coarse mesh would be suitable for certain insensitive variables while others would necessarily have to be subdivided on a finer grid. For example, if there are only four decision variables and each is assigned five possible values, the number of combinations or possible simulations is 4^5 or 1024. A finer grid could result in combinations that require years of simulation on high speed computers. Consequently, except in the most simple situations, uniform grid sampling is highly inefficient.

The random sampling approach consists of randomly selecting different designs, that is feasible sets, of decision variables . Quantitative statements about the reliability of the results can be made. Consider, for example, the results of 30 simulations of 30 (n=30) sets or combinations of decision variables (X_1, X_2 --- X_{30}).The simulations result in 30 values of the objective function B(Xi)(i.e.,30 points on the response surface). Assume that the probability that all 30 values of B(X) are less than some value Bp is 0,9 (p=0,9). The probability that each B(Xi) is less than Bp is also 0,9 or p. Hence the pro-

bability that all 30 objective function values (BX_1)____ B(Xn) are less than 0,9 is $0,9^{30}$ or p^n. Thus the probability that at least one of the 30 B(Xi) exceeds Bp is $1-0,9^{30}(1-p^n)$, or 0,957. In other words, the probability that the best of the objective function values (the least cost for example) falls in the upper 10% (100p%) of all the values yielded by all possible sets of decision variables is approximately 96% ($100(1-p^n)$%). While the probability that the best of 30 trial designs is in the upper 30% of all designs is 96%, one does not know how large the absolute difference between the optimum value of B and the best of those observed may be.

The nature of the results (i.e., the shape of the response surface) is a useful indicator of how many samples should be taken. Fewer samples are required for response surfaces which are relatively flat and smooth near the optimum.

Sequential search procedures utilise previous results to calculate what adjustments might result in 'better' performance with respect to the objective function. Loucks et al (1981) states that the most frequently used sequential search procedure in water resources analysis is trial and error. This is used because it is simple and because the problems are too large to be helped much by formal sequential search procedures. The trial-and-error method moves in the direction the user 'feels' will result in the greatest change in the performance. This depends very much on the user's understanding of the system being simulated.

Another sequential search approach is to use the partial derivatives of the objective function to identify the direction in which to change the decision variables in order to maximise the rate of change of the objective. If each design or set of decision vectors

consists of k decision variables x_1, x_2, ---- x_k, then each variable can be marginally adjusted and the model can be run. The difference ΔB in the objective function B for the marginal change Δx_j in x_j can be used as an approximation to the partial derivative so that

$$\frac{\partial B}{\partial x_j} = \frac{\Delta B}{x_j - (x_j - \Delta x_j)} \qquad j = 1, 2, \text{---- } k$$

This approach is explained in greater detail in Meta Systems Inc. (1975). Stark et.al. (1972) give useful examples on steepest gradient search techniques.

Each of the search and sampling methods has its own advantages. It follows that the most used procedure often involves a combination of all these methods. This hybrid sampling approach could make use of random or grid sampling to locate initial 'interesting' regions of the response surface followed by a directed steepest gradient search to locate the optimum. There is no guarantee that the global optimum will be found in any of these or more sophisticated procedures unless the problem satisfies a number of very restrictive mathematical conditions.

If a response surface appears smooth and devoid of abrupt discontinuities then fewer sample points are indicated. The identification of the exact optimal solution may not even be worth the cost of investigation. Conversely, if the response surface is characterised by abrupt peaks with near vertical walls, the sampling procedure must be more refined (and consequently more expensive) in order to be sure that the highest peak is not overlooked. All these approaches must be augmented by sound engineering judgement as there is no easy rule for judging the adequacy of a particular alternative chosen for simulation.

CHAPTER SIX

6 A SIMPLIFIED MODEL OF THE WATER RETICULATION SYSTEM IN UNISEL GOLD MINE

The simplified model of the water reticulation system in Unisel Gold Mine is shown in fig. 6.1. Use of water for the various mining activities continuously circulated in the mine is described in chapter two. At various points in the cycle water leaves the mine in the following ways: by windage and evaporation from surface cooling towers and spray ponds; with the ore mined; with mud pumped out; by evaporation from within the mine and by periodic overflow of the surface dams.

In the simplified model, water lost is assumed to be replaced by make up water from the nearby surface supply dam and/or from the Regional Water Board. The volume of water in the simplified model is therefore assumed to be constant.

During evaporation, pure water is removed and any inorganic salts which were present in the water are left behind in the system. Make up water added to replace the evaporation loss contains more salts and results in an increase in the mass of salts in the system. During circulation, water comes in contact with the ore being mined and salts are leached from the ore, further increasing the mass of salts in the water. If no water other than by evaporation were removed then the concentration of salts in the system would theoretically increase indefinitely. In practice, the dissolved salts are removed from the system with the non-evaporative water losses from the system, described above, (overflow, mud, ore and windage). Whatever the initial salt concentration of the water in the system, the concentration will eventually reach an equilibrium value. At that stage the mass flow rate of salts leaving the system will equal the inflow rate.

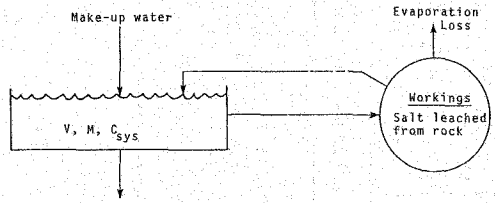
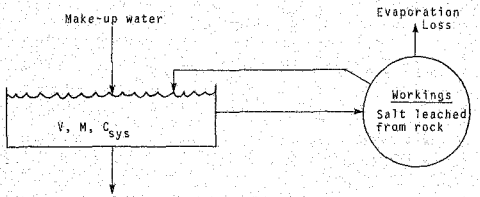


Fig. 6.1 Simplified Model of Unisel Gold Mine



Losses = overflow + mud + ore + windage

Fig. 61 Simplified Model of Unisel Gold Mine

The various concentrating and diluting effects of water flows into and out of the system are described in detail in chapter two.

The way in which the average salt concentration of the system changes with time from some initial value to some other value and eventually to a constant equilibrium value is predicted using the simple model shown. The model is mathematically described by a single first-order differential equation, which, due to its simplicity, is solved analytically to give relationships which are used to check the numerical solution of the differential equation in the simulation program.

6.1 THE MATHEMATICAL MODEL

The following symbols are used:

- t time
- M Mass of salts in the system at time t.
- V Constant volume of water in the system.
- C Concentration of salts (salt mass per unit volume).
- Co Initial concentration of salts in the system at time to.
- Cf Final concentration at time tf.
- C_{sys} The average salt concentration of the system.
- L Mass of salts leached per unit time.
- Q Flowrate.

The differential equation

The rate of increase of salt mass in the system equals the salt mass inflow rate minus the salt mass outflow rate, i.e.

$$\frac{dM}{dt} = (\Sigma Q.C)_{make\text{-}up} + L - (\Sigma Q)_{losses}.C_{sys} \qquad (6\text{-}1)$$

therefore

$$\frac{dC_{sys}}{dt} = \frac{1}{V}\frac{dM}{dt}$$

$$= K_1 - K_i.C_{sys} \qquad (6\text{-}2)$$

$$K_1 = \frac{(\Sigma Q.C)_{make-up}}{V} + L$$

and

$$K_2 = \frac{(\Sigma Q)_{losses}}{V} \qquad (6-3)$$

are both constants in the model.

6.2 ANALYTICAL SOLUTION OF THE MODEL

Rearranging equation (6-2) and integrating as follows:

$$\int_{Co}^{Cf} \frac{dC_{sys}}{K_1 - K_2 . C_{sys}} = \int_0^{tf} dt$$

$$\left[-\frac{1}{K_2} . \ln(K_1 - K_2 C_{sys}) \right]_{Co}^{C_f} = t \qquad (6-4)$$

The following relationships are obtained from equation (6-4):

a) Time for the average salt concentration of the system Csys to change from Co to Cf is

$$t = \frac{1}{K_2} \ln \left[\frac{K_1 - K_2 . Co}{K_1 - K_2 . Cf} \right] . \qquad (6-5)$$

b) The final system salt concentration after a time lapse of t and an initial salt concentration of Co is

$$Cf = \frac{K_1 - (K_1 - K_2 . Co) e^{-K_2 t}}{K_2} \qquad (6-6)$$

c) The equilibrium salt concentration of the system after an infinite time of operation is

$$Cf = \frac{K_1}{K_2} \qquad (6-7)$$

It should be noted that the final concentration Cf is independent of the initial salt concentration Co and depends only on K_1 and K_2.

Example

The above equations are valid for any system of consistent

units. In this example, volume, mass and time are measured in megalitres (Mℓ), kilograms (kg) and days (d) respectively. Concentration is often expressed in units of milligrams per litre (mg/ℓ), which is numerically the same as in kg/Mℓ units. Following is a list of basic input assumptions for this example.

Average Flow (Mℓ/d)		Concentration (kg/Mℓ)
Make up Water		
Supply dam	1,5	10 000
Rand Water Board	1,0	500
	2,5	
Water losses		
Overflow	0,2)	
Mud pumped	0,8)	
Ore loss	0,3)	Csys (variable)
Windage	0,3)	
Evaporation	0,9	0
	2,5	

The average volume of water in the system is estimated to be 13,2 Mℓ and about 3000 kg of salts is leached per day by water which comes into contact with the ore and remains in the system.

The constants, K_1 and K_2 above are calculated as follows:

$$K_1 = \frac{(1,5.10000 + 1,0.500)+3000}{13,2}$$

$$= 1401,52 \text{ Kg/Mℓ/d} \qquad (6\text{-}8)$$

$$K_2 = \frac{(0,2+0,8+0,3+0,3)}{13,2}$$

$$= 0,121212/\text{d} \qquad (6\text{-}9)$$

Equation (6-6) is used to find the system salt concentration after 20 days, assuming an initial salt concentration of 500 kg/Mℓ (or mg/ℓ).

$$Cf = \frac{1401,52-(1401,5\ 0,1212.500)e^{-0,121212.20}}{0,121212}$$

$$= 10583 \text{ kg/M}\ell$$

similarly C_f = 11562,5 kg/Mℓ after 100 days

Using equation (6-7), the equilibrium salt concentration is

$$C_f = \frac{1401,52}{0,121212}$$

$$= 11562,5 \text{ kg/M}\ell$$

which agrees to within one decimal place with the concentration calculated above after 100 days.

6.3 NUMERICAL SOLUTION OF THE MODEL

The single differential equation, (6-1) above, is solved numerically using the simulation program. The equation is written as a function of the variables, A(1), A(2),---A(11), even though some of the values are parameters of the system and do not change with time, for example the volume of water in the system. Expressing (6-1) into variables facilitates changing any parameter or variable by simply keying in a new value before or during an interrupted simulation, without having to modify the model equation(s).

Equation (6-2),

$$\frac{dC_{sys}}{dt} = K_1 - K_2.Csys,$$

is written in BASIC as

```
F(1) = K1-K2*A(1)                                    (6-10)
```

and K_1 and K_2, calculated in the example above (see 6-8 and 6-9), appear as :

```
K1 = (A(4)+A(5)*A(3)+A(10)/A(11)                     (6-11)
```

and

```
K2 = (Q1+A(6)+A(7)+A(8))/A(11).                      (6-12)
```

Only variables (or parameters) in the form A(i), where i = 1,2,3 ----, can be changed or displayed as output by

the simulation program. Q and C, in the list of symbols below, denote flow and salt concentrations respectively.

Program Variable	Description	Value
A(1)	C system	500 kg/Mℓ*
A(2)	C supply dam	10000 "
A(3)	C_{RWB}	500 "
A(4)	Q supply dam	1,5 Mℓ/d
A(5)	Q_{RWB}	1,0 "
A(6)	Q mud pumped	0,8 "
A(7)	Q ore loss	0,3 "
A(8)	Q windage	0,3 "
A(9)	Q evaporation	0,9 "
A(10)	Mass of salts leached	3000 kg/d
A(11)	System water volume	13,2 Mℓ
Q1	Overflow	0,2 Mℓ/d**

* C system is the only value which changes during the simulation.

** Q1 is a variable not recognised by the program and can only be defined, changed or displayed as a result of statements written by the user in the modules MODEL, INITIAL and FINAL.

6.3.1 Entering the Model and any Pre- and Post- Simulation Instructions.

The tape cartridge is inserted into the Hewlett-Packard HP-85 computer and the simulation program is loaded from tape into memory with the command

```
LOAD "MASTER".
```

The modules INITIAL, MODEL and FINAL when listed with the command

```
LIST 4630,
```

contain no model and user instructions and should therefore result in the following listing:

```
4630 ! ----------MODEL
4640 REM MAIN SUBR TO CALC F(i),
     K(i,z)FOR ALL i AND z=1,2,3
     ,,,
7960 FOR J=1 TO N0
7970 K(J,Z)=H*F(J) ! Z=1,2,3OR4
7980 NEXT J
7990 RETURN
8000 ! ----------INITIAL
8800 ! DATA FOR 1)INIT VALS
8850 ! DATA FOR 4)PRT LIST
8870 ! DATA FOR 6)PLOT INPT
8900 ! DATA FOR 10)TABLES
8970 ! DATA FOR 11)QUEUES
8999 RETURN
9000 ! ----------FINAL
9010 ! SUBR TO PERFORM ANY USER-
     DEFINED OPERATIONS AFTER A
     RUN
9999 RETURN
```

The above statements, written in BASIC, are essential and must not be changed by the user when entering the model and instructions.

Once the simulation program has been loaded from tape into memory the model statements and any pre- and post-simulation instructions can be entered into the modules MODEL, INITIAL and FINAL respectively.

1) The model in this example simply consists of the single differential equation (6-10) and is entered as shown below on lines 4650, 4660 and 4670.

```
4630 ! ----------MODEL
4640 REM MAIN SUBR TO CALC F(i),
     K(i,z)FOR ALL i AND z=1,2,3
     ,,,
4650 K1=(A(4)*A(2)+A(5)*A(3)+A(1
     0))/A(11)
4660 K2=(Q1+A(6)+A(7)+A(8))/A(11
     )
4670 F(1)=K1-K2*A(1) ! dTsys/dt=
     K1-K2*Tsys
7960 FOR J=1 TO N0
7970 K(J,Z)=H*F(J) ! Z=1,2,3OR4
7980 NEXT J
7990 RETURN
```

Models are entered using any line numbers between 4670 and 7960.

2) *INITIAL* is a module which is called just before simulation begins. The listing of INITIAL shown below illustrates how this module is used to print headings and the initial values and parameters used in the simulation. The variable Q1(daily overflow) calculated on line 8180 equals the total inflow less the remaining outflows. Q1 is a parameter (a constant) and is used on line 4660 in MODEL.

The lines 8800 to 8970 are a permanent part of INITIAL and must not be removed by the user. Their purpose, when used, is to create a permanent record of unit values and parameters which can be read repeatedly from data statements every time the program is used. This facility is used in the example in chapter 7 , but not in this one.

```
8000 ! ----------INITIAL
8010 ! SUBR DONE BEFORE SIMUL'N
8020 DISP "----------------------
     ----------"
8030 DISP "SIMPLIFIED MINE SYSTE
     M"
8040 DISP "STEADY FLOW,VARIABLE
     SALTS"
8050 DISP "----------------------
     ----------"
8060 DISP "UNITS:Ml,d,kg.NOTE-kg
     /Ml=mg/l."
8070 DISP "SALT CONCENTRATIONS:"
8080 DISP " SYSTEM";TAB(16);A(1)
8090 DISP " SUPPLY DAM";TAB(16);
     A(2)
8100 DISP " RWB";TAB(16);A(3)
8110 DISP "FLOWS(Ml/d):"
8120 DISP " SUPPLY DAM";TAB(16);
     A(4)
8130 DISP " RWB";TAB(16);A(5)
8140 DISP " MUD";TAB( 6);A(6)
8150 DISP " ORE LOSS";TAB(16);A(
     7)
8160 DISP " WIND LOSS";TAB(16);A
     (8)
8170 DISP " EVAPORATION";TAB(16)
     ;A(9)
8180 Q1=A(4)+A(5)-A(6)-A(7)-A(8)
     -A(9)
8190 DISP " OVERFLOW";TAB(16);Q1
8200 DISP "LEACHED kg/d";TAB(16)
     ;A(10)
8210 DISP "SYSTEM VOLUME";TAB(16
     );A(11)
8800 ! DATA FOR 1)INIT VALS
8850 ! DATA FOR 4)PRT LIST
8870 ! DATA FOR 6)PLOT INPT
8900 ! DATA FOR 10)TABLES
8970 ! DATA FOR 11)QUEUES
8999 RETURN
```

3) FINAL is a module called after the simulation is complete. The listing below illustrates how the modulo is used to display the time step and the solution algorithm used.

```
9000 ! ------------FINAL
9010 ! SUBR TO PERFORM ANY USER-
     DEFINED OPERATIONS AFTER A
     RUN
9020 DISP "TIME STEP=";H;"DAYS"
9025 DISP "ALGORITHM:";
9030 IF F2=1 THEN DISP "EULER"
9040 IF F2=2 THEN DISP "MOD.EULE
     R"
9050 IF F2=3 THEN DISP "4th ORDE
     R R-KUTTA"
9999 RETURN
```

The variables H and F2 are variables used by the simulation program and are explained in appendix D.

6.3.2 Running the Simulation Program

1) After the model has been entered as shown above, the RUN-key is pressed. After a few seconds delay, the question is asked whether the heading and notes must be printed or displayed. Typing P for printing results in the following:

```
CONTINUOUS SIMULATION OF A
SYSTEM DESCRIBED BY ORDINARY
DIFFERENTIAL EQUATIONS WITH
INITIAL BOUNDARY CONDITIONS.

M.C.HOLTON-WITS UNIVERSITY.
**********************************
NOTE
1)Press key k1 WHILE EXECUTING
  to get back into input mode
2)Space is provided inF&K for up
  to 20 differential equations
3)Space is provided in A;A0&B
  for up to 105 variables in the
  prgm
4)Space is provided in A1 for
  printing up to 50 variables at
  each step
5)File space provided for<=4000
  graph points.M has space for
  <=20graphs.
6)Space is provided in D1 for
  <=10 tables and in D2&D3 for a
  total of<=100start times and
  <=100data points
7)Space is provided in E1&E2for
  <=20queues and a total of 100
  values
**********************************
```

Note one above reminds the user that key k1 can be pressed during simulation if the output indicates the onset of instability or if, for some reason, it is desired to change the input data and begin simulating again. Notes two to seven give the dimensions of arrays and matrices in the program. The dimensions may be changed to suit the requirements of the models and the memory space available, (see lines 110 to 150 in appendix C).

2) In the model there is one differential equation,F(1) and eleven variables,A(1) to A(11)

```
DIFFERENTIAL EQUATIONS&VARIABLES

dA(J)/dT=F(J) J=1 to?
1

F(J)=func(T,A(1)..A( 1 ),..A(N1))
EXTRA VARIABLES ARE A( 2) .A(N1)
(IF NO EXTRAS,ENTER N1= 1) N1=?
?
11
```

3) The initial values of the eleven variables are requested next.

```
A0( 1 )?
500
A0( 2 )?
10000
A0( 3 )?
500
A0( 4 )?
1.5
A0( 5 )?
1
A0( 6 )?
.8
A0( 7 )?
.3
A0( 8 )?
.3
A0( 9 )?
.9
A0( 10 )?
3000
A0( 11 )?
13.2
```

It should be noted that all the input data is requested by displaying a statement on the screen, followed by two questions. The following computer is what appeared on the screen and preceded the above

paper printout of initial values.

```
ENTER THE INITIAL VALUE FOR EACH
 VARIABLE
1)USE PREDEFINED DATA
2)KEYBOARD INPUT
(1or2)?
2
PRINT OR DISPLAY(PorD)
?
P
```

The same questions are asked with each of the data inputs below but are excluded from the discussion below.

4) Only the value of variable A(1), i.e. C_{sys} will be printed as output during simulation as it is the only variable which varies with time. The other variables A(2) and A(11) are actually constant parameters which are stored as variables so that they can easily be changed in between simulation runs.

```
HOW MANY VARIABLES
A(1)..A(11)MUST BE PRINTED
?
1
ENTER THE  1 NUMBER(S) BETWEEN
1 AND 11 IN ANY ORDER.
(NO. 1 )?
1
```

5) When the simulation time equals 0 days, the program will commence to print the value of variable A(1) and will continue to do so until the simulation time equals 100 days. The value will only be printed after every 10 simulation time-steps. If, for example, the time-step H equals 0,5 days then the value of A(1) will be printed 20 times.

```
PRINT OUTPUT FROM T=T2 TO T8
EVERY S0 TIME STEPS
(T2,T8,S0)?
0,100,10
```

6) A graph of the value of A(1) versus time is required. Data points required for plotting are stored on a tape file which has space for 2000 points (see note 5 in 1) above). The unit spacing of 10 days along the time axis and 1000 kg/Mℓ along the variable A(1)-axis, refers to the tic-marks on the graph plotted. If any of the values plotted are outside the range of 0 to 13000 kg/Mℓ (MN to MX) then the program will automatically increase MX or decrease MN accordingly, and enlarge the scale of the graph.

```
NO.PLOTS,MAX NO.PTS.(See note 5)
?
1,2000
UNIT SPACING ALONG T-AXIS?
10
FOR EACH VARIABLE TO BE PLOTTED
ENTER:
V-VARIABLE NO.,MN-MIN.VALUE,MX-
MAX.VALUE,U-UNIT SPACING ALONG
VARIABLE AXIS
(V,MN,MX,U)?
1,0,13000,1000
```

7) Variable A(1) will be plotted for time between 0 and 100 days. A check is performed to ensure that the time interval lies within the time range, specified in 8), for the simulation. A maximum of 50 points will be stored for plotting A(1). Depending on the time-step size and the time interval for plotting, the program will automatically select data points for plotting at suitable time intervals to ensure that no more than 50 points will be plotted. If there are only 10 points available during simulation, for example, then only 10 points will be plotted.

```
PLOT SPECIFIED VARIABLES FROM
T=T3 TO T4,USING ABOUT 50 PTS.
(T3,T4,C8)?
0,100,50
```

The graph on the screen and that copied onto paper has a length along the time axis of 250 dots. No benefit

can therefore be gained by specifying a number greater than 250 for C8 above. The larger the value of C8 and the number of graphs to be plotted, the longer the simulation run will take.

8) The simulation is to be carried out from 0 to 100 days using a time increment step size of one day. In this example the output, plotting and execution time range is the same, but this is not necessary as it may be desirable, in some instances, to have a 'warm up' period only after which output is printed and/or plotted.

```
EXECUTE FROM T=T0 TO T9 WITH TIM
E STEP H
(T0,T9,H)?
0,100,1
```

9) The Fourth-Order Runge-Kutta algorithm is selected.

```
EULER,MOD.EULER OR 4TH ORDER
RUNGE-KUTTA(1,2or3)?
3
```

10) Tables and queues are used and explained in the example in chapter 7.

```
USE TABLES (orN)?
N

USE QUEUES(YorN)?
N
```

The above input data is entered before the first simulation run. After this initial input and after any simulation run, the following list of options is displayed on the screen so that any changes or corrections can be made before the next run.

```
1)CHANGE ALL INIT. VALUES
2)RE-USE INIT.VARIABLES&QUEUES
3)CHANGE SOME VARIABLE VALUES
4)CHANGE PRINT LIST
5)CHANGE PRINT TIMES
6)CHANGE PLOTTING DATA
7)CHANGE TIMES FOR PLOTTING
8)CHANGE EXECUTION TIMES
9)CHANGE ALGORITHM
10)CHANGE FUNCTION TABLES
11)CHANGE QUEUE PARAMETERS
12)EXECUTE PROGRAM
(LAST OPTION 4 )
ENTER NEW OPTION 1TO 12?
12
```

No changes are required after checking the input in steps 1) to 10) above, and option 12 is selected.

The following output results from the instructions coded into INITIAL.

```
-------------------------------
SIMPLIFIED MINE SYSTEM
STEADY FLOW,VARIABLE SALTS
-------------------------------
UNITS:Ml,d,kg.NOTE-kg/Ml=mg/l
SALT CONCENTRATIONS:
 SYSTEM          500
 SUPPLY DAM      10000
 RWB             500
FLOWS(Ml/d):
 SUPPLY DAM      1.5
 RWB             1
 MUD              .8
 ORE LOSS         .3
 WIND LOSS        .3
 EVAPORATION      .9
 OVERFLOW         .2
LEACHED kg/d     3000
SYSTEM VOLUME    13.2
```

The average salt concentration of the system water Csys is printed out every ten days, i.e. every 10 time steps of 1 day, as shown in fig.62 below.

```
1)CHANGE ALL INIT. VALUES
2)RE-USE INIT.VARIABLES&QUEUES
3)CHANGE SOME VARIABLE VALUES
4)CHANGE PRINT LIST
5)CHANGE PRINT TIMES
6)CHANGE PLOTTING DATA
7)CHANGE TIMES FOR PLOTTING
8)CHANGE EXECUTION TIMES
9)CHANGE ALGORITHM
10)CHANGE FUNCTION TABLES
11)CHANGE QUEUE PARAMETERS
12)EXECUTE PROGRAM
(LAST OPTION 4 )
ENTER NEW OPTION ITO 12?
12
```

No changes are required after checking the input in steps 1) to 10) above, and option 12 is selected.

The following output results from the instructions coded into INITIAL.

```
-----------------------  ----------
SIMPLIFIED MINE SYSTEM
STEADY FLOW,VARIABLE SALTS
-----------------------  ----------
UNITS:Ml,d,kg,NOTE-kg/Ml=mg/l
SALT CONCENTRATIONS:
 SYSTEM          500
 SUPPLY DAM      10000
 RWB             500
FLOWS(Ml/d):
 SUPPLY DAM      1.5
 RWB             1
 MUD             .8
 ORE LOSS        .3
 WIND LOSS       .3
 EVAPORATION     .9
 OVERFLOW        .2
LEACHED kg/d     3000
SYSTEM VOLUME    13.2
```

The average salt concentration of the system water Csys is printed out every ten days, i.e. every 10 time steps of 1 day, as shown in fig.62 below.

```
**********************************
INITIAL VALUE(S):T= 0
A( 1 )= 500
T= 10
A( 1 )= 8270.67470853
T= 20
A( 1 )= 10582.9642938
T= 30
A( 1 )= 11271.8233527
T= 40
A( 1 )= 11475.7664227
T= 50
A( 1 )= 11536.6910253
T= 60
A( 1 )= 11554.8201233
T= 70
A( 1 )= 11560.2147289
T= 80
A( 1 )= 11561.8199808
T= 90
A( 1 )= 11562.2976494
  100
    )= 11562.4397874
  t**********************************
```

Fig. 6.2 Salt Concentration (Runge-Kutta using 1 day Time-Steps)

At the end of the simulation the graphs are plotted by reading the recorded data from the data tape file. Fig. 6.3 shows the graph of salt concentration versus time plotted sideways with the specified scale information printed at the bottom of the graph; the minimum and maximum T (time) and variable axes values and the unit tic mark spacing . Fifty points were plotted from an available 101 points (0 to 100 with a step of 1).

The following output results from the instructions coded into FINAL:

```
TIME STEP= 1 DAYS
ALGORITHM:4th ORDER R-KUTTA
```

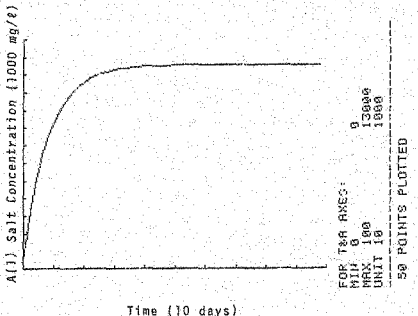


Fig. 6.3 Salt Concentration Versus time (Runge-Kutta using 1 day time-steps)

If another run is requested then the same list of options shown earlier is again displayed on the screen as shown in fig.6.4.

```
ANOTHER RUN(YorN)?
Y

1)CHANGE ALL INIT  VALUES
2)RE-USE INIT.VARIABLES&QUEUES
3)CHANGE SOME VARIABLE VALUES
4)CHANGE PRINT LIST
5)CHANGE PRINT TIMES
6)CHANGE PLOTTING DATA
7)CHANGE TIMES FOR PLOTTING
8)CHANGE EXECUTION TIMES
9)CHANGE ALGORITHM
10)CHANGE FUNCTION TABLES
11)CHANGE QUEUE PARAMETERS
12)EXECUTE PROGRAM
(LAST OPTION 12 )
ENTER NEW OPTION 1TO 12?
2
```

Fig.6.4

In the next run (fig.6.5), the time-step was changed to 10 days and output printed every time-step. Option 2 was chosen (fig.6.4) to reset the variables A(1) to A(11) to the initial values originally specified. This has the effect of changing only the current value of variable A(1), 11562,5 kg/Mℓ, back to 500 since the values of A(2) to A(11) were not changed during simulation. If option 2 had been excluded simulation would have continued for a further 100 days using 11562,5 as the starting value of A(1). It can be seen from the graph (fig. 6.3) that this would have resulted in a negligible change in the salt concentration. The initial and current values of some or all of the variables can be changed by selecting options 3 or 1 respectively. The output for the second run is shown in fig.6.6.

```
VARIABLES SET TO INITIAL VALUES.

EXECUTE FROM T=T0 TO T9 WITH TIM
E STEP H
(T0,T9,H)?
0,100,10

PRINT OUTPUT FROM T=T2 TO T8
EVERY S0 TIME STEPS
(T2,T8,S0)?
0,100,1
```

Fig. 6.5

```
---------------------------------
SIMPLIFIED MINE SYSTEM
STEADY FLOW,VARIABLE SALTS
---------------------------------
UNITS:Ml,d,kg.NOTE-kg/Ml=mg/l.
SALT CONCENTRATIONS:
 SYSTEM          500
 SUPPLY DAM      10000
 RWB             500
FLOWS(Ml/d):
 SUPPLY DAM      1.5
 RWB             1
 MND              .8
 ORE LOSS         .3
 WIND LOSS        .3
 EVAPORATION      .9
 OVERFLOW         .2
LEACHED kg/d    3000
SYSTEM VOLUME   13.2
```

Fig. 6.6

```
**********************************
INITIAL VALUE(S):T= 0
A( 1 )= 500
T= 10
A( 1 )= 8870.88583477
T= 20
A( 1 )= 10460.4553014
T= 30
A( 1 )= 11214.6658865
T= 40
A( 1 )= 11452.7144617
T= 50
A( 1 )= 11527.8488144
T= 60
A( 1 )= 11551.5631801
T= 70
A( 1 )= 11559.0480538
T= 80
A( 1 )= 11561.4104756
T= 90
A( 1 )= 11562.1561177
T= 100
A( 1 )= 11562.3914618
**********************************
```

Fig. 6.7 Salt Concentration (Runge-Kutta using 10 day time-steps)

Fig. 6.7 consists of printed output of C_{sys} every 10 days as in fig.6.2 but using a 10 day instead of a 1 day time-step. Fairly large discrepancies exist between this and the previous run at T equals 40 days for example. After T equals 100 days the value of A(1) agrees to 1 decimal place for the two simulations and shows that the final or equilibrium salt concentration is independent of the time-step size. The graph (fig. 6.8) for this run is similar to the first graph (fig.6.3) but the straight-line-segment effect in fig.6.8 of only having 11 points to plot

instead of 50 is apparent.

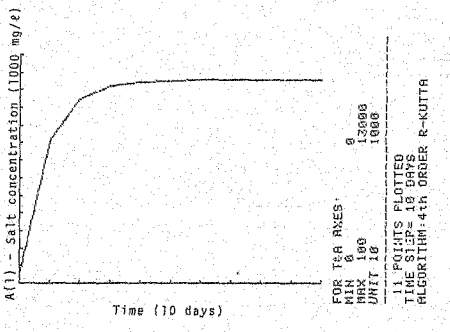


Fig. 68 Salt Concentration Versus Time (Runge-Kutta using 10 day time-step).

The Euler algorithm is used in the third run with the same 10 day step size as above. The printed and graphical results are shown in figures 6.9 and 6.10. A comparison of the last two graphs (figures 6.8 and 6.9) gives an indication of the accuracy of the more powerful Fourth-Order Runge-Kutta method when compared with the Euler method.

```
**********************************
INITIAL VALUE(S):T= 0
A( 1 )= 500
T= 10
A( 1 )= 13909.0909091
T= 20
A( 1 )= 11064.7382921
T= 30
A( 1 )= 11648.0858169
T= 40
A( 1 )= 11540.1030086
T= 50
A( 1 )= 11567.250877
T= 60
A( 1 )= 11561.4922383
T= 70
A( 1 )= 11562.7137677
T= 80
A( 1 )= 11562.4546554
T= 90
A( 1 )= 11562.5096186
T= 100
A( 1 )= 11562.4979598
**********************************
```

Fig. 69 Salt Concentration (Simple Euler using 10 day time-steps)

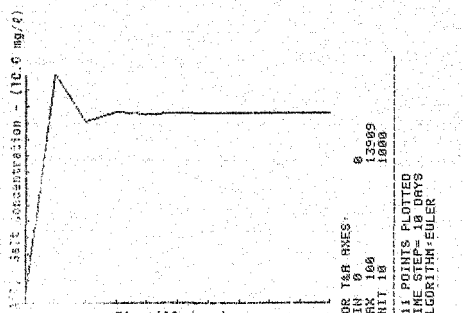


Fig. 69.0 Salt Concentration Versus Time (Simple Euler using 10 day time-steps)

After 100 days the value of A(1) in fig. 6.9 has converged to an equilibrium value which differs by only 0,05 mg/ℓ and indicates that the equilibrium salt concentration is independent of both the time step size and the method used. The salt concentration during the unsteady stage, before equilibrium, is dependent on the method used and the time step size. Generally the smaller the step size and the more efficient the algorithm selected, the more accurate the results.

6.3.3 Truncation Errors and Estimation of the Maximum Time-Step Size.

The first two runs, (figs. 6.2 and 6.7), using the Runge-Kutta method, were made using time steps of 1 and 10 days (h1 and h2). At 20 days the two answers are 10582 and 10460 mg/ℓ (A1 and A2) respectively. It can be estimated using the results of the above two simulations what, for example, the maximum time step must be which will produce a result at 20 days, accurate to 3 decimal places. Letting the new error E_3 equal $\pm$ 0,0005 mg/ℓ, the new step size h_3 is estimated using equation (3-11) derived in section 3.5. The Runge-Kutta is a fourth order method i.e. $O(h)=4$

$$\text{new step size } h_3 = h_1 \left| E_3 (1-h_2/h_1)^{O(h)} / (A_2 - A_1) \right|^{\frac{1}{O(h)}}$$

$$= 1 \left| .0005 (1-10/1)^4 / (10460-10582) \right|^{1/4}$$

$$\simeq 0{,}45 \text{ say } 0{,}5 \text{ days.}$$

Fig. 6.11 below lists the results of another run using a time step of 0,5 days and the Runge Kutta method.

```
**********************************
INITIAL VALUE(S):T= 0
A( 1 )= 500
T= 10
A( 1 )= 8270.68217843
T= 20
A( 1 )= 10582.9697394
T= 30
A( 1 )= 11271.0253368
T= 40
A( 1 )= 11475.7672099
T= 50
A( 1 )= 11536.6913181
T= 60
A( 1 )= 11554.8202279
T= 70
A( 1 )= 11560.2147653
T= 80
A( 1 )= 11561.8199932
T= 90
A( 1 )= 11562.2976537
T= 100
A( 1 )= 11562.4297888
**********************************
TIME STEP= .5 DAYS
ALGORITHM:4th ORDER R-KUTTA
```

Fig. 6.11 Salt Concentration (Runge-Kutta using 0,5 day time-steps)

Comparing the results in fig.6.10 with the exact analytical results in Table 6.2 it can be seen that the numerically calculated value at 20 days is correct to 3 decimal places as predicted.

Table 6.2- Exact analytical values

Time (days)	System concentration (mg/ℓ)
0	0
10	8270,683
20	10582,969
30	11271,025
40	11475,767
50	11536,691
60	11554,820
70	11560,215
80	11561,820
90	11562,298
100	11562,440

From a practical point of view, it would be desirable to use the largest time-step size (h_3) which would result in an answer accurate to $\pm$ 200 mg/ℓ (E_3) Comparing figures 6.7 and 6.11, using step sizes 10 and 0,5 days (h1 and h2) respectively, the maximum discrepancy occurs at T equals 10 days (A1 = 8071 and A2 = 8270). The desired step size h3 is calculated as before.

$$h_3 \approx 10\left|200.(1-0,5/10)^4/(8270-8071)\right|^{1/4}$$
$$\approx 9,5 \text{ say } 10 \text{ days.}$$

This confirms the fact that the 10 day step size used for fig. 6.11 would result in a maximum error or $\pm$ 200 mg/ℓ (compare fig. 6.7 with table 6.11 at 10 days).

6.3.4 Simulating in the Reverse Time Direction

The following run was made starting with the result at the end of the last run (fig. 6.11above), i.e., option 2 was not selected to re-initialise the variable values. The print-out time, the execution time and time-step were reversed as shown in fig. 6.12. It should be noted that the error in A(1) after the forward and backward simulation (at T=0) in fig. 6.13 is only 0,02 mg/ℓ. This can be used as an indication of the accuracy and stability of the calculation.

```
PRINT OUTPUT FROM T=T2 TO T8
EVERY S8 TIME STEPS
(T2,T8,S8)?
100,0,20

EXECUTE FROM T=T8 TO T9 WITH TIM
E STEP H
(T8,T9,H)?
100,0,-.5
```

Fig. 6.12.

```
-------------------------------
SIMPLIFIED MINE SYSTEM
STEADY FLOW,VARIABLE SALTS
-------------------------------
UNITS:Ml,d,kg,NOTE-kg/Ml=mg/l.
SALT CONCENTRATIONS:
 SYSTEM          11562.4397888
 SUPPLY DAM      10000
 RWB             500
FLOWS(Ml/d):
 SUPPLY DAM      1.5
 RWB             1
 MUD             .8
 ORE LOSS        .3
 WIND LOSS       .3
 EVAPORATION     .9
 OVERFLOW        .2
LERCHED kg/d     3000
SYSTEM VOLUME    13.2
**********************************
INITIAL VALUE(S):T= 100
A( 1 )= 11562.4397888
T= 90
A( 1 )= 11562.2976538
T= 80
A( 1 )= 11561.8199943
T= 70
A( 1 )= 11560.2147694
T= 60
A( 1 )= 11554.8202421
T= 50
A( 1 )= 11536 6913651
T= 40
A( 1 )= 11475.7673667
T= 30
A( 1 )= 11271.02586
T= 20
A( 1 )= 10582.9704833
T= 10
A( 1 )= 8270.6879933
T= 0
A( 1 )= 500.019389182
**********************************
TIME STEP=-.5 DAYS
ALGORITHM:4th ORDER R-KUTTA
```

Fig. 6.13 Salt Concentration during a reverse simulation

The results of an identical forwards and backwards simulation, but conducted with the least accurate Euler algorithm are given in figures 6.14 and 6.15. The starting value after the simulation contains an error of 5760 mg/ℓ. The values at other times during the simulation can be compared with the exact answers in Table 6.2. The accuracy of results using the Modified Euler algorithm could

be expected to be somewhere between those of the Fourth-Order Runge-Kutta and the Euler methods.

```
**********************************
INITIAL VALUE(S):T= 0
A( 1 )= 300
T= 10
A( 1 )= 8394.3308346
T= 20
A( 1 )= 10655.1738207
T= 30
A( 1 )= 11302.652513
T= 40
A( 1 )= 11488.0827531
T= 50
A( 1 )= 11541.1877806
T= 60
A( 1 )= 11556.3964325
T= 70
A( 1 )= 11560.7520105
T= 80
A( 1 )= 11561.9993966
T= 90
A( 1 )= 11562.3566331
T= 100
A( 1 )= 11562.4589414
**********************************
TIME STEP=  .5 DAYS
ALGORITHM:EULER
```

Fig. 6.14 Salt Concentration during forward simulation (Euler method using 0,5 day time-steps)

```
**********************************
INITIAL VALUE(S):T= 100
A( 1 )= 11562.4589414
T= 90
A( 1 )= 11562.3668856
T= 80
A( 1 )= 11562.0679165
T= 70
A( 1 )= 11561.0983173
T= 60
A( 1 )= 11557.952928
T= 50
A( 1 )= 11547.7492567
T= 40
A( 1 )= 11514.6484518
T= 30
A( 1 )= 11407.2691327
T= 20
A( 1 )= 11058.9296243
T= 10
A( 1 )= 9928.91302251
T= 0
A( 1 )= 6263.12866653
**********************************
TIME STEP=-.5 DAYS
ALGORITHM:EULER
```

Fig. 6.15 Salt Concentrations during reverse simulation (Euler method using 0,5 day time-steps)

CHAPTER SEVEN

7. DETAILED MODEL OF UNISEL GOLD MINE WATER RETICULATION SYSTEM

7.1 INTRODUCTION

The simple model discussed in chapter 6 assumes steady or average flow and a uniform salt concentration at any time for all the water in a single constant volume element representing the system. The model presented in this section was evolved from a number of simpler models which initially dealt with water quality and quantity aspects separately but considered the elements of the real water system individually. Fig. 7.1 (the same as fig. 2.1) shows the physical layout and the individual elements of Unisel Gold Mine. As a greater understanding of the water system was gained, and as more information became available from mine visits, communication with mining personnel and chemical results from sampling, so the model has developed to the stage that it is presented in here.

Complete data concerning flows and operating relationships at the mine as well as the chemical results from leaching tests conducted at the University were not available. Certain data used in this model are therefore inaccurate but, nonetheless, based on the best available data. It should in any case be recognised that such models are always in a state of evolution because of the very nature of a gold mine. Physical changes due to excavation, policy changes resulting in different equipment, and changes in operation conditions as a result of larger pumps, different valves etc., are examples of changing factors which affect the model. With this thought in mind, the model has been written in as general a form as possible to enable any parameter or variable to be changed during simulation by using the facilities of the simulation program.

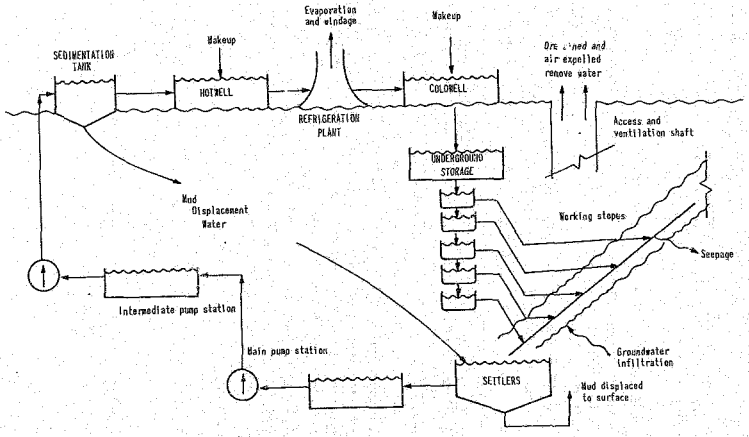


Fig. 7.1 Unisel Gold Mine Water Reticulation System

The model is divided into two sections which deal separately with the unsteady flow and unsteady salt masses in each of the 8 storage elements of the system. The model can be used to simulate either water quantity or both quantity and quality variations. Water quantity refers to volumes of water in storage elements, cumulative flows, flows between system elements and external flows into and out of the system. Water quality refers to the mass of salts in storage volumes, the cumulative mass of salts and the concentration of salts in flows. When only water quantity is simulated then salt mass and concentration is excluded from the model and the simulation is facilitated.

The water reticulation system in this model (see fig. 7.1) consists of 8 water storage elements: underground settlers; main pump station sump; intermediate pump station sump; surface sedimentation tank; hotwell; cold-well; underground storage dam; the cascade dams. The volume of water stored in all elements changes significantly with time except that of the underground settlers which is considered constant. The differential equations F(1) to F(7) describe the water volume changes in the elements. The change with time of the total mass of salts in each of the 8 elements is described by the 8 differential equations F(8) to F(15). The simulation program numerically solves the 15 differential equations simultaneously for each time increment to obtain the 7 water volumes A(1) to A(7) and 8 salt masses A(8) to A(15). These values are used to calculate other useful information. The variation with time of only one particular type of salt can be studied using this model. Repeated simulations can be made for different dissolved salts, or the model could be extended to involve more salts and any chemical relationships between them. In this model total dissolved salts are simulated (considered as a single salt).

A number of features of the simulation program, not shown in the previous example (chapter 6), are illustrated in this example: the use of tables to describe relationships; the use of queues for the effects of time lag; the use of data statements for large amounts of input data. How to load the simulation program and how to enter the model and any pre-and post-simulation instructions into MODEL, INITIAL and FINAL, is discussed in chapter 6 and is not repeated here. The three user-defined modules MODEL, INITIAL and FINAL are listed together with a list of program symbols and their meaning. Each element in the model is then discussed and the governing equations for each are derived. The results of a few simulation runs are presented and discussed in chapter 8.