AN INTERNET SERVICE CENTRE ON WATER MODELLING SYSTEMS FOR THE MINING INDUSTRY

MR Howard • JJ Heymans

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Water Research Commission

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AN INTERNET SERVICE CENTRE ON WATER MODELLING SYSTEMS FOR THE MINING INDUSTRY

by

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Report to the Water Research Commission on the project

Development of an Internet Service Centre on Water Modelling Systems for the Mining Industry

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NOTE

Answers to any queries regarding the application and operation
of the Internet Web Site, are obtainable from
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EXECUTIVE SUMMARY

Recent changes to South African legislation place more emphasis on the prediction of a mine's impact on the environment both now and in the future. The use of predictive models, therefore, is becoming a more important aspect of mine water management. This includes the use of models for internal water reticulation (such as stormwater management and water balances) and for external applications (such as effluent discharge options and geohydrological impacts).

Although this approach to predicting the impact a mine may have on the surface water environment is to the benefit to all the users of the catchment water resources, a reality is that most mines do not have the resources to undertake such modelling in-house. There is a need therefore, to provide some mechanism whereby mines and regulators can obtain independent evaluations of water models in order to assist in the decision-making process.

This project was aimed at identifying those models which are currently in use in South Africa, as well as those models which could be used, but which are currently only used internationally. In terms of the mining environment, there are a number of areas where no locally used model is available, and consequently potential options need to be identified from overseas. This is particularly relevant in the areas of geochemistry and acid generation. It was this motivation that resulted in the development of internet web site which evaluates a range of typical water models and which makes this evaluation available to anyone with access to the internet

The research project ream identified the following modelling areas: hydrology, water quality, geochemistry, groundwater and water and salt balances. The team investigated three global types of model: firstly those which are freely available, widely used and can be downloaded from the Internet; secondly, those which must be bought from the supplier; and thirdly, models which need not be bought, or which cannot be bought, but which can be run by the supplier.

Details provided about the models include:

- availability
- applicability (strengths and weaknesses)
- usability
- data requirements
- computer requirements
- case studies (local and international)

This site has been developed and is located at:

http://www.ccwr.ac.za/iscp

The original intent with web site was to populate it with up to 50 models. This has not been achieved during the course of the project for a number of reasons:

- The project team evaluated the models used by them and in which they had sufficient expertise to evaluate the model. This restricted the number of models.

- Appeals were made by way of personal letters, letters to organisations and numerous publications in a variety of periodicals for anyone with models to approach the project team for the inclusion of their model on the site. This proved to have little success.

In the end, a total of thirty models were evaluated and are included in the web site. It is hoped that as the web site becomes more widely known, additional models will be added to the site and that a larger number of models will be available to the end-user.

The site will be maintained and upgraded periodically by the Water Research Commission.

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The Project Team wishes to express its gratitude to the Project Steering Committee for their guidance of the research:

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- University of Natal - Department of Chemical Engineering
- University of the Free State - Institute for Groundwater Studies
- Ninham Shand
- Stewart Scott Inc.

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Additionally, a number of other researchers contributed to the Internet site. These researchers are listed on the site on the applicable web page.

1. INTRODUCTION

Recent changes to South African legislation place more emphasis on the prediction of a mine's impact on the environment both now and in the future. The new National Water Act (Act No. 36 of 1998) presents a strategy on how the Department of Water Affairs & Forestry will manage the national water resource. This strategy is divided into two key areas: the national water resource strategy (Part 1) and the catchment management strategy (Part 2). There are currently a number of initiatives underway to facilitate the implementation of the strategy. Also inherent in the National Water Act (NWA) is the concept of licensing water use. All mines and industries that have significant impacts on the water resource will require licensing. The NWA stipulates certain conditions for the issue of general authorisations and licences. A selective excerpt of these conditions is:

"(1) A responsible authority may attach conditions to every general authorisation or licence–
(b) relating to water management by-
(i) specifying management practices and general requirements for any water use, including water conservation measures;
(ii) requiring the monitoring and analysis of and reporting on every water use and imposing a duty to measure and record aspects of water use, specifying measuring and recording devices to be used;
(iii) requiring the preparation and approval of and adherence to, a water management plan;
(iv) ....

(c) relating to return flow and discharge or disposal of waste, by-
(i) specifying a water resource to which it must be returned or other manner in which it must be disposed of;
(ii) specifying permissible levels for some or all of its chemical and physical components; and
(iii) specifying treatment to which it must be subjected, before it is discharged;

(d) in the case of a controlled activity-
(i) specifying the waste treatment, pollution control and monitoring equipment to be installed, maintained and operated; and
(ii) specifying the management practices to be followed to prevent the pollution of any water resource;

(e) in the case of taking or storage of water-
(i) setting out the specific quantity of water or percentage of flow which may be taken;
(ii) ....

In order for licensees to submit license applications, they need to set up water quality models that are capable of predicting the quantity and quality of water that they wish to seek approval to discharge, for different management strategies applied within the mines.

Although this approach to predicting the impact a mine may have on the surface water environment is to the benefit to all the users of the catchment water resources, a reality is that most mines do not have the resources to undertake such modelling in-house. The result is an increased use of consultants to undertake modelling exercises. The consequence of this is the wide variety of models which are used in the modelling process. There are a number of drawbacks with this series of events:

- In the first instance, the mine as the client may have no knowledge as to the applicability of a particular model to their own circumstances;
- The model may not be widely used in South Africa because of certain deficits within the programme; and
- The information generated by the model may not be verifiable because of the site-specific nature of the model.

The mining industry is primarily faced with two options:

- Either continue down the path as is; or
- Develop in-house expertise in the field of water modelling.

In either event, independent information on the range of models available, the appropriateness of the model to specific circumstances and the degree of technical capability required to run the models would prove invaluable to the mine in the decision making process. These considerations also apply to the regulators.

This project was aimed at identifying those models which are currently in use in South Africa, as well as those models which could be used, but which are currently only used internationally. In terms of the mining environment, there are a number of areas where no locally used model is available, and consequently potential options need to be identified from overseas. This is particularly relevant in the areas of geochemistry and acid generation. It was this motivation that resulted in the development of an internet web site which evaluates a range of typical water models and which makes this evaluation available to anyone with access to the internet.

This project had the following objectives:

1. To develop an Internet based service which provides sufficient information to the mining and water industries to select appropriate predictive mathematical models.

To achieve this objective, the following sub-objectives need to be satisfied:

(a) Utilise existing expertise to identify appropriate models in the fields of:

- hydrology
- water quality
- geochemistry
- groundwater
- water and salt balances

(b) Prepare evaluation information on each of the identified models, which will include:

- availability
- applicability
- usability
- data requirements
- computer requirements
- case studies

2. Compose and implement an Internet service centre with links to other sites on the Internet where models can either be found or ordered.

2. METHODOLOGY

This project was designed to utilise recognised local modelling specialists to prepare the information required for the Internet Service Centre (ISC). Each of the identified experts has extensive experience in the use of the models locally and internationally, and is in the best position to supply information pertaining to case studies.

The project started with the identification of all potential models. This was done by each specialist for their particular field of expertise. Once this was completed, the specialists started with the model evaluation and preparation of the information required for the ISC.

In parallel to this, the following tasks were undertaken to gather additional information:

- searches were undertaken both locally, via the Internet, and internationally via experts, on the range of models available.

- letters were sent out to local consulting companies inviting them to participate in the project.

- advertisements were placed in the SA Water Bulletin, various mining journals including Mining News and SA Gold, Coal and Base Minerals, and Water Sewage & Effluent soliciting companies and individuals to submit information on models at their disposal for inclusion on the web site.

- the Internet site was opened earlier than scheduled to provide an additional mechanism for companies or individuals to make an input.

Once all the models were identified, evaluated and relevant documentation prepared, the information was converted into a format acceptable for the Internet.

The Internet Service Centre (ISC) contains a number of pages detailing various aspects of each model as well as its availability and use locally and internationally. A series of pages and links cover the following aspects:

- availability
- applicability (strengths and weaknesses)
- usability
- data requirements
- computer requirements
- case studies (local and international)

The system is structured in such a way as to allow the user to browse the pages for the above information using standard Internet software. Should the user wish to download free software, a link is available for this, should the software be for sale, the appropriate firm will be accessed, and should the software be proprietary, then the relevant e-mail information will be available for the company concerned.

The total package therefore allows the user to:

- identify the range of models available for a particular water related aspect;
- ascertain its applicability to the specific circumstances;
- evaluate the information and system requirements;
- identify where the model can be obtained, or who can undertake the modelling for the user.

Links to other related web sites are also established.

The ISC is housed at the CCWR in Pietermaritzburg. Although not directly responsible for the maintenance of the site in the future, the CCWR will provide technical support to the maintenance team.

This document includes a hardcopy of the web pages as well as the method to be used to update and add to the information. This will form the basis for future maintenance of the ISC.

3. INTERNET SITE

3.1 Introduction

The Internet Service Centre for Mine Related Water Models is located at:

http://www.ccwr.ac.za/iscp

The opening page of the web site is presented in Figure 1.

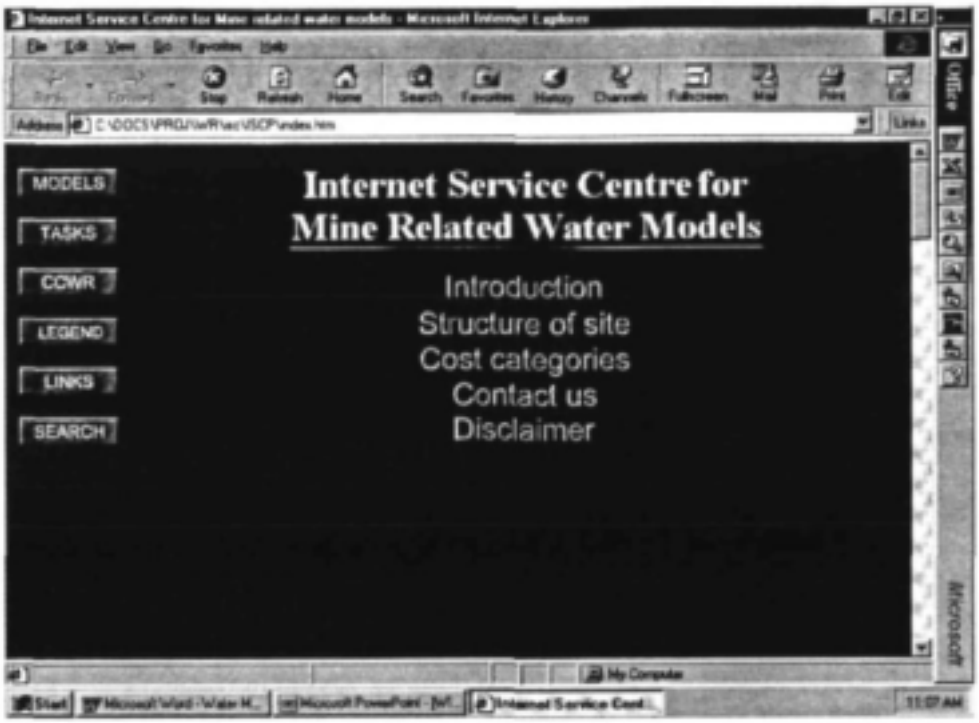

Figure 1 : Opening Page of Internet Service Centre for Mine Related Water Models

There are two ways to navigate this web site:

1. Go to a specific model – The models are arranged in separate categories, depending on the water media concerned (i.e. groundwater modelling, surface water modelling, etc.);

2. Task based selection of models – The models can be selected depending on the task required by the user (i.e. tailings dam modelling, etc.).

On selecting the Models option, the user can select which category of model they wish to view. This is presented in Figure 2.

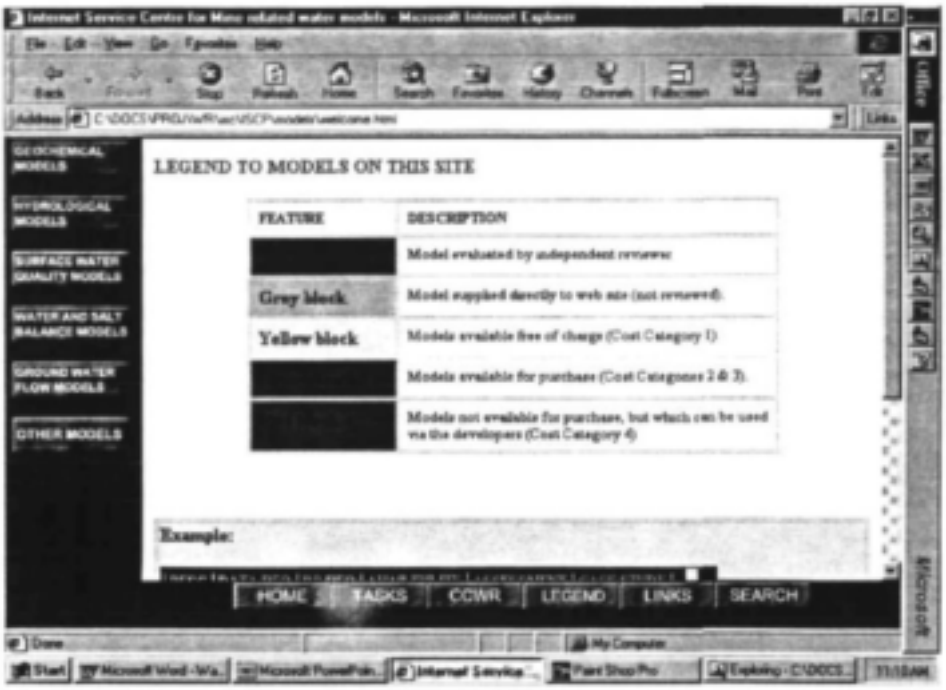

Figure 2: Selection by model category

The user can now select the model by model category (hydrological models, geohydrological models etc.). Once selected the user is presented with the names of available models for his selection to view the evaluation.

The evaluation does not provide the content of each model, but rather refers to the concept on which the model is based. The following information is provided for each of the models:

- **Description**: Summary of the purpose of the model and its applications;
- **Data**: Information necessary to feed into the model;
- **Availability**: Where to access the model;
- **Assessment**: Evaluation of applications, disadvantages and advantages, level of expertise required, tasks used in the mining context, what it is used for and the principles under which it operates;
- **Computer requirements**: Hardware, software and computer language necessary to run the model; and
- **Case Study**: Examples of practical applications.

Additionally, the various specialists were requested to supply the following information for each model:

1) Grade the model to indicate the level of competency required to use it.
2) Technical keywords
3) Range of applications for which the model is capable
4) Information regarding the applicable algorithms and main mathematical limitations (where applicable)
5) Supply an indication of how widely the model is used or how well established it is in the industry.

6) Supply related references.
7) Provide an inventory of data sources.
8) Provide general links to organizations such as the EPA.
9) Name of person, organization and email address undertaking the review.

A legend is used to inform the user of the following:

- The model was independently reviewed;
- The model was not independently reviewed but was submitted directly by the developer;
- The model is available free of charge;
- The model can be purchased; and
- The model cannot be purchased but the developers can be contacted to run the model.

Additionally, the following cost categories are applied to the models.

Cost Category 1) Free models;
Cost Category 2) Models less than US$ 2 000,00;
Cost Category 3) Models more than US$ 10 000,00;
Cost Category 4) Models not for sale.

Links

Links are available to the following organisations:
- Centre for Exposure Assessment Modelling
- Water Research Commission
- Institute for Water Quality Studies
- Weather Bureau
- Department of Water Affairs & Forestry
- Department of Mineral & Energy Affairs
- Department of Agriculture
- Department of Environment Affairs
- US Geological Survey
- CSIRO in Australia

Model evaluation

Hardcopy versions of the detailed evaluations on the web site are reproduced in Appendix 1. A summary of each model appears below.

3.2 Geochemical Models

ACIDROCK

ACIDROCK is a model designed to evaluate acidic drainage in waste rock piles. The conceptual basis for this model was the program RATAP, which was designed to assist in the prediction of acid generation caused by hydrological events and chemical reactions occurring in mine tailings sites. The transport, heat generation

and oxygen flux portions of RATAP were replaced to reflect the difference in chemical and physical environments between waste rock piles and reactive tailings sites. It has been reported that the formulation of chemical equations used in RATAP were used for this model. The chemistry was expanded to include uranium and radium, including sorption on mineral solids and organic surfaces. Furthermore, the co-precipitation of radium with gypsum and radioactive decay have been included. ACIDROCK uses measured fundamental rate laws for the dissolution on sulphide minerals.

AQUACHEM

AquaChem is a fully integrated software package developed specifically for graphical and numerical analysis of geochemical data sets. AquaChem features a powerful database that can be customized and configured to include an unlimited number of attributes per sample and a built-in database of inorganic chemicals that are commonly-used for geochemical analyses, calculations and plotting. AquaChem covers a wide range of calculations frequently used for the analysis, interpretation and comparison of aqueous geochemical data. The analysis tools in AquaChem range from simple unit transformations, mixing calculations, statistics and charge balances to more complex calculations involving correlation matrices and geothermometrics. These powerful analytical capabilities in AquaChem are complimented by a comprehensive selection of commonly used graphical techniques to portray the chemical characteristics of geochemical and water quality data for single samples and groups of samples.

MINEQL 4.0

MINEQL+ is a geochemical model written by Environmental Research Software, USA. It is capable of calculating equilibrium aqueous speciation, adsorption, gas phase partitioning, solid phase saturation states, and precipitation-dissolution of metals. MINEQL+ can solve a broad range of chemical equilibrium problems, but since it is purely an equilibrium model, it cannot be used to evaluate systems with significant kinetic constraints. MINEQL+ was originally designed to be a research tool but it is currently used in over 500 colleges and universities world-wide as an aid in teaching aquatic chemistry.

MINTEQA2

MINTEQA2 is a geochemical equilibrium speciation model written by the US EPA (Environmental Protection Agency). It can compute equilibria between dissolved species in dilute aqueous solutions and adsorbed, solid and gas phases in laboratory or natural aquatic systems. The model is purely an equilibrium model, hence it cannot be used to evaluate systems with significant kinetic constraints. MINTEQA2 is used extensively around the world, but especially in the USA. The US EPA requires MINTEQA2 investigations to be undertaken for site investigations and assessments.

PHREEQC

PHREEQC is a multipurpose geochemical program written by the US Geological Survey. It can perform speciation, inverse modelling, and reaction-path and one dimensional advective reaction-transport modeling. The model is based on an ion-association aqueous model. It lacks the ability to do true kinetic modelling and cannot model dispersion. PHREEQC is widely used, but is better known by the name of an older version PHREEQE, which has been superceded by PHREEQC.

WATTAIL

A computer program (WATAIL) has been developed to assist in the management of water quality associated with disposal of sulphide tailings. The objective of the program is to provide comparisons in loading rates of the major oxidation products to surface water draining from the local watershed in which the tailings basin is contained. The program focuses on rehabilitation strategies based on engineered covers, including underwater scenarios. The output of the model provides concentration values of dissolved iron and sulphate that can be converted to mass loadings or release rates when the discharge flow rates are considered.

3.3 Hydrological Models

ACRU

The ACRU agrohydrological modelling system is a multi-purpose model which integrates the various water budgeting and runoff producing components of the terrestrial hydrological system with risk analysis. It can be applied in design hydrology, crop yield modelling, reservoir yield simulation and irrigation water demand/supply, regional water resources assessment, planning optimum water resource utilisation and resolving conflicting demands on water resources. It is widely used in agricultural studies but would have application in the mining context when considering rehabilitation options. It can be run on a daily timestep.

Hydrological Simulation Program Fortran (HSPF)

The Hydrological Simulation Program—FORTRAN (HSPF) is a comprehensive package for the simulation of watershed hydrology and water quality for both conventional and toxic organic pollutants. The model is extensively used in the USA. In South Africa use is also growing and is set to increase rapidly with the installed modelling system requirements which will be necessary in order to manage water resources in an integrated manner under the new water law.

Water Resource Simulation Model (WRSM90) and Catchment Rainfall Programme (HDYP08)

WRSM90 is a monthly timestep hydrological model of a modular construction, with four different types of module (runoff, reservoir, irrigation and channel) linked by means of arcs or routes. The arcs represent lines along which water flows, such as river reaches.

WRSM90 has become the de-facto model for water resources studies undertaken on behalf the South African Department of Water Affairs and Forestry (DWAF). Listed below are some of the more important catchments studied using WRSM90 and its predecessor, HDYP09.

- Limpopo, Sand, Luvuvhu, Letaba, Lephalala, Olifants (Mpumalanga & W Cape), Crocodile (North West Province & Mpumulanga), Mogalakwena, Sabie, Vaal, Orange, Breede, Berg, Kei, Mgeni, Thukela, Mvoti, Mhlatuze and Komati.

Daily Flow Modelling (DAYFLOW)

A cost effective option for a daily version of WRSM90 resulted in the development of DAYFLOW. DAYFLOW is a batch file that allows the user to run any of the following three programs:

- HDYP16 - Updated daily rainfall-runoff simulation model
- SCPLOT - Plotting of various graphs depicting monthly flow
- DAYPLOT - Plotting of graphs depicting daily flow

Essentially DAYFLOW uses a daily time-step whereas WRSM90 uses a monthly timestep. However, unlike WRSM90 it does not have the capability to simulate a complex network in a single run.

HEC-RAS

HEC-RAS assesses water levels and velocities in open channel river systems. It has the ability to model:

- Steady flow water surface profiles
- Branched or looped channel networks
- Bridges, culverts, weirs and spills
- Subcritical, supercritical or mixed flow regimes

The original computer program HEC-2, Water Surface Profiles, originated from a step-backwater program written as early as 1964. This early version was revised in 1966 and released by the Hydrologic Engineering Centre (HEC) in the USA. Since then the program has been revised several times and HEC-RAS, first released in 1995, represents the latest version. HEC-RAS (and its earlier derivatives) has been widely used in the USA but the extent of its use in South Africa is not known.

3.4 Water Quality Models

CE-QUAL-R1

CE-QUAL-R1 (R1) simulates the vertical distribution of thermal energy and chemical and biological materials in an impoundment. The model is thus designed as a one-dimensional description of a water body. The model was developed to study water quality problems, to develop management methods, and fine tune system operation. The model has been extensively used in the United States by the US Corps of Engineers. Evaluation and development of the model involved the use of

the DeGray Lake and the Eau Galle Reservoir data sets. In South Africa, the two-dimensional version of the model has been used.

DYRESM

DYRESM-1D is a one-dimensional hydrodynamic reservoir simulation model for the prediction of the vertical temperature and salinity distribution in small to medium size lakes and reservoirs. DYRESM was used to assess the application and capabilities of the model to provide a description of the hydrodynamics and thermal stratification in a number of South African impoundments. The model has been widely distributed both within Australia and overseas for use in teaching, research and industry in a wide variety of applications. These applications include the use of the model for reservoir management and the design of destratification systems.

QUAL2E

The enhanced stream water quality model (QUAL2E) is a steady state riverine quality model with some dynamic features. Steady state hydraulics (flows) are combined with water quality parameters that can optimally be steady-state or reflect daily variations in river flow. QUAL2E has been used widely and is an accepted standard particularly for wasteload allocation studies of stream systems. The model has been used successfully to simulate the conservative and non-conservative behaviour of rivers in South Africa. The simulations include simulation of TDS, N, P, DO and *E. coli*. In each case the model has provided a rapid and efficient tool for the assessment of water quality.

WASP

The Water Quality Analysis Simulation Program (WASP) is maintained by the Environmental protection Agency, is a generalized modelling framework for simulating aquatic systems, including rivers, reservoirs, estuaries and coastal waters. Problems that have been studied using WASP include biochemical oxygen demand, dissolved oxygen dynamics, nutrients/eutrophication, bacterial contamination, and toxic chemical movement. WASP has been successfully used in the USA for numerous applications in the field of water resource and quality management. The model requires a high level of computer literacy.

CE-QUAL-RIV1

The Waterways Experimental Station model CE-QUAL-RIV1 is a fully dynamic one-dimensional flow and water quality simulation model for rivers and streams. The model package includes two stand alone programs RIV1H and RIV1Q. RIV1Q is the water quality program. The model is similar to QUAL2E in that it simulates temperature, dissolved oxygen, BOD, nutrient kinetics, iron, manganese and coliform bacteria. The difference between the models QUAL2E and CE-QUAL-RIV1 is that RIV1 is fully hydrodynamic and can simulate sharp changes in river flow and water quality constituent concentration. In South Africa, the model has been tested using the flow and quality data for the Berg River, Western Cape.

IMPAQ

IMPAQ (**I**mpoundment/ river **m**anagement and **p**lanning **a**ssessment tool for water **q**uality simulation) was developed as part of numerous water resource system analysis studies for the Department of Water Affairs and Forestry (Directorate of project Planning). The model was developed so that it could import monthly hydrology from the *Water Resource Yield Model* and then simulate water quality at various points in a river system. IMPAQ was used to fine-tune system operating rules and also assess the impact of contaminant sources (point and diffuse).

FLUX, BATHTUB, PROFILE

These simplified procedures for eutrophication assessment and prediction were developed by Dr W. W. Walker for the US Army Corps of Engineers, Waterways Experiment Station. It consists of three interrelated programs, FLUX, PROFILE and BATHTUB. In South Africa, the FLUX model has been used in a number of studies to calculate mass loadings.

REMDSS

REMDSS - Reservoir Eutrophication Model Decision Support System, is designed to simulate the phosphorus dynamics in a reservoir. The model is mainly used to assess the impact of phosphorus control measures on eutrophication in reservoirs. The REMDSS model can not be used to simulate phosphorus dynamics in a small reservoir or weir where the water residence time is less than one week.. REMDSS has been extensively used in South Africa to predict the impact of phosphorous management actions on in-lake trophic status.

BETTER

The BETTER model, Box Exchange Transport Temperature and Ecology of a Reservoir Model, was designed to simulate seasonal patterns of temperature, dissolved oxygen, nutrients, pH and algal biomass in reservoirs. The BETTER manual printed in 1991 includes a bibliography of 17 reports describing the application of the model to 10 reservoirs in Tennessee Valley Authority. Since the publication of the manual, the applications of the model have been extensive, including the reservoirs of the Lesotho Highlands Water Project.

NACL01

NACL01 is a daily time step catchment hydro-salinity model. It combines catchment hydrology with the related salinity. NACL01 is designed to run on a PC. NACL01 is not screen-interactive, and the user needs to enter the resulting model output into processing software or other programs. Typically this model provides daily time series of catchment runoff and salinity, which is then fed as input to the channel routing model NACL02

NACL02

NACL02 is a daily time step model for routing flow and salt through a river system. NACL02 has been used in a number of detailed studies. These include the RSA Department of Water Affairs Vaal River Salinity Study and the Vaal River System Analysis Update Study. It has also been used as part of an environmental impact assessment for the Blesbokspruit, which includes the sensitive Blesbokspruit wetland (a designated RAMSAR convention site).

WQT

WQT is a monthly time hydro-salinity model. It is written in modular form and combines catchment hydrology with the related salinity. This PC based model is screen-interactive, allowing the user to view statistics and plots, adjust input variables and save output files repetitively without the need to exit the program or re-read the input data. The model has been used in a number of river system analyses carried out on behalf of the RSA Department of Water Affairs and Forestry. These include the Vaal, Orange and Crocodile Rivers (which together constitute a large proportion of the surface water resources of the country). The model has also been used on the Waterval, Free State Goldfields, Blesbok and Mooi River Situation Assessment studies, and the development of a Water Management Plan for the Free State Goldfields catchment. Smaller studies include hydro-salinity modelling of the Molopo River system.

OTIS

OTIS is a mathematical simulation model used to characterize the fate and transport of water-borne solutes in streams and rivers. The governing equation underlying the model is the advection-dispersion equation with additional terms to account for transient storage, lateral inflow, first-order decay and sorption. It is used widelely in the US where its applications include instream mixing.

OTEQ

OTEQ is a mathematical simulation model used to characterize the fate and transport of trace metals in streams and rivers. OTEQ couples the transport capabilities of OTIS (One-Dimensional Transport with Inflow and Storage) with the chemical equilibrium capabilities of MINTEQ (U.S.EPA). The coupled model considers a variety of physical and chemical processes including advection, dispersion, transient storage, the transport and deposition of water-borne solid phases, acid-base reactions, complexation, precipitation/dissolution and sorption.

At present, the model is used exclusively within the U.S. Geological Survey (USGS). Use outside of the USGS will begin after publication of user documentation.

3.5 Water and salt balance models

AQUABAT

Aquabat is a modular water and salt balance simulation software programme. The heart of the programme is the graphical interface using Microsoft Windows 95. The programme is based on unit processes which are linked using point and click technology. The water and salt balances are solved using the simultaneous solution of equations and the code is written in such a way as to generate these equations as the programme is executed. Its ease of use makes it applicable in most mining environments.

3.6 Groundwater Models

AQUAMOD

AQUAMOD for Windows is a 2D-triangular finite element Groundwater Modelling Package. AQUAMOD for Windows is used by the following institutions: IGS, CSIR, and consulting companies in SA and Nawater, Namibia.

ASMWIN

ASMWIN is a 2D finite difference program written by Chiang, Kinzelbach and Rauch, especially for teaching purposes. It can do flow and mass transport modelling. For mass transport either the finite difference or random walk method could be selected. This beta version has been tested and used in some short courses.

PMWIN

Processing Modflow for Windows (PMWIN) is an integrated system for modelling that includes:

- Groundwater flow and solute transport with the USGS groundwater flow model MODFLOW;
- The particle tracking model PMPATH;
- The solute transport model MT3D; and
- The parameter estimation program PEST.

MODFLOW can simulate the effects of wells, rivers, drains, head-dependent boundaries, recharge and evapotranspiration. PMWIN also supports the simulation of cut-off walls and the calculation of subsidence of the ground surface due to changes of hydraulic heads. The particle-tracking model PMPATH can be used for the delineation of catchment area or for the calculation of groundwater paths and travel times. The MT3D transport model can be used to simulate changes in concentration of single species miscible contaminants in groundwater considering advection, dispersion and some simple chemical reactions. The chemical reactions included in the model are currently limited to equilibrium-controlled linear or non-linear sorption and first-order irreversible decay or biodegradation. The purpose of PEST is to assist in data interpretation and in model calibration. If there are field or laboratory measurements, PEST can adjust model parameters and/or excitation data

in order that the discrepancies between the pertinent model-generated numbers and the corresponding measurements are reduced to a minimum

4 UPDATING WEB PAGES

The Internet Service Centre for Mine Related Water Models is intended to be dynamic. Thus it should continuously be changed and updated as new models become available. However, a strict protocol is required to update the site. The following section details the technical procedure to follow. The implemenattion procedure should be obtained from the CCWR (see web site).

Web Directories

All NEW models will be placed into either of the following directories

iscp/models/geochem/new model
iscp/models/grndwaterf/new model
iscp/models/hydro/new model
iscp/models/other/new model
iscp/models/surwaterq/new model
iscp/models/watersaltb/new model

Model Frames

Each model consists of three HTML pages

- The "welcome.html" file will launch the frame of that particular model
- The file "top_frame.htm" contains the legend and subheadings (with links) of that particular model
- The file "modelmain.htm" contains the actual model information and "bookmarks"

Bookmarks and links

The file "modelmain.htm" has bookmarks on the following words

1.Description
2.Data Requirements
3.Computer / PC Requirements
4.Availability
5.Assessment
6.Case Study

The file "top_frame.htm" has links to the above-mentioned bookmarks

1.#desc
2.#data
3.#pcreq
4.#avai

5.#assess
6.#case

Linking a model to the main page of a model Category

All models are listed in their appropriate categories - They also have their own legends.

The following are category pages which contain links to every model on the site

/iscp/models/geochem/main.htm
/iscp/models/grndwaterf/main.htm
/iscp/models/hydro/main.htm
/iscp/models/other/main.htm
/iscp/models/surwaterq/main.htm
/iscp/models/watersaltb/main.htm

When linking a model to any of these pages there should be a target frame specified - this target frame is "_parent"

Located on the site is a template for all future models. This must be copied and pasted into any one of the categories - then renamed to the name of your new Model.

All links are already setup - all that is required is to paste the correct information under the correct headings on the page modelmain.htm.

The page top_frame.htm will only need to be edited for the legend.

Once completed, then the model's welcome.html page must be linked to the appropriate main page as mentioned above.

5 CONCLUSIONS

The primary objective of this project was to develop an Internet Service Centre for Mine Related Water Models. This site has been developed and is located at:

http://www.ccwr.ac.za/iscp

The original intent with web site was to populate it with up to 50 models. This has not been achieved during the course of the project for a number of reasons:

- The project team evaluated the models used by them and in which they had sufficient expertise to evaluate the model. This restricted the number of models.
- Appeals were made by way of personal letters, letters to organisations and numerous publications in a variety of periodicals for anyone with models to approach the project team for the inclusion of their model on the site. This proved to have little success.

In the end, a total of thirty models were evaluated and are included in the web site. It is hoped that as the web site becomes more widely known, additional models will be

added to the site and that a larger number of models will be available to the end-user.

The site will be maintained and upgraded periodically by the Water Research Commission.

APPENDIX

MODEL: **ACIDROCK**

EVALUATED BY: **Dr RH Boer, Pulles Howard & De Lange Inc.**
www.phd.co.za

1) Description:

ACIDROCK is a model designed to evaluate acidic drainage in waste rock piles (Scharer et al., 1994)[1]. The conceptual basis for this model was the program RATAP, which was designed to assist in the prediction of acid generation caused by hydrological events and chemical reactions occurring in mine tailings sites. The transport, heat generation and oxygen flux portions of RATAP were replaced to reflect the difference in chemical and physical environments between waste rock piles and reactive tailings sites. Scharer et al., (1994) reported that the formulation of chemical equations used in RATAP were used for this model. The chemistry was expanded to include uranium and radium, including sorption on mineral solids and organic surfaces. Furthermore, the co-precipitation of radium with gypsum and radioactive decay have been included. ACIDROCK uses measured fundamental rate laws for the dissolution on sulphide minerals.

ACIDROCK simulates the waste rock pile as an equivalent rectangle of specified dimensions, which is divided into 20 layers, each interconnects to the other. Water flows downwards and exits as seepage at the base. Various parameters can be changed over a simulation to model the effects of different covers, re-profiling, changes in infiltration, etc.

The model is currently limited in the chemical constituents (minerals, aqueous species and complexes) that it includes. The pH in the model is estimated using electroneutrality. This model is not a detailed geochemical model and can not make a detailed assessment of the reactions, which occur between a fluid and solid phases. It is rather designed to examine implications of various containment options, using a simplified geochemical model with a restricted set of minerals and aqueous species.

The following list include the important processes that could be simulated during geochemical modelling:

1) Acid generation due to biological and chemical oxidation of sulphide minerals
2) Diffusion of oxygen into heaps and tailings, and also into tailings rock particles
3) Convective transport of oxygen into waste rock heaps
4) Production and transport of heat (conductive and advection)
5) Temperature with depth and effect of temperature on oxidation rates
6) Release (leaching) of metals
7) Transport of dissolved chemical species (e.g. sulphate, aluminium, calcium, magnesium, iron, metals)
8) Dissolution of solid buffering minerals (e.g. calcite, dolomite, sericite)

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[1] Scharer JM, Pettit CM, Chambers D and Kwong EC 1994. Mathematical simulation of a waste rock heap. Proc. 3rd Int. conf. Abatement of Acidic Drainage, U.S. Dept. Int. Bur. Mines Special Pub. SP 06A-94, V.1, 30-39.

9) Formation (precipitation) of secondary minerals (e.g. ferric hydroxides, jarosite)
10) Solubility of solid phases (e.g. precipitates, minerals)
11) Speciation of dissolved constituents
12) Estimation of the pH
13) Solid solution equilibria for metals
14) Adsorption of metals onto aluminium and ferric hydroxides, jarosite and organic carbon surface
15) Co-precipitation

2) Data requirements:

Data requirements for geochemical modelling using ACIDROCK are summarised below. The accuracy of the model predictions depends on the amount and quality of the data available.

Climatic:
Monthly mean surface temperature
Monthly precipitation/evaporation/evapotranspiration

Physical:
Surface area, depth
Bulk density, porosity/void volume
Moisture content/saturation level (% void volume)
Particle size distribution

Hydrological:
Hydraulic conductivity (vertical & horizontal)
Infiltration flow
Seepage flow

Water Quality:
Infiltration waters
Background water quality (surface & groundwater)
Porewater quality (with depth)
Seepage quality

Mineralogical:
Mineralogical composition
Estimate of percentage leachable pyrite (sulphide minerals)
Chemical and elemental analysis of solids
Chemical formulae of minerals
Proportion pre-oxidised (easily soluble metals and radionuclides)

Kinetic:
Biological and chemical oxidation rates for sulphide minerals
Weathering rates for silicates and carbonates
Miscellaneous data:
Description of historic as well as current activities
Visual observations reported during field visits

Transport related properties:
Diffusion coefficients
Convective air flow
Thermal conductivity
Temperature measurements with depth
Solid-liquid distribution coefficients (Kd) for metals

3) Computer requirements:

The system can run on almost all platforms from the smallest PC to the largest super computer using FORTRAN. The power of the computer naturally affects the run time.

4) Availability:

The ACIDROCK model is a proprietary software package, which could only be accessed through Senes Consultants Limited (121 Granton Drive, Unit 12, Richmond Hill, Ontario, Canada L4B 3N4).

4.1) Costs:

This model is not for sale, but can be obtained from the developers: Senes Consultants Ltd.
http://www.senes.on.ca

5) Assessment:

The following quote is from the MEND report (MEND Project 1.42.1).

> *" The current waste rock engineering models ACIDROCK and --- are the state-of-the-art in geochemical modelling of waste rock piles. They are clearly insufficient to make detailed predictions of ARD chemistry, as their chemical components are not complete enough. They can however be used for making relative comparisons and for data analysis. Even if they are currently evolving these models cannot be expected to evolve beyond of including detailed geochemistry in the near future. "*

5.1) Level of competency required:

The fundamental determinant of the levels of competency required are those of the potential users knowledge of the real world system that he/she is trying to model. If one has the scientific knowledge of the systems that one is modelling then the competency required to run the model is trivial by comparison. However, if one does not know the science behind the systems that one is modelling then any model is difficult and should not be used.

5.2) Keywords for task-based search:

Integrated, water resources, simulation, modelling, hydrological modelling, water quality modelling, conflict resolution, dissolution *(kinetic or equilibrium controlled)*, complexation *(from equilibrium and stoichiometry of several complexes)*, and precipitation *(formation of complexes and secondary minerals; (pH phase equilibria) (sulphate, iron, acidity, etc.)*, dissolution *(thermodynamic and sorption equilibrium)*, adsorption and coprecipitation of several metals and radionuclides.

5.3) Application algorithms and main mathematical limitations:

The model operates at a one-month time step. The spatial and temporal scale must however be matched realistically. This naturally requires the model user to be fully aware of the scientific systems being modelled.

Ancillary programs such as SoilCover and HELP are commercially available and these are highly recommended for optimization of the input data.

5.4) How widely is the model used and how well is it established in the industry:

The model is extensively used in North America, in particular Canada, as well as Germany and South Africa.

5.5) Related References:

Scharer JM, Pettit CM, Chambers D and Kwong EC 1994. Mathematical simulation of a waste rock heap. Proc. 3rd Int. conf. Abatement of Acidic Drainage, U.S. Dept. Int. Bur. Mines Special Pub. SP 06A-94, V.1, 30-39.

5.6) Links to organisations:

ACIDROCK was developed and is maintained as proprietary software by Senes Consultants Limited
http://www.senes.on.ca

5.7) Range of applications:

The ACIDROCK model was developed to simulate the generation and neutralization of acidic drainage in a waste rock heap. Empirical methods and mathematical

modelling were used to provide long-term predictions of acidic drainage for application of several different covers on acid generating heaps e.g. compacted clay, semi-compacted clay, non-compacted clay and pervious till. *(Equity Silver Mines, British Columbia, Canada).*

The ACIDROCK model was expanded to support the simulation and evaluation of various decommissioning alternatives for an *in-situ* uranium leach pile, including: reclamation with a cover; re-profiling the pile into an extension and mixing the relocated waste rock with lime; and removal, mixing with lime, and placement in the bottom of an open pit and flooding. *(Ronneburg, Thuringia, Germany).*

ACIDROCK was applied for simulation of acid generation in four coal refuse test piles constructed to evaluate several treatment alternatives (e.g. compaction, limestone addition, and bactericide treatment) and investigate the effect of pile size on acid generation through simulation of the actual large pile *(Eastern Canada).*

6) Case study:

The geochemical modelling of the Durban Navigational Colliery (Durnacol) Dump No. 7 has provided predictions for the possible short-term and long-term geochemical behaviour of the discard dump if it was to remain uncovered (Base Case). The modelling also supported a comparison of the advantages of placement of three different covers: Simple, Intermediate and Ideal cover.

According to field data collected from the site and laboratory analyses of samples of discard collected from the surface of the dump, the discard is currently acid-generating, but the overall seepage from the dump is neutral. The short-term simulation of the Base Case scenario suggests that the seepage from the dump could become acidic (pH 4 to 5 range) within the next ten years.

The long-term simulation of the Base Case scenario indicates that the discard could become strongly acid-generating (seepage pH < 3) and release high levels of sulphate, iron, acidity and metals within 100 years. The simulations of the cover options showed that the development of acidic and contaminated seepage could be prevented for the Ideal cover scenario, or significantly delayed for the Simple and Intermediate cover scenarios.

The modelling provided long-term predictions for the concentrations and loadings of contaminants that could be released from the dump under different decommissioning scenarios. At the time of placement of the cover, the discard is simulated as acid generating, but the combined dump seepage is currently neutral. If the placement of the cover did not take place until several years into the future, the dump would be simulated as containing more oxidized discard and the porewaters would be more acidic. Therefore, the simulated time for placement of the cover could have a significant effect on the predicted seepage quality and contaminant loadings for the cover options.

Relative cost estimates have been provided for the three cover scenarios. The major portion of the cost for cover construction is in re-profiling the dump for placement of the cover, vegetating the cover, and rehabilitating the borrow sites. These costs

have been compared with estimated expenses associated with different water treatment options.

It has been accepted, based on information provided by the mine, that there is no direct cost for excavation of imported soil materials, or for reclamation of the borrow sites for the imported materials. As a result of this hypothetical assumption, there is little difference between the estimated costs for the Simple and Intermediate covers. The Ideal engineered cover provides an order of magnitude reduction in the possible contaminant loadings, although the cost for the Ideal cover is only 30% higher than the cost of the Intermediate cover. Therefore, it would appear to be very cost-effective to construct an engineered cover on the dump. It is imperative that the rates used for the costing exercise need to be critically evaluated in the context of local contracting rates to better define the costs of the different covers.

Cost-benefit estimates indicate that an engineered cover would be the preferred option for rehabilitation of dump 7. Placement of a Simple cover would be substantially more expensive compared to the costs associated with either the Ideal or Intermediate cover options. However, the final selection of a cover will mainly depend on the target pollution load reductions, which are currently not well defined. Furthermore, the capital and operating costs associated with the various water treatment options need to be refined. Under the current guidelines approximately 300 tons/annum of pollution would be allowed to emanate from dump 7. These conditions suggest that an Intermediate cover option, together with a passive treatment plant would be the most cost-effective combination that would enable the mine to adhere to these guidelines.

MODEL: **ACRU**

EVALUATED BY:

1) Description:

The ACRU model has its hydrological origins in a distributed catchment evapotranspiration based study carried out in the Natal Drakensberg in the early 1970s (Schulze, 1975). The acronym ACRU is derived from the Agricultural Catchments Research Unit within the Department of Agricultural Engineering of the University of Natal in Pietermaritzburg.

CONCEPTS OF THE ACRU MODEL

The ACRU agrohydrological modelling system (Schulze, 1984; 1986; 1988a; 1989a; 1994) is centred around the following aims:

- It is a physical conceptual model, i.e. it is conceptual in that it conceives of a system in which important processes and couplings are idealised, and physical to the degree that physical processes are represented explicitly.
- ACRU is not a parameter fitting or optimising model and variables (rather than optimised parameters) are, by and large, estimated from physical characteristics of the catchment.
- It is a multi-purpose model, which integrates the various water budgeting and runoff producing components of the terrestrial hydrological system with risk analysis. It can be applied in design hydrology, crop yield modelling, reservoir yield simulation and irrigation water demand/supply, regional water resources assessment, planning optimum water resource utilisation and resolving conflicting demands on water resources.
- The ACRU model revolves around daily multi-layer soil water budgeting and the model has been developed essentially into a versatile total evaporation model. It has therefore been structured to be highly sensitive to climate and to land cover/use changes on the soil water and runoff regimes, and its water budget is responsive to supplementary watering by irrigation, to changes in tillage practices or to the onset and degree of plant stress.
- ACRU has been designed as a multi-level model, with either multiple options or alternative pathways (or a hierarchy of pathways) available in many of its routines, depending on the level of available input data available or the detail of output required. Thus, for example, reference potential evaporation, interception losses, values of soil water retention constants, maximum (i.e. "potential") as well as total evaporation ("actual evapotranspiration"), leaf area index, components of the peak discharge estimation, hydrograph routing, reservoir storage: area relationships or the length of phenological periods in crop growth, all may be estimated by various methods according to the level of input data at hand or the relative accuracy of simulation required.
- ACRU can operate as a point or as a lumped small catchments model. However, for large catchments or in areas of complex land uses and soils ACRU can operate as a distributed cell-type model.
- The model includes a dynamic input option to facilitate modelling the hydrological response to climate or land use or management changes in a time series, be they long term/gradual changes (e.g. forest growth, urbanisation,

expansion of irrigation project or climate trends), abrupt changes (e.g. clearfelling, fire impacts, construction of a dam, development of an irrigation project, introduction of new land management strategies such as tillage practices), or changes of an intra-annual nature (e.g. crops with non-annual cycles, such as sugarcane).

2) Data requirements:

The ACRU modelling system is made up of a number of discrete, but interlinked components. The ACRU model requires both an input menu file and a file containing hydrometeorological data, and may contain an optional dynamic file.
What type of hydrometeorological data is needed?

The model uses daily time steps and thus daily rainfall input, thereby making optimal use of available data. Certain more cyclic, conservative and less sensitive variables (e.g. temperature, reference potential evaporation), for which values may have to be input at monthly level (if daily values are not available), are transformed internally in ACRU to daily values by Fourier Analysis.

The generation of stormflow in ACRU is based on the premise that, after initial abstractions (through interception, depression storage and infiltration before runoff commences), the runoff produced is a function of the magnitude of the rainfall and the soil water deficit from a critical response depth of the soil. The soil water deficit antecedent to a rainfall event is simulated by ACRU's multi-layer soil water budgeting routines on a daily basis. The critical response depth has been found to depend, inter alia, on the dominant runoff-producing mechanism

2.1) Inventory of data sources:

Deterministic hydrological models, particularly when operating in distributed mode, require intensive soils, vegetation and climatic information and the collection and inputting of this information is both time consuming and laborious. It is to this end that a suite of software programs, called ACRU Utilities, has been developed to aid users in preparing input information for, and output information from, the ACRU hydrological simulation model.

The ACRU Menubuilder

The ACRU Menubuilder is an interactive, user friendly program of over 250 subroutines which prompts the user with questions for information, guides (with internal help and error checking facilities) the user through the various options available and facilitates rapid information input through a MENU file. It contains pre-programmed Decision Support Systems. Technical details on the Menubuilder are given in Chapter 5 of the ACRU User Manual.

Information is input into the Menubuilder in a sequential mode, dealing with individual processes one at a time. A feature of the Menubuilder, which can assist in editing a previously created MENU, is the facility to proceed to any selected section of the MENU, and skip over previously input information. In addition, the user can

end the session at any time and all information will be written to the user-selected output MENU file name.

ACRU caters for several levels of information availability. Detailed information is often not available and the user can then resort to the "experience" that has built into ACRU and the Menubuilder through a Decision Support System by way of default values and pre-programmed information.

The two areas where this facility is particularly useful are in inputting soils and vegetation information. In each case, if catchment information is limited or considered "inadequate", the user can select from a range of classes of input and the program assigns realistic default values to the variables.

Area-Weighting Soil Type And Land Cover Information

Although ACRU can be run in distributed mode with a catchment discretised into a number of subcatchments, each with relatively homogeneous hydrological response, it is still often the case that more than one soil type or vegetation/land cover is present within a subcatchment. When this occurs, it is necessary to weight input values according to their respective areas, which can be a tedious undertaking. Hence stand-alone routines are provided to area-weight soil type and land cover information for each subcatchment. The programs are run independently of the Menubuilder, and the area-weighted information may be entered into the Menubuilder. Alternatively, routines are provided which will automatically insert output from the area- weighting programs into an existing MENU. The MENU containing the inserted information may already contain the remaining information for the simulation (i.e. the Menubuilder has already been run) or, alternatively, the MENU can be used as the input MENU to the Menubuilder program.

Land Type Soils Information

When detailed soils information is not available for the catchment area of interest, Land Type (soils) information published by the erstwhile Soil and Irrigation Research Institute, now the Institute for Soil, Climate and Water (ISCW) may be used. A routine converts ISCW Land Type information into hydrological information, which can be utilised directly by ACRU.

Conversions From GIS

A routine is included which will area-weight and convert into ACRU format relevant information from land cover and Land Type (soils) polygons that have been digitised using the ARC/INFO GIS package. This interface with GIS greatly enhances ACRU's versatility.

Generation Of A Stochastic Time Series Of Daily Rainfall

Often, for planning purposes, a stochastic time series of daily rainfall values is used in preference to historical data, which may be difficult to obtain or which may contain missing data. A routine may be called to generate a stochastic time series of daily rainfall, for any one of over 5 000 station locations in South Africa, based on

an original study by Zucchini and Adamson (1984), and subsequent updates of that research. The user merely inputs latitude and longitude co-ordinates for the location of interest, and then selects any one of the 10 computer selected rainfall stations closest to the location and appearing on screen, before selecting any length of record desirable. The generated daily rainfall series can be automatically formatted to an ACRU format, ready for use; alternatively the user can request that the stochastic series be output in any one of a number of other formats.

Extraction Of Gridded Images

The Department of Agricultural Engineering at the University of Natal has developed gridded images of mean monthly A-pan equivalent evaporation and monthly means of daily maximum and minimum temperatures, at a resolution of one minute by one minute of a degree latitude/longitude covering southern Africa. A routine is included which will extract values from the gridded image for a user input rectangular catchment boundary.

Lagging Of A Time Series

A daily time series can be "lagged" by a number of hours, based on the assumption that the daily values making up the time series are distributed uniformly over the day in the long run. This may be useful, for example, when using historical daily rainfall data, which are recorded for the 24 hour "day" starting at 08:00, in conjunction with observed daily streamflow data, which are derived from digitised data and are normally outputted for the 24 hour period starting at 00:00. The streamflow data, being of a more continuous rather than the "pulsar" nature of the rainfall, would then be computed in a time-weighted manner to coincide with the rainfall "day". This "lagging" of a time series can improve simulations markedly (e.g. Herpertz, 1994).

Other Utilities

A number of other utilities are included. For example, daily rainfall data can be converted or re-converted into a number of different formats (e.g. SAWB, ACRU).

3) Computer requirements:

Distributed hydrological models require intensive soils, vegetation and climatic information and the collection and inputting of this information is both time consuming and labourious. It is to this end that a series of programs have been developed to aid users in running the ACRU hydrological simulation model. These programs have been written in ANSI FORTRAN 77 and make use of the ANSI.SYS device driver of the DOS operating system and will therefore only run on IBM compatible personal computers. If these programs output garbage to the screen on execution the ANSI.SYS driver statement should be added to the CONFIG.SYS file and the machine must then be rebooted. The input data file of variables and parameters that is required by the ACRU simulation model is called a menu.

4) Availability:

ACRU can be obtained from:

University of Natal,
Private Bag X01,
Scottsville 3209,
Pietermaritzburg,
South Africa.
Phone +27 331 260-5489
Fax: + 27 331 260-5818

Or downloaded from the CCWR's home page: http://www.ccwr.ac.za/~lynch2/acru/index.html

For questions regarding ACRU contact Prof. R. Schulze at: schulze@aqua.ccwr.ac.za

4.1) Costs:

5) Assessment:

5.1) Level of competency required:

5.2) Keywords for task-based search:

5.3) Application algorithms and main mathematical limitations:

ACRU operates in conjunction with the interactive ACRU Utilities, which is a suite of software tools to aid in the preparation of input information (e.g. the ACRU Menubuilder) and output information (e.g. the ACRU Outputbuilder). The ACRU Menubuilder prompts the user with unambiguous questions, leading the user into inputting, for example, complex distributed catchment information easily. The Menubuilder contains alternative decision paths with pre-programmed Decision Support Systems. Furthermore, the Menubuilder includes a help facility, built-in default values as well as warning and error messages. Details of the various Utilities are presented in ACRU User Manual.

OUTPUT SIMULATED BY ACRU

The "heart" of the ACRU model is a daily multi-layer soil water budget, and hence the model simulates the components and processes of the hydrological cycle affecting this soil water budget, including:

- Canopy interception of rainfall by vegetation;
- Net rainfall reaching the ground surface;
- Infiltration of net rainfall into the soil;
- Total evaporation (transpiration as well as soil water evaporation) from the various horizons of the soil profile to root depth;
- Suppression of soil water evaporation by litter or mulch;

- The redistribution of soil water in the soil profile, both saturated and unsaturated; and
- Percolation of soil water into the intermediate groundwater zone.

The model can output any of the above components. In the present output routines, provision has been made to output on a daily basis, or as monthly and annual totals of the daily values, inter alia:

- Rainfall;
- Effective rainfall;
- Reference potential evaporation;
- Maximum evaporation (i.e. "potential evapotranspiration") from the vegetation under conditions of freely available soil water;
- Total evaporation (i.e. "actual evapotranspiration") in the form of transpiration and soil water evaporation from top- and subsoil horizons respectively; and
- Soil water content of top- and subsoil layers and drainage into the intermediate zone.

From the soil water budget, the model is capable of outputting simulated elements of streamflow on a daily time step, or as monthly or annual totals of daily values. These include:

- Stormflow depth (or volume);
- Baseflow depth (or volume);
- Accumulated streamflow from all upstream catchments when simulating distributed, multiple subcatchments; and
- Peak discharge (including hydrograph routing when simulating distributed multiple subcatchments).

The components of the water budget are integrated with modules embedded within the ACRU model to enable output of:

- Reservoir yield analysis (overflow, reservoir status, abstractions, transfers);
- Sediment yield analysis (daily, monthly, annual; reservoir sedimentation);
- Irrigation water demand (for different crops, application efficiencies, modes of scheduling);
- Irrigation water supply (from streams, reservoirs and combinations; off-channel reservoir storage);
- Wetlands hydrological responses;
- Effects of abstractions from the stream (e.g. for domestic purposes) on catchment water yield;
- Fluctuations of shallow groundwater under certain conditions;
- Hydrological impacts of afforestation;
- Effects of other land cover, land use and management (e.g. tillage) changes (gradual or abrupt);
- Seasonal crop yields (maize, sugarcane and winter wheat - dryland or irrigated, as well as for non-crop specific net above-ground primary production); and
- The effects of enhanced atmospheric CO2 levels on transpiration suppression and hence on crop yield and water resources.

Being a daily time step model, ACRU does not, in most of its standard routines, account for the temporal variability within individual storm events. However, the

distributed version of the ACRU model has the ability to take account of the spatial variability not only of rainfall, but also of land uses and soils to provide a more accurate representation of where, within the catchments, the hydrological responses are occurring and with what magnitude.

Inter-Subcatchment Streamflow

The lumped model's soil water budgeting routine is performed on a point scale with all units expressed in mm. Stormflow and baseflow, which together make up streamflow, are thus also expressed in mm. In order to direct outflow to downstream cells, the streamflow depth calculated by the model has to be converted to a volume (m^3), because each subcatchment may have a different area. The presence or absence and the identity of upstream subcatchments are determined by interrogation of the menu.

5.4) How widely is the model used and how well is it established in the industry:

Other than in southern Africa (South Africa, Botswana, Namibia, Lesotho, Swaziland and Zimbabwe), lectures on the ACRU system have been given in Australia, Austria, Canada, Chile, Czech Republic, France, Germany, Hungary, Kenya, Portugal, Switzerland, the UK and the USA. The model has been verified widely on data from southern Africa and the USA (Schulze, 1994, Chapter 22), used extensively in decision making in southern Africa and by 1994 the model had been applied internationally in research in Botswana, Chile, Germany, Lesotho, Namibia, Swaziland and the USA.

5.5) Related References:

http://www.ccwr.ac.za/~lynch2/acru/index.html

5.6) Links to organisations:

http://www.ccwr.ac.za/~lynch2/acru/index.html

5.7) Range of applications:

- Water Resources Assessments;
- Design Flood Estimation;
- Irrigation Water Demand And Supply;
- Crop Yield And Primary Production Modelling;
- Assessments Of Impacts Of Land Use Changes On Water Resources;
- Assessments Of Hydrological Impacts Of Wetlands;
- Groundwater Modelling; and
- Assessments Of Potential Impacts Of Global Climate Change On Crop Production And Hydrological Responses.

6) Case study:

Water Resources Assessments

Regional runoff production in the Qwa-Qwa area within South Africa was simulated by Schulze, Schäfer, and Lynch (1990) who applied ACRU on a minute by minute grid of latitude/longitude of the area. The simulated streamflow at each grid point was then totalled in order to assess the regional production of runoff in average, wet and drought-stricken years. A semi-distributed subcatchment approach was used by Schulze (1988b) in a regional assessment of water resources in the Winterton area of KwaZulu-Natal for complex, multiple irrigation abstractions. In the regionally most comprehensive application of the ACRU modelling system to date, Tarboton and Schulze (1990; 1991; 1992) successfully modelled the hydrology of the 4354 km^2 Mgeni River catchment in South Africa. The model was applied in a spatially distributed mode consisting of 123 sub-catchments and was linked to a Geographic Information System (GIS) in order to integrate geographically spatial information for input into the model and to display output from the model. More recently ACRU has simulated streamflow from the Bröhl, a 300 km2 tributary catchment of the Rhine in Germany, very successfully (Herpertz, 1994).

Design Flood Estimation

Verified stormflows simulated by the ACRU model from catchments in the USA, representing a range of climates and sizes, were used in the development of SCS design flood estimation techniques for southern Africa by Schulze (1982), Dunsmore, Schulze and Schmidt (1986) and Schmidt and Schulze (1987a). In the latter study, the ACRU model was used to integrate risk analysis with simulated soil moisture changes antecedent to design events, and was also used to estimate design streamflow by considering the joint association between rainfall and antecedent soil moisture conditions. The lagging and attenuation of floods through river reaches and reservoirs is important in the estimation of peak discharge from a catchment consisting of numerous subcatchments. The hydrograph routing routines developed and verified by Smithers and Caldecott (1993), were used by Tarboton and Schulze (1992) in the hydrological modelling of the Mgeni River system.

Irrigation Water Demand And Supply

One of the ACRU model's strengths is the integration of water demand and supply on a catchment scale. This attribute has been used extensively in reconciling and optimising irrigation water demand and supply. Crop water requirements for irrigation planning in southern Africa were determined by Dent (1988) and Dent, Schulze and Angus (1988) using the ACRU model. The sensitivity of crop water requirements to estimates of reference evaporation was investigated by Lecler, Kunz and Schulze (1993). Crop water requirements have been integrated with catchment water yield (e.g. Dent, 1988; Schulze, 1988b; Lecler and Schulze, 1994) and the effect of different irrigation strategies have been studied, inter alia, by Furniss, Dent and Schulze (1988), Furniss and Schulze (1989) and Lecler and Schulze (1994). The optimum utilisation of the limited water resource for irrigation planning has been investigated by Furniss et al. (1988), Furniss and Schulze (1989) and Lecler and Schulze (1994). Schulze and George (1987b) include an economic analysis in assessing the implications of deficit irrigation in Namibia while the paper by Lecler, Schulze, Mottram, De Jager and Bennie (1993) compares ACRU with other models used in South Africa as an irrigation management tool.

Crop Yield And Primary Production Modelling

The ACRU model has options to simulate seasonal yields of maize (with the ACRU maize model developed by Domleo, 1990), winter wheat (Domleo, 1990), sugarcane (Hughes, 1992) as well as primary production (Schulze, 1984). Schulze (1985; 1986; 1989b) has reviewed ACRU's crop yield output with particular reference to risk analysis and irrigation, while Furniss and Schulze (1989) used the maize yield simulation option to investigate crop yield in relation to soil properties and optimum irrigation applications at four climatically diverse locations in South Africa. Schulze (1991a) also used the maize yield option to examine likely shifts in maize production regions as a consequence of elevated levels of atmospheric CO_2. A version of the CERES suite of crop growth models has been linked to ACRU to form a tool, which can simulate crop growth and hydrological events at regional scale. This hybrid model has been used by Schulze, Kiker and Kunz (1993) to simulate possible changes in maize production as a consequence of likely global climate change and associated CO_2 fertilisation.

Assessments Of Impacts Of Land Use Changes On Water Resources

The ACRU model has been developed and shown to be sensitive to land cover, land use and land management changes and has been used frequently in assessing this impact on streamflow. An important background paper in this regard was that by Schulze (1987). Tarboton and Schulze (1990; 1992; 1993) investigated three development scenarios on streamflow responses in the Mgeni River catchment. The first scenario investigated was the impact of small farm dams on streamflow, the second scenario examined the impacts of afforestation and the third scenario analysed the impact of urbanisation on streamflow. In another series of studies, this time on catchment responses to sugarcane cultivation under different agricultural practices, Haywood and Schulze (1990; 1991) illustrated the simulating potential of ACRU, also in a comparison with other models.

The model has been used frequently to study the hydrological effects of afforestation. For example, Schulze (1990b), Schulze and George (1987a; 1987c) and Tarboton and Schulze (1990, 1992) examine the effects of afforestation on catchment water yield, while Kienzle and Schulze (1992) used the ACRU model to simulate the effect of afforestation on shallow groundwater resources in deep sandy soils. The integration of soil properties and climate within the model has enabled the model to be used to assess and map the potential of sites for forestry production (Donkin and Schulze, 1990; Schulze, 1990c). In a comparison with recorded data, Scott and Schulze (1992) used the ACRU model successfully to simulate the hydrological effects of a wildfire in an afforested research catchment at Ntabamhlope. A major development to ease the application of ACRU in impacts studies on afforestation was the development of a forest Decision Support System in ACRU (Jewitt and Schulze, 1991), which has also been verified on a range of instrumented afforested catchments (Jewitt and Schulze, 1993).

Assessments Of Hydrological Impacts Of Wetlands

A wetland sub-model for the ACRU model was initially developed by Schulze, Chapman, Angus and Schmidt (1987) and used to assess the hydrological impacts of

upstream reservoirs on wetlands in East Griqualand. Smithers (1991) further refined and verified the model against observed data. The model was then applied by Smithers and Schulze (1993) to investigate the influence of wetlands on streamflow regulation and flood attenuation.

Groundwater Modelling

The use of ACRU's shallow groundwater module to simulate likely long term consequences of afforestation on fluctuations in groundwater level using historical climate and borehole data was demonstrated for deep sandy soils in northeastern KwaZulu Natal by Kienzle and Schulze (1992). ACRU was furthermore the hydrological simulator of recharge from the soil to groundwater in a study by Lynch, Reynders and Schulze (1994) which applied the DRASTIC equation to map groundwater vulnerability over South Africa using a GIS approach.

Assessments Of Potential Impacts Of Global Climate Change On Crop Production And Hydrological Responses

A number of studies utilising the ACRU model have been conducted to assess the potential impact of elevated CO2 and temperature levels and possible changes in precipitation and potential evaporation on crop and runoff production in southern Africa. Likely shifts in maize production regions in southern Africa as a consequence of global climate change were simulated using the ACRU model by Schulze (1991a). This work was greatly improved when the hybrid ACRU/CERES model was used subsequently by Schulze, Kiker and Kunz (1993) to simulate possible changes in maize production under different fertiliser scenarios over southern Africa. In regard to possible hydrological responses to climate change Schulze (1990a; 1991b) applied ACRU to scenarios of design stormflow production as well as potential water yield changes. Kunz and Schulze (1993) used ACRU to assess the sensitivity of runoff production at several locations in southern Africa to climate change and also used the model to ascertain critical climate thresholds of the hydrological system to change.

Other Applications Of ACRU

ACRU has in recent years been applied to diverse other hydrological problems, inter alia, assessing:

- Potential impacts of cloud seeding on streamflow production (Howard and Görgens, 1993);
- Urban runoff responses of both the formal and informal sectors (Tarboton and Schulze, 1993);
- Water quality under urban conditions (Schmitz, De Villiers and Schulze, 1993); as well as
- Establishing groundwater vulnerability to contamination (Lynch et al., 1994).

The model has also been selected as the "engine" which "drives" simulations used by a series of user manuals now in standard use by practitioners in southern Africa, including one on irrigation planning (Dent et al., 1988) and on design hydrographs from small catchments (Schmidt and Schulze, 1987a; Schulze, Schmidt and Smithers, 1993).

MODEL: **AQUABAT**
EVALUATED BY: **Mike Howard, Pulles Howard & de Lange Inc.**
www.phd.co.za

1) Description:

AQUABAT is a water and salt balance simulation model. It was developed primarily for the mining industry but can be used in any industry where water management is important.

Water and salt balances remain the most powerful potential tools available to mine water managers. Despite this fact, most mines do not have access to proper dynamic water balances, which are updated on a regular basis to serve as management tools. The efficient management of water can reduce costs, it can reduce the volume of "lost" water and it can reduce the volume of water leaving the mine and purchased by the mine.

The water balance must identify all water circuits across the mine, and ascribe accurate flow rates to each of the circuits. Once the water is in balance, salt concentrations can be added, to identify pollution sources.

Tables of flow and water quality data also have limited practical management value until they are converted to dynamic schematic representations. These schematic representations indicate the paths and volumes of water in circuit around the mine. Once the information has been collected, it can be placed on a computer programme. The use of a computer model has the following benefits:

- Access to up-to-date and accurate water and salt balances at all times.
- Reduction in manpower required to prepare regular water and salt balances.
- Access to a powerful tool which assists mine personnel in managing their water systems, thereby reducing impact on the water environment and reducing wastage of valuable and costly water.
- Ability to audit water usage and wastage on the mine and instantly identify problem areas.
- Ability to provide accurate water balances when preparing EMPRs, when monitoring or auditing compliance with EMPR provisions and when entering into negotiations with water authorities.

AQUABAT uses the functionality of Windows' Graphic User Interface and Drag and Drop features to allow the user to create the water balance diagram. Thereafter a grid system (similar to a spreadsheet) is the interface for data entry into the system. The water flow diagram and the data can be printed.

AQUABAT uses the simultaneous solution of equations to solve for unknown flows and concentrations. The model uses the solution of mass balances to determine the

unknowns. It works accurately on conservative substances and should not be used on non-conservative substances.

2) Data requirements:

If the user has only flow data available, one unknown stream per unit can be calculated. However, if the user has salt data available, two unknown flows can be calculated.

The user can choose between any 4 conservative salts:
- Total dissolved salts;
- Sulphate;
- Sodium;
- User defined.

The flow data needs to be supplied in m3 per day and salt data in mg/l.

3) Computer requirements:

The following minimum requirements are needed to install and run AQUABAT:

- 486 CPU
- 16 Mbytes RAM
- 10 Mbytes hard disk space
- VGA monitor operating at 800 X 600 dpi
- Mouse
- Windows 95

4) Availability:

AQUABAT is available from Pulles Howard & de Lange in South Africa (e-mail phd@phd.co.za).

4.1) Costs:

It is a price category 2 model (< US$ 2000).

5) Assessment:

AQUABAT has been used successfully in a number of mines in South Africa to manage water resources. Its graphical user interface makes it easy to use.

5.1) Level of competency required:

A moderate level of computer literacy is required. Knowledge of water balances and their use in management are required.

5.2) Keywords for task-based search:

AQUABAT, water balance, salt balance, mine water management, pollution loads, what-if? Scenarios

5.3) Application algorithms and main mathematical limitations:

AQUABAT uses the simultaneous solution of equations to solve for unknown flows, therefore in any unit process the number of unknowns that can be solved for is equal to the number of input fields. Thus, if only flow data is available, one unknown can be calculated, but if flow and salt data is available, two unknown streams can be calculated.

5.4) How widely is the model used:

Due to the recent launch of AQUABAT its use has been restricted to the South African mining industry.

5.5) Related References:

Van Heerden, J.J., Van Der Spuy, D. and Le Roux, P.J. (1986). Manual For The Planning, Design And Operation Of River Gauging Stations. *Department of Water Affairs Report No. TR126.*

Anon. (1991). Degremont Water Treatment Handbook, *Sixth Edition.*

Connely, R.J., Abrams, L.J. and Schultz, C.B. (1989). An Investigation Into Rainfall Recharge To Groundwater. *WRC Report No 149/1/89.*

Van Zyl, W.H. and de Jager, J.M. (1992). Errors In Micro-Meteorological Estimates Of Reference Crop Evaporation Due To Advection. *Water SA, Vol. 18, No. 4, pp 255 - 264.*

Hammer, A. (1992). Creating Freshwater Wetlands, *Lewis Publishers, p28.*

Brezny, O., Mehta, I. and Sharma, R.K. (1973). Studies On Evapo-transpiration Of Some Aquatic Weeds. *Weed Science, Vol. 21, No. 3, pp 197 - 204.*

Marsalek, J. (1990). Evaluation Of Pollutant Loads From Urban Nonpoint Sources. *Wat. Sci. Tech. Vol. 22, No. 10/11. pp 23 - 30.*

Russ, H.J. and Uhl, M. (1990). Comparison Of Pollutant Load Calculation Methods Based On Measured Data - State Of The Investigation, *Wat. Sci. Tech. Vol. 22, No. 10/11. pp 95 - 102.*

Pulles, W., Heath, R. and Howard, M. (1995). A Manual To Assess And Ameliorate The Impact Of Gold Mining Operations On The Surface Water Environment. *WRC Report in preparation.*

5.6) Links to organizations:

http://www.phd.co.za

5.7) Range of applications:

- water and salt balance modelling
- identification of pollution loads
- water management
- assessment of water monitoring requirements

6) Case Study:

In order to demonstrate how water balances are developed, a worked example is presented here. A single typical circuit is used as the example, but the principles would apply to any water circuit on any mine.

Surface water domestic circuits
A schematic diagram indicating the surface water domestic circuits is presented in Figure 1. The water balance for the domestic circuits is as follows (all figures are M ℓ/month):

$$(1) = (2) + (3) + (4) + (5) + (6) + (7) + (12) \approx (2) + (9) + (10) + (11) + (12) + (5) + x$$

where x represents a net consumption for the domestic system.

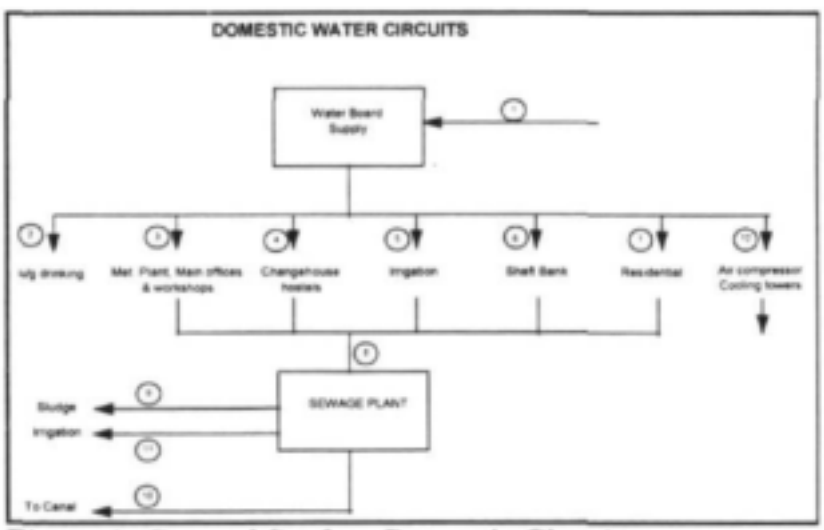

Figure 1: General Surface Domestic Circuits.

This equates to:

$$\text{In (185)} = 6 + 14 + 59 + y + 18 + 51 + 1$$

In terms of the volume of water distributed to the various circuits, all are metered except the volume of water for irrigation. This is solved from the equation to give 36 Mℓ/month.

Out	=	6 + z + 0,5 + 126,5 + 1 + 36 + x
Therefore x + z	=	15 Mℓ/month

This calculation generates a net consumption loss for the system of 15 Mℓ/month. This figure is attributable to losses within the system, the portion of water within the sewage sludge, physical consumption, domestic garden irrigation, washing use and any discrepancies between the Water Board meter readings and the mine's own water meter readings.

MODEL: **AQUACHEM**

EVALUATED BY: Scientific Software Group, E-mail: info@scisoftware.com
And
Dr. Rudy Boer, Pulles Howard & De Lange Inc.
Email: rudy@phd.co.za

1) Description:

AquaChem is a fully integrated software package developed specifically for graphical and numerical analysis of geochemical data sets. AquaChem features a powerful database that can be customized and configured to include an unlimited number of attributes per sample and a built-in database of inorganic chemicals that are commonly-used for geochemical analyses, calculations and plotting. AquaChem covers a wide range of calculations frequently used for the analysis, interpretation and comparison of aqueous geochemical data. The analysis tools in AquaChem range from simple unit transformations, mixing calculations, statistics and charge balances to more complex calculations involving correlation matrices and geothermometrics. These powerful analytical capabilities in AquaChem are complimented by a comprehensive selection of commonly used graphical techniques to portray the chemical characteristics of geochemical and water quality data for single samples and groups of samples. The fully customizable graphical features of AquaChem facilitate the understanding and interpretation of the many complex interactions between the groundwater and aquifer materials. AquaChem's graphical plotting techniques include Piper, Stiff, Durov, Langelier-Ludwig, Schoeller and ternary diagrams, radial plots, scatter graphs, frequency histograms, pie charts, geothermometer plots and time series graphs. In addition, AquaChem features a graphical interface to the popular geochemical modeling program PHREEQC for calculating equilibrium concentrations (or activities) of chemical species in solution and saturation indices of solid phases in equilibrium with a solution.

2) Data requirements:

AquaChem Database Features

- **Data Structure**

AquaChem is built around a customizable database that can be configured to include an unlimited number of attributes per sample (e.g., chemical elements, gas concentration, isotopic composition, physical parameters, etc. Each sample in AquaChem can be characterized according to five basic parameter groups including: (1) Header Information (Sample ID, Location, Date, Geology, etc.), (2) Physical Data (Coordinates, sample depth, head, pH, Conductivity, etc.), (3) Cations (Ca, Mg, Na, K, etc.), (4) Anions (Cl, Br, SO_4, NO_3, etc.), and (5) Uncharged Compounds (Al, As, CO_2, etc.).

Each of these parameter groups contains predefined parameters, which can be used to create a data structure that is customized for your sampling and reporting requirements. The built-in database in AquaChem contains most major cations and anions and the chemical properties of each. Additional parameters that are not included can be easily added to the database together with guideline exceedence values for each parameter.

The AquaChem database offers standard database functionality for performing queries or adding and subtracting samples from the selected data set. A powerful search engine allows you to find and group data records according to virtually any search criterion associated with the data set. The selected samples can be easily saved in subgroups or temporarily isolated from the other records for further data processing and interpretation by AquaChem.

- **Data Analysis**

AquaChem uses the common measured values (cations and anions) for each sample to calculate additional geochemical parameters including water type, sum of anions, sum of cations, ion balance, TDS, hardness, alkalinity, common geochemical ratios, and dissolved minerals. In addition, AquaChem also performs more advanced calculations including:

- Basic statistical calculations such as average value, standard deviation and linear correlation matrices.
- Similarity analysis to calculate a linear regression between a single sample and all other samples of the record list.
- Mixing of two samples can be performed and the results written to the database and a new sample record.
- Chemical facies can be calculated based on the elements that are present by more than 20% of the total of all elements in equivalent concentration.
- Geothermometric calculations can be performed to estimate the original temperature at depth of sampled water.
- Upper and lower tolerance and guideline limit exceedences can be identified for every numeric parameter in the sample set.

AquaChem also produces printed reports for each record or for the entire database containing general sample information, isotope summaries, and a list of samples. All sample records can be exported to a tab-delimited ASCII file.

3) Computer requirements:

AquaChem Requirements: PC 486DX/Pentium with 8 MB RAM, 10 MB free disk space and Windows 95/NT.

4) Availability:

Scientific Software Group,
P.O. Box 23041,
Washington, DC 20026-3041
Phone (703) 620-9214
Fax (703) 620-6793
E-mail info@scisoftware.com

4.1) Costs:

Cost Category 2: < US$ 2000

Prices include shipping and tech support provided by the developer.

5) Assessment:

AquaChem is a fully-integrated software package developed specifically for graphical and numerical analysis of geochemical data sets. AquaChem features a powerful database that can be customized and configured to include an unlimited number of attributes per sample and a built-in database of inorganic chemicals that are commonly-used for geochemical analyses, calculations and plotting.

AquaChem covers a wide range of calculations frequently used for the analysis, interpretation and comparison of aqueous geochemical data. The analysis tools range from simple unit transformations, mixing calculations, statistics and charge balances to more complex calculations involving correlation matrices and geothermometrics. These powerful analytical capabilities in AquaChem are complimented by a comprehensive selection of commonly-used graphical techniques to portray the chemical characteristics of geochemical and water quality data for single samples and groups of samples. The fully customizable graphical features in AquaChem facilitate the understanding and interpretation of the many complex interactions between the groundwater and aquifer materials. AquaChem's graphical plotting techniques include Piper, Stiff, Durov, Langelier-Ludwig, Schoeller and ternary diagrams, radial plots, scatter graphs, frequency histograms, pie charts, geothermometer plots and time series graphs.

In addition, AquaChem features a graphical interface to the popular geochemical modeling program PHREEQC for calculating equilibrium concentrations (or activities) of chemical species in solution and saturation indices of solid phases in equilibrium with a solution.

Once you start using AquaChem, you will see that it is truly one of the most powerful tools available for anyone dealing with the interpretation, analysis and modeling of simple or complex aqueous geochemical data sets.

AquaChem Main Features

- Automatic unit conversions (mg/l, mol/l, mmol/l, ppm, meq, SiO_2 in Si, H_2Si_3, etc.)
- Flexible data input methods (import from ASCII file or manual keyboard entry)
- Standard database functionality for performing queries and grouping data
- Built-in selection of common geochemical calculations and analysis methods
- Comprehensive selection of graphical techniques for representing and interpreting aqueous geochemical data
- Graphical interface to PHREEQC for geochemical modeling (PHREEQC executable included!)

AquaChem Graphical Display Features

AquaChem's powerful graphical tools utilize 15 techniques commonly used by hydrogeologists and geochemists for analyzing and interpreting aqueous

geochemical data sets for hundreds and even thousands of different samples. All text on each graphical display can be customized using a full selection of Windows true type fonts. The various graphical methods and the display options of AquaChem are discussed below.

Common Features for all Graphs

One of the most powerful features of AquaChem is the ability to simultaneously display and modify multiple plots, and to easily identify selected data points within each plot. This unique feature allows you to perform a comprehensive analysis of the data using several interpretation methods. Futhermore, each sample record in the database is directly linked to the graphs, so that any changes to the data are immediately updated on the graphs. This also allows you to easily identify specific sample records on each plot. Other common features include: fully customizable axes scale settings and unit selections for applicable graphs; complete selection of Windows True Type fonts for plot titles, legends, axis labels, and symbol labels; and proportional symbol sizes using concentration value for any measured or calculated parameter.

Site Map Diagrams

Detailed site maps can be imported from DXF files and overlaid with sample point locations. This provides a familiar point of reference when you are analyzing sample data by simultaneously displaying several plot types on the same screen. The symbols representing the sample locations can be customized according to shape and color. In addition, the map plot can be used to display the location of different water facies or the symbols can be scaled according to the concentration of a selected measured element. The highlighted sample points indicate samples that are selected in the database and are also highlighted on all other open graphical displays.

Stiff Diagrams

The Stiff diagrams in AquaChem are plotted for individual samples as a method of graphically comparing the concentration of selected anions and cations for several individual samples. The shape formed by the Stiff diagrams will quickly identify samples that have similar compositions and are particularly useful when used as map symbols to show the geographic location of different water facies.

Radial Diagrams

The radial diagrams in AquaChem are plotted for individual samples as a method of graphically comparing the concentrations of measured parameters for several individual samples. The shape formed by the radial diagrams will quickly identify samples that have similar compositions and are particularly useful when used as map symbols to show the geographic location of different water facies.

Pie Charts

The pie charts in AquaChem are used to plot the concentrations ratio of the major ions (or any combination of parameters) for individual samples. As with the Stiff

and radial diagrams, the pie chart is used to graphically compare the concentration ratios of several measured parameters for several different samples. The color and patterns used to identify each parameter are customizable.

Piper Diagrams

The Piper diagram in AquaChem plots the major ions as percentages of milli-equivalents in two base triangles. The total cations and the total anions are set equal to 100% and the data points in the two triangles are projected onto an adjacent grid. This plot reveals useful properties and relationships for large sample groups. The main purpose of the Piper diagram is to show clustering of data points to indicate samples that have similar compositions.

The Piper diagram in AquaChem can be used to plot all samples in the open database or selected sample groups. In addition, the symbols representing the sample values can be customized according to shape and color. The highlighted sample points indicate samples that are selected in the database and are also highlighted on all other open graphical displays.

Durov Diagrams

The Durov diagram in AquaChem is an alternative to the Piper diagram. The Durov diagram plots the major ions as percentages of milli-equivalents in two base triangles. The total cations and the total anions are set equal to 100% and the data points in the two triangles are projected onto a square grid that lies perpendicular to the third axis in each triangle. This plot reveals useful properties and relationships for large sample groups. The main purpose of the Durov diagram is to show clustering of data points to indicate samples that have similar compositions.

The Durov diagram can be used to plot all samples in the open database or selected sample groups. In addition, the symbols representing the sample values can be customized according to shape and color. Other options include individual multiplication factors for each selected ion to prevent data point accumulation along a base line. The highlighted sample points indicate samples that are selected in the database and are also highlighted on all other open graphical displays.

Ternary Diagrams

A ternary diagram in AquaChem is also used to identify trends and relationships between groups of samples. However, it is generally easier to understand than Piper or Durov diagrams since it involves fewer parameters and does not involve projections of data points onto a grid. Like the Piper diagram, the ternary diagram plots the ions as percentages of their concentration values. The ternary diagram is not limited to using only meq units.

The ternary diagram can be used to plot all samples in the open database or selected sample groups. In addition, the symbols representing the sample values can be customized according to shape and color. Other options include individual multiplication factors for each selected ion to prevent data point accumulation along

a base line. The highlighted sample points indicate samples that are selected in the database and are also highlighted on all other open graphical displays.

Langelier-Ludwig Diagram

The Langelier-Ludwig square diagram in AquaChem is similar to the projection areas of the Piper and Durov diagrams. Suitable groupings of cations and anions are selected and plotted as percentages of milli-equivalents. By convention, the sums of the selected cations are plotted on the y-axis, and the sum of the selected anions are plotted on the x-axis. Each axis ranges from 0 to 50 meq%.

All major elements can be displayed in one plot with the Langelier-Ludwig diagram. However, like the Piper and Durov diagrams, it displays relative ratios rather than absolute concentrations.

The Langelier-Ludwig diagram can be used to plot all samples in the open database or selected sample groups. In addition, the symbols representing the sample values can be customized according to shape and color. The highlighted sample points indicate samples that are selected in the database and are also highlighted on all other open graphical displays.

Schoeller Diagrams

These semi-logarithmic diagrams were developed to represent major ion analyses in meq/l and to demonstrate different hydrochemical water types on the same diagram. This type of graphical representation has the advantage that unlike the trilinear diagrams, actual sample concentrations are displayed and compared.

The Schoeller diagram in AquaChem can be used to plot all samples in the open database or selected sample groups only. Up to 10 different parameters can be included along the x-axis and the symbols representing the sample points can be customized according to shape and color. The highlighted lines indicate specific samples that are selected in the database and are also highlighted on all other open graphical displays.

Scatter Plots

The X-Y scatter plots are the most simple initial approach to the interpretation of geochemical data. Single plots of ion relationship and parameters that show significant data can be easily created and patterns are quickly identified and easily understood. Both normal scale and log scales are supported for the x and y axes and multiplication factors can be applied to either the x or y element. Element ratios and sums may also be included for either axes.

The scatter plot in AquaChem can be used to plot all samples in the open database or selected sample groups. The symbols representing the sample points can be customized according to shape and color. The highlighted data points indicate specific samples that are selected in the database and are also highlighted on all other open graphical displays.

Frequency Histograms

Frequency histograms are most commonly used to check the number of populations within a given range of measured values. This allows you to view a large number of samples without the diagram becoming too cluttered with data points. The frequency of samples within the given ranges can be plotted according to percentages or numbers of samples.

The frequency histogram can be used to plot all samples in the open database or selected sample groups. The range of values can be customized up to 10 or more groups and the individual samples can be identified at the associated value along the x-axis. The highlighted data points indicate specific samples that are selected in the database and are also highlighted on all other open graphical displays.

Time Series Graphs

The evolution of physical and chemical parameters for a given sampling location is a standard technique for interpreting hydrochemical and hydrogeological processes in natural waters. AquaChem allows you to plot time-series graphs for any numeric parameter in your database, and axes are customizable to suit your display requirements.

The time series graph plot can be used to plot all samples in the open database or selected sample groups. The symbols representing the sample points can be customized according to shape and color. The highlighted data points indicate specific samples that are selected in the database and are also highlighted on all other open graphical displays.

Geothermometer Plots

Geothermometer plots can be used to test the quality of geothermometer estimates for a given geological and hydrogeological condition.

The Giggenbach Triangle

The Giggenbach triangle is composed of three zones; (1) immature waters along the base; (2) partially equilibrated waters in the middle; and (3) fully equilibrated waters along the upper curve. Depending on where the composition of a given sample lies within this triangle, you can estimate the extent of rock-water equilibrium based on the concentrations of K, Mg and Na.

Log (K)-1000/T Plots

The linear log (K)-1000/T plots can be used for samples from boreholes where you know the insitu temperature of the formation. It can be used to: (i) check the usability of thermometers on a set of samples; (ii) plot the chemistry versus formation temperature; (iii) search for the geothermometer with the best fit; and (iv) develop new chemical geothermometers for parameters which show linear behavior.

Printing Results

AquaChem prints all reports and graphical displays to any printer or plotter supported by Windows 95/NT. The printing utility allows you to size and arrange the location of an unlimited number of open graphical displays on the page. This is particularly useful for comparing Stiff and radial diagrams from multiple samples or for using several different graphical displays to interpret groups of samples in each plot. Two lines of titles can be added at the top of the page while a single line of footer information can be added at the bottom of the page.

The PHREEQC Interface

PHREEQC is a program for performing aqueous geochemical calculations and modeling including:

> Speciation and saturation-index calculations;
> Reaction-path and advective-transport calculations involving specified irreversible reactions, mixing of solutions, mineral and gas equilibria, surface complexation reactions, and ion-exchange reactions; and
> Inverse modeling to find sets of mineral and gas mole transfers that account for composition differences between waters, within specified compositional uncertainties.

As the name might suggest, PHREEQC is written in the C programming language and is derived from the Fortran program PHREEQE (Parkhurst et al., 1980). PHREEQC is essentially an upgrade from the previous versions of PHREEQE since it retains all of the functionality and incorporates many improvements and new features.

Creating PHREEQC Input Files

AquaChem provides a direct interface to PHREEQC for creating the input files and running the simulations (WATEQ data files can also be read by PHREEQC). A full working version of PHREEQC is included with AquaChem and can be executed directly from the interface.

In order to run a geochemical simulation using PHREEQC, you must specify at least one solution to use in the simulation. The main advantage of the AquaChem interface is that it provides a direct link between PHREEQC input and output files and the AquaChem database files. This database link allows for instantaneous preparation of hundreds of solutions using samples from the database. Alternatively, you can also use the interface to load modeled solutions from previous simulations or to manually prepare solutions. These features will save you an incredible amount of time and hassle when you are dealing with a large number of samples (e.g., simultaneous speciation of many samples).

The AquaChem PHREEQC interface also provides a link between the specified solutions and other PHREEQC operations including adding reactions to the solutions; defining mineral phases for equilibration with the solutions; mixing solutions; adding gas phases to the solutions; specifying ion exchanges; performing 1-D transport simulations, and inverse modeling.

Once the properties of the solutions have been defined, you simply execute the PHREEQC program directly from the AquaChem interface and the simulation calculations will take place. If additional modifications are required, AquaChem allows you to edit the PHREEQC input text file directly from the interface.

Importing PHREEQC Results

AquaChem allows you to import the PHREEQC modeling output file (.pun file) into your database for creating graphs and tables for reports and for statistically analyzing the results. When the appropriate PHREEQC simulation output file is selected and imported, the results will be displayed in a spreadsheet. These results can be copied and pasted to other Windows applications or imported into your AquaChem database.

5.1) Level of competency required:

The fundamental determinant of the levels of competency required are those of the potential users knowledge of the real world system that he/she is trying to model. If one has the scientific knowledge of the systems that one is modelling then the competency required to run the model is trivial by comparison. However, if one does not know the science behind the systems that one is modelling then any model is difficult and should not be used.

5.2) Keywords for task-based search:

AquaChem - aqueous geochemical analysis, plotting and modeling, hydrogeochemical, water quality, geochemical

5.3) How widely is the model used and how well is it established in the industry:

AquaChem is the most comprehensive software package for aqueous geochemical analysis, plotting and modeling.

5.4) Range of applications:

The Most Comprehensive Software Package for Aqueous Geochemical Analysis, Plotting and Modeling

6) Case study:

MODEL: **AQUAMOD for Windows**

EVALUATED BY: **Gerrit van Tonder, University of the Orange Free State**
gerrit@igs-nt.uovs.ac.za

1) Description:

AQUAMOD for Windows is a 2D-triangular finite element Groundwater Modelling Package, consisting of six programs:

- Network Generator, NETGEN,
- Groundwater Modelling program, AQUA,
- DATASIM for the graphic presentation of the modelling results,
- TIMEGRPH for the display of time-dependent data,
- RPTSOLV, a pumping-test procedure for fractured-rock aquifers, and
- TRIPOL, a Kriging and Bayesian interpolation program.

1.1) NETGEN (GRID GENERATOR)
NETGEN generates a finite triangular mesh between a finite set of user-defined data points.

1.2) AQUA

This program consists of eight subprograms, namely:

1.2.1) AQUA-FLOW: (FLOW PROGRAM)

AQUA-FLOW solves the Galerkin finite element method in two dimensions for groundwater flow.
Special features of AQUA include the ability to specify:

(i) Variable pumping rates;
(ii) Time-dependent recharge values as percentage of monthly rainfall; and
(iii) A confined or water-table aquifer.

The output of AQUA yields:

(i) Monthly simulated water levels at each node (e.g. for contouring purposes) or water levels at specific user-defined nodes;
(ii) Groundwater velocities in the centre of each element (optional); and
(iii) A groundwater balance.

1.2.2) AQUA-INV (INVERSE PROGRAM FOR FLOW):

AQUA-INV is an automated parameter identification program which uses the flow program AQUA and the Marquardt optimisation algorithm to obtain the following choice of parameter combinations for zones in an aquifer which simultaneously produce the best fit between observed and simulated historical water-level data:

1. T- and S-variables
2. T
3. S
4. Recharge
5. T and recharge
6. Neumann inflow flux at boundary

7. T, S and inflow flux at boundary.

1.2.3) AQUA-MASS:

This program solves the convection diffusion equation in two dimensions for mass transport problems.

1.2.4) MASS-INV (INVERSE MASS TRANSPORT PROGRAM):

This program is the equivalent of the AQUA-INV program, and can be used for the automated calibration of the mass transport problem. The parameters, which could be inverse, are the T-values and the longitudinal and transversal dispersivities.

1.2.5) AQUA-MAN (MATHEMATICAL OPTIMIZATION):

AQUA-MAN links the distributed parameter groundwater flow simulation model, AQUA, with mathematical optimisation methods using a technique known as the response matrix approach. Linear programming formulation of the management problem is solved by a simplex routine obtained from Kinzelbach (1986).

1.2.6) SVF (RECHARGE ESTIMATION):

This program estimates the groundwater recharge of an aquifer with the aid of the SVF-method and was originally programmed for the WRC-project of Kirchner *et. al.* (1991). It is also possible to calculate cumulative rainfall departures (CRD) with this program (Bredenkamp *et. al.*, 1995).

1.2.7) AQUA-MC AND MASS-MC:

Two program modules (AQUA-MC and MASS-MC) were added to the AQUAMOD package to cover the aspects of groundwater flow and pollution risk respectively. The programs are based on the Bayes approximation, which requires the specification of probability density functions (p.d.f.) for the different variables. The p.d.f. approach is much less complicated and less time-consuming than the geostatistical approach and can be performed with ease on a PC.

1.2.8) MASS-MC:

MASS-MC utilises Monte Carlo simulations in the determination of pollution risk using a Bayes approximation.

1.3) RPTSOLV:

Bredenkamp and co-workers (Bredenkamp, 1992, and Bredenkamp *et. al.*, 1995) demonstrated that the calculated S-values in fractured-rock aquifers (if analysed with the Theis-model or any analytical fractured model, e.g. Moench) are a function of the distance between the abstraction and observation boreholes (the larger the distance, the smaller the estimated S-values).

Prof. Wolfgang Kinzelbach suggested that a 2D-radial flow model might be the solution to the problem. The necessary software, RPTSOLV, was written and is included as part of the AQUAWIN software suite.

1.4) DATASIM AND TIMEGRPH:

DATASIM is an animation program and can be used for the display of contours, velocities, maps and finite element meshes, while TIMEGRPH is a line graph viewer.

1.5) TRIPOL:

TRIPOL is an interpolation program using the Kriging and Bayesian methods to estimate data values at unknown points.

2) Data requirements:

- Aquifer Geometry: Boundaries, zones with different T, S and recharge values, initial groundwater levels.
- Measured water levels in boreholes with time for inverse calibration
- (only for solute transport) Concentration of groundwater, dispersivity values

3) Computer requirements:

Hardware:
Personal computer running Microsoft Windows 95/98 or Windows NT 3.51 or later
16 MB of available memory (32MB or more recommended)
A hard disk
VGA or higher-resolution monitor
Microsoft Mouse or compatible pointing device

4) Availability:

This software is free and could be extracted from:

FTP:\\igs-nt.uovs.ac.za

4.1) Costs:

Cost category 1: Free of charge

5) Assessment:

5.1) Level of competency required:

Very high level of expertise required for the program

5.2) Technical keywords for task-based search:

groundwater model, flow, solute transport, inverse model, automatic calibration, interpolation, risk analysis

5.3) Applicable algorithms and main mathematical limitations:

- A direct solver using Gaussian elimination.
- The inverse part uses the Levenberg-Marquardt method to solve the non-linear regression problem.
- Risk is performed with a Monte Carlo technique

5.4) How widely is the model is used or how well is it established in the industry:

AQUAMOD for Windows is used by the following institutions: IGS, CSIR, and consulting companies in SA and Nawater, Namibia

5.5) Related references:

Kinzelbach, W. (1986). Groundwater Modelling: An introduction with sample programs in BASIC. Evelopments in Water Science NO. 25, Elsevier, 333p.

Kirchner, J., Van Tonder, G.J. and Lukas, E. (1991). Exploitation potential of Karoo Aquifers. WRC Report No. 170/1/91. Pretoria.

Bredenkamp, D.B., Botha, L.J., Van Tonder, G.J. and Van Rensburg, H.J. (1995). Manual on quantitative estimation of groundwater recharge and aquifer storativity. WRC Report No. 353, Pretoria.

Bredenkamp, DB (1992) Estimation of the Yield of the Polfontein Compartment. Technical Report GH 3783, Directorate Geohydrology, Pretoria.

Van Tonder, G.J., Buys, J., Lukas, E. and Staats, S. (1998). Extension and refinement of the AQUAMOD computer software. WRC report No. 640/1/98, Pretoria.

5.6) Links to organisations:

5.7) Range of applications for which the model is capable.

Simulation of steady-state and transient two dimensional groundwater flow and solute transport.

6) Case Study:

The AQUAMOD for Windows program was applied to more than 40 case studies in South Africa, Botswana and Namibia

MODEL: **ASMWIN - ASM for Windows 6.0 (Beta)**

EVALUATED BY: **Gerrit van Tonder, University of Orange Free State**
gerrit@igs-nt.uovs.ac.za

1) Description:

ASMWIN is a 2D finite difference program written by Chiang, Kinzelbach and Rauch, especially for teaching purposes. It can do flow and mass transport modelling. For mass transport either the finite difference or random walk method could be selected. This beta version has been tested and used in some short courses. The manual and the Windows-help file are not ready for release. The use of ASMWIN is, however, similar to PMWIN. When in doubt, you should first try PMWIN. It has a very extensive Windows-help.

Installation Instructions:

- Download the files ASMDISK1.ZIP, ASMDISK2.ZIP, ASMDISK3.ZIP into a clean subdirectory.
- Unzip the files.
- Run setup.exe from the File Manager (or Explorer) and follow the screen.

After having installed ASMWIN, you should add the following entries to the file CONFIG.SYS and reboot your computer.

For Windows 95
FILES=80
DEVICE=C:\WINDOWS\COMMAND\ANSI.SYS

Note that you should change the above paths (C:\DOS\ or C:\WINDOWS\COMMAND) to the correct one if you have installed the operating systems on other directories.

2) Data requirements:

1) Geometry of the aquifer, T, S, recharge
2) (only for solute transport) Concentration of groundwater, dispersivity and distribution coefficient
3) Other hydrological information such as river stage, rain fall, etc.

3) Computer Requirements:

Hardware

- Personal computer running Microsoft Windows 3.1 or later or Windows 95/NT
- 16 MB of available memory (32MB or more are recommended)
- A 3.5" high-density disk drive and a hard disk.
- EGA or higher-resolution monitor
- Microsoft Mouse or compatible pointing device.

Software
A FORTRAN compiler is required if you intend to modify and compile the models ASMSIM1, ASMT2SIM, ASMWINMC and ASMOPTI.

4) Availability:

http://ourworld.compuserve.com/homepages/w_h_chiang/

4.1) Costs:

Free of charge. Cost Category 1.

5) Assessment:

This program is excellent for teaching purposes.

5.1) Level of competency required:

This program is very easy to use.

5.2) Technical keywords for task-based search:

groundwater model, flow, solute transport, particle tracking,

5.3) Applicable algorithms and main mathematical limitations:

- Preconditioned conjugate-gradient (Hill, 1990), and
- The particle-tracking model uses a semi-analytical particle-tracking scheme developed by Pollock (1988) to calculate the groundwater paths and travel times.
- The transport model uses a random walk or finite difference method to solve for the advective-dispersive-reactive transport equation.

5.4) How widely is the model used and how well is it established in the industry.

Used world wide for training of students in groundwater modelling

5.5) Related references:

- Hill, M. C., 1990a, Preconditioned Conjugate-Gradient 2 (PCG2), A computer program for solving groundwater flow equations, U. S. Geological Survey, Denver.
- Pollock, D. W. 1988. Semianalytical computation of path lines for finite difference models. Ground Water (26)6, 743-750.

http://ourworld.compuserve.com/homepages/w_h_chiang/

5.6) Links to organisations such as the EPA:

http://ourworld.compuserve.com/homepages/w_h_chiang/

5.7) Range of applications for which the model is capable.

Simulation of steady-state and transient two dimensional groundwater flow and solute transport.

6) Case Study:

ASMWIN is a teaching programme and the evaluator does not know of any case studies.

MODEL: **BETTER - A Two-dimensional Reservoir Water Quality Model**

EVALUATED BY: Nico Rossouw, Environment and Forestry Technology, CSIR
Email: nrossouw@csir.co.za

1) Description:

BETTER Model Overview:

The BETTER model, Box Exchange Transport Temperature and Ecology of a Reservoir Model, was designed to simulate seasonal patterns of temperature, dissolved oxygen, nutrients, pH and algal biomass in reservoirs. The BETTER model is a branched two-dimensional box reservoir water quality model. A reservoir is segmented into an array of volume elements or boxes. Inflow, outflow, meteorologic conditions, and inflow concentrations are normally specified on a daily time step (subdaily allowed). Heat budget calculations govern surface heat exchange that contributes to temperature (density) stratification. Reservoir geometry, flows, and thermal stratification determine flow and mixing patterns within the reservoir. Various chemical and biological processes are simulated within each volume element. The resulting two-dimensional concentration patterns are calculated and can be displayed graphically. Effects of different inflow conditions or the influence of reservoir processes can be explored by making comparative simulations.

Modelled Geometry: The reservoir volume is divided vertically and longitudinally into an array of volume elements, or boxes. This simple representation of reservoir geometry is used to determine flow patterns, temperature stratification, travel time characteristics, and other water quality patterns within the reservoir. The BETTER model uses a floating layer scheme, whereby the same layer thicknesses are used even though the reservoir surface raises and lowers. Normally, shallow layers (1.5 m) are specified near the surface to preserve strong gradients that develop in the epilimnion and metalimnion. Deeper layers (3-6 m) can be specified below this region.

Flow patterns in the lake or reservoir, are modelled as longitudinal and vertical flow transfers between the array of volume elements. Daily flow patterns are calculated using inflows and outflows from the system as specified by the user. Flow patterns are influenced by temperature patterns because the density of water is controlled by temperature. Inflow temperature, specified by the user, governing where inflow will enter the water column, and flows move through the reservoir along matched density pathways. Thermal stratification arising from surface heat exchange and mixing processes determines the ambient reservoir conditions into which the inflow is moving. In addition to horizontal and vertical flows (advection), vertical mixing (exchange) is simulated. Mixing may be caused by wind surface cooling (convective mixing), or turbulent flows (dispersion). The BETTER model uses two other variables to simulate travel times (called AGE) and track dilution of effluents (called DYE) or movement of particular inflow events.

Inorganic suspended solids are simulated to account for settling of inorganic particles entering the reservoir and to calculate the vertical absorption of light in the reservoir. The suspended solids formulation uses a constant settling rate and does not include resuspension or size fraction. An average light level is calculated for each volume element based on both inorganic suspended solids and organics such as algae.

Biochemical variables included in the BETTER model are: a) nutrients required to estimate algal growth, and b) organic matter. Both have effects on the Dissolved Oxygen balance. Time series of concentrations of each modelled chemical and biological variable are required input for each inflow. **Phosphorus** is simulated as dissolved and available for algal uptake. During anaerobic conditions, phosphorus is released from sediments. **Ammonia- and nitrate-nitrogen** are simulated because of the strong effect that nitrification (oxidation) has on the oxygen budget. Both are assumed available for algal uptake. During anaerobic conditions, denitrification of nitrate to nitrogen gas is simulated. The model then estimates algal biomass based on light or nutrient limited growth and respiration formulations. **Dissolved oxygen** is often the most important variable from the standpoint of water quality and fisheries management.

Modelled Processes: Only a few processes in BETTER are unique to this model, and fairly standard kinetic formulations are used. The strength of the BETTER model is relatively easy simulations of seasonal water quality patterns, generated by these representations of dominant processes, without major execution problems such as numerical instabilities.

Physical processes simulated with BETTER largely involve the flow, mixing, and temperature circulations. Inflow placement can be considered a physical process in which buoyancy forces associated with the density of the inflow are balanced within the water column by entering at the matched density (temperature). A second process, involving the densimetric Froude number, is simulated that may override the matched density deflection process.

Surface heat exchange: The surface heat exchange is calculated with terms for longwave radiation from the sky and water surface, evaporative cooling and advective heat loss;, and near surface absorption of infrared and ultraviolet solar radiation. A light extinction coefficient for each volume element is calculated from the suspended solids and algal concentrations. The same extinction coefficient applies to solar heating and photosynthetic radiation.

Three **mixing mechanisms** are included in the BETTER model, wind mixing, turbulent mixing and surface cooling during the night. These flow, mixing, and heat exchange processes result in transport and exchange flows between the entire array of volume elements. Simple mass balances are then calculated in each volume element for each modelled water quality variable. Internal processes act within each volume element to increase, reduce, transform, or transfer additional mass of the variables.

Biochemical processes include several **oxidation and decay** processes that transform variables, consume oxygen, and release carbon dioxide and associated

nutrients. **Settling** is simulated for several variables, transferring mass to the layer below, or to the reservoir bottom. **Algal uptake** of nutrients is directly coupled with growth using constant nutrient contents (stoichiometry) for algae. **Algal respiration** and mortality release nutrients and consume oxygen. **Sediment oxygen demand** (SOD) is simulated as an areal oxygen consumption rate. Surface exchange of oxygen and carbon dioxide are simulated as a function of saturation concentrations and windspeed. All of these biochemical process rates depend on temperature. Mixing coefficients, kinetic process rate coefficients, and temperature rate coefficients are input by the user.

Animation and Graphics Portfolio Manager (AGPM) overview:

The Animation and Graphics Portfolio Manager (AGPM) version 2.0 for Windows (98/95, NT 4.0, 3.1x) is post-processing software for graphically displaying results of two-dimensional reservoir water quality models such as CE-QUAL-W2, BETTER, and WASP. It lets the modeler build a series of plots using an intuitive Windows interface for one simulation, and then efficiently reproduce all the same plots for a subsequent simulation. The software dramatically reduces the time and expense of plotting multi-constituent model results, shortening calibration times while expanding capability for presentations and professional reports. Calibration requires display of numerous water quality constituents in many plot types (time-depth contours, distance-depth contours, time-series, vertical profiles, etc) for each of a large number
of simulations. These plots can now be produced at the click of a button.

It is becoming more common for water resources professionals to make presentations on reservoir behaviour to the lay public. Animation and other powerful depictions of water quality patterns allow modelers to provide insights to a range of audiences about the effects of major
influences on local reservoirs (e.g., dam operations, watershed changes, inflow loadings, hydrology, meteorology, channel morphometry).

2) Data requirements:

The BETTER model requires two input files.

The **Geometry File** contains all the model input that are not expressed as time series. These include:
- Cell (box) volumes and areas
- Tributary connectivity
- Outlet levels
- Process rates and coefficients
- Initial conditions

The **Inflow File** contains all the model inputs that are expressed as time series. These include daily or sub-daily values for:
- River inflows
- Local inflows
- Dam discharges
- Inflow water quality

- Meteorology

2.1) Inventory of data sources:

Model geometry:	Reservoir basin maps or GIS
Parameter values:	User's Manual or local studies
Hydrology:	Department of Water Affairs & Forestry (Directorate of Hydrology), WR90 series of publication, Computing Centre for Water Research (CCWR) or simulated inflow time series
Water quality:	Department of Water Affairs & Forestry (Directorate of Hydrology) or simulated water quality time series
Meteorological data:	Weather Bureau (Department of Environmental Affairs & Tourism) or CCWR.

3) Computer requirements:

BETTER model - Personal computer, MS DOS
AGPM visualization software - Personal computer, Windows 3.1 or Windows 95

4) Availability:

BETTER Model Contact information (USA):
Dr Gary Hauser
Engineering Laboratory
Tennessee Valley Authority
129 Pine Road
Norris, TN 37828 USA
Fax: 091-615-632-1840
Email: ghauser@tva.com

AGPM Visualization Software Contact information (USA)
Loginetics, Inc.
7304 Foxlair Rd
Knoxville, TN 37918 U.S.A.
E-mail: support@loginetics.com
Fax: 091-423-922-5768

Technical support (South Africa):
Nico Rossouw
Environmentek, CSIR
PO Box 395
Pretoria 0001
Tel: 012 841 4576
Fax: 012 841 2506
Email: nrossouw@csir.co.za

4.1) Costs:

BETTER Model - Free from the TVA

AGPM Visualization Software – Cost Category 2 (< US$2000)

5) Assessment:

5.1) Level of competency required:

In order to use the BETTER model, a user needs at least experience in limnology and water quality, be a proficient PC users and able to manipulate data, have an understanding of reservoir hydrodynamics and understand physical-biochemical reservoir processes.

5.2) Keywords for task-based search:

Reservoir water quality model, temperature, eutrophication, reservoirs, nutrients, dynamic, reservoir management.

5.3) Application algorithms and main mathematical limitations:

Application algorithms:

The application algorithms are well documented in the user manual. These include processes such as flow placement, heat exchange and mixing caused by wind, turbulence and surface cooling. Biochemical processes include oxidation and decay, settling, algal uptake of nutrients, algal respiration and sediment oxygen demand.

General model limitations:

Model limitations are well documented in the User's Manual. These include:
- Two-dimensional model (longitudinal and vertical changes in water quality), not 3-D
- No momentum equation
- Simplified sediment oxygen demand and anaerobic processes
- Mixed SI and US units

Limits on model dimensions:

Number of modelled reservoir branches (including main river branch): 5
Number of local diffuse inflows (not tributaries): 5
Number of longitudinal columns in system: 55
Number of vertical layers: 50
Number of outlets at the dam wall: 3
Number of local discharges directly into dam: 10
Number of local withdrawals directly from dam (can be diffusers): 10

5.4) How widely is the model used and how well is it established in the industry:

The BETTER manual printed in 1991 include a bibliography of 17 reports describing the application of the model to 10 reservoirs in Tennessee Valley Authority. Since the publication of the manual, the applications of the model have been extensive, including the reservoirs of the Lesotho Highlands Water Project.

5.5) Related References:

User's manual:

Bender, M.D., Hauser, G.E., Shiao, M.C. and Proctor, W.D. (1990). *BETTER: A Two-Dimensional Reservoir Water Quality Model. Technical Reference Manual and User's Guide.* Report No. WR28-2-590-152, Tennessee Valley Authority.

South African applications:

CSIR (1997). *Baseline Water Quality and Aquatic Communities Studies Phase 1B. Volume 2. Technical Report.* Lesotho Highlands Water Project. Lesotho Highlands Development Authority. (Application to Katse Dam)

CSIR (1997). *Baseline Water Quality and Aquatic Communities Studies Phase 1B. Volume 2. Water Quality Modelling Report.* Lesotho Highlands Water Project. Lesotho Highlands Development Authority. (Application to Fika Patso Dam and Mohale Dam)

5.6) Links to organisations:

AGPM Visualisation software - http://209.75.5.187/agpm.html

5.7) Range of applications:

The BETTER model has been applied to simulate:
- Seasonal water quality changes in reservoir water quality
- Water quality released from a reservoir
- Interpretation of reservoir monitoring data
- Design of reservoir monitoring programmes
- Impact of management actions on in-lake water quality
- Impact of outlet structure design on water quality
- Impact of operating rules on in-lake and downstream water quality

6) Case study:

Application of the BETTER model to predict water quality impacts in Mohale Dam, Lesotho Highlands Water Project.

Mohale Reservoir is the second reservoir to be constructed in the Lesotho Highlands Water Project. In a joint project between the CSIR and Rankin International (USA), the impacts on reservoir, release and Katse-Mohale Tunnel water quality were estimated using the BETTER two-dimensional reservoir water quality model.

The BETTER model was selected from the available two-dimensional water quality models because the data requirements were modest, creation of input files is more straight forward and less expensive than similar two-dimensional models, the model has been successfully applied to numerous reservoirs around the world, and the

model can easily accommodate complex multiple reservoir arms and hydraulic structures such as multi-level offtakes at any reservoir location.

The modelling assessment was organised into two phases. The first phase involved calibration of the model to Fika Patso Dam, development of a daily water balance for Phase 1B reservoirs, input development for a 14-year simulation, and an initial application of the model to explore Mohale reservoir water quality patterns. In the absence of actual reservoir data from Mohale, relevant model coefficients were determined by calibrating the model to Fika Patso, a grassy highlands reservoir in the region with available data. The second phase involved improvement of the reservoir model, final calibration of Fika Patso, and refinement of inflow quality estimates with longer available record; and use of the revised water quality model to assess Mohale Reservoir quality, offtake implications, and the quality of the environmental release.

Modelling results indicated that Mohale Dam water quality will be significantly affected by the hydrologic regime of the Senqunyane River. Extreme dam level fluctuations in Mohale will be governed by multi-year weather cycles of wet and dry periods, upon which smaller fluctuations from the annual cycle will be superimposed. Wet summers will introduce high inflows into a thermally stratified reservoir, producing a high degree of variability in water quality at the Mohale-Katse Transfer Tunnel offtake, especially during low pool elevations. Complete thermal destratification of the reservoir forebay occurred in only about a third of the 14 simulation years, suggesting a multi-year persistence of water quality patterns in Mohale Reservoir.

Sensitivity of the reservoir water quality to inflow loadings and reservoir sediment oxygen demand were revealed in first phase modelling. This was explored further in the second phase using expanded inflow data from Phase 1B monitoring efforts and an improved sediment release/oxygen demand model. The second phase also incorporated limnological insights gleaned from a review of Natal reservoir projects.

Three scenarios were simulated with the BETTER model to explore effects of loading uncertainties and use of two offtake levels. Case 1 included a low range of reasonable organic and nutrient loadings based on available data. Case 2 included a high range of reasonable organic and nutrient loadings. Cases 1 and 2 both assumed exclusive use of the lower offtake (elevation 1998 m). Case 3 included the high range of loadings and use of the upper offtake (elevation 2025 m), whenever possible. Cases 1 and 2, therefore, bracketed inflow loading effects within the range of uncertainty, and Cases 2 and 3 illustrated the effects of withdrawal from different offtakes.

The main water quality concern with case 1 (low loads) was periodic low dissolved oxygen (DO) concentrations. DO as low as 2 mg/L occurred at the offtake location in Case 1. With Case 2 (high loads), the DO was even lower and inorganic nitrogen was low enough to become the limiting nutrient during some years. The upper offtake could sometimes be used to increase the DO in the tunnel. However, use of the upper offtake 1) could yield lower DO concentrations; 2) could result in higher algae concentrations in the Mohale Reservoir forebay; and 3) could often yield the

same water quality as the lower offtake. Model results, therefore, indicate that long-term use of the upper offtake could impact water quality at lower depths.

In general, simulated algal concentrations in the reservoir were in the acceptable range and anoxic products were found to be insignificant. The water quality of the environmental release is expected to be acceptable for downstream uses, based on modelled forebay water quality and the flexibility allowed by the multi-level outlet structure. Analysis of predicted and available data shows that construction of Mohale Dam will greatly impact the flow magnitude, duration, and frequency of Senqunyane River below Mohale.

Source: CSIR (1997). *Baseline Water Quality and Aquatic Communities Studies Phase 1B. Volume 2. Water Quality Modelling Report.* Lesotho Highlands Water Project. Lesotho Highlands Development Authority.

MODEL: **CE-QUAL-R1**
EVALUATED BY: *Dr. Andrew Bath, Ninham Shand*
ftp://ftp.shands.co.za, bath@iafrica.com

1) Description:

CE-QUAL-R1 (R1) simulates the vertical distribution of thermal energy and chemical and biological materials in an impoundment. The model is thus designed as a one-dimensional description of a water body. The model was developed to study water quality problems, to develop management methods, and fine tune system operation (WES, 1986).

The model uses a conceptual view of an impoundment as a series of vertical sequence of layers with thermal energy and materials uniformly distributed in each layer. The primary physical processes modelled include surface heat transfer, shortwave and long wave radiation and penetration, convective mixing, wind and flow induced mixing, entrainment of ambient water by pumped-storage inflows, inflow density current placement, selective withdrawal, and density stratification as impacted by temperature and dissolved and suspended solids. Chemical and biological processes simulated by R1 include the effects on dissolved oxygen, of atmospheric interchange, photosynthesis, respiration, organic matter decomposition, nitrification, and chemical oxidation of reduced substances, uptake, excretion, and regeneration of nitrogen and phosphorus, carbon cycling and alkalinity-pH-CO_2 interactions. Outflows from the reservoir can be specified as a schedule of releases, or set as user criteria for volume and water temperature (Wurbs, 1995).

2) Data Requirements:

The time varying (daily) input requirements include: temperature, quality and flow of the inflowing rivers, starting conditions in the reservoir, meteorological data, inflow and outflow data. In addition, bathymetric data are required to configure the shape and extent of the inundated basin.

2.1) Inventory of Data Sources:

CE-QUAL-R1/CE-THERM-R1, Installation guide, Civil/Environmental Computer Model Library Department of Civil and Environmental Engineering, Old
URL: www.cee.odu.edu/cee/model/cequal_inst.html

ODU Version of Enhanced USACE WES CE-THERM-R1, Civil/Environmental Computer Model Library Department of Civil and Environmental Engineering, Old
URL: www.cee.odu.edu/cee/model/odu_therm.html

CE-QUAL-R1/CE-THERM-R1 Model - A Numerical One-Dimensional Model of Reservoir Water Quality, Civil/Environmental Computer Model Library
URL: www.cee.odu.edu/cee/model/cequal.html

Environmental/Water Resources Computer Model Library in the Department of Civil and Environmental Engineering, ODU
URL: www.cee.odu.edu/cee/model/

3) Computer Requirements:

The minimum requirements to run the model include a 80486 personal computer equipped with a math coprocessor. A minimum of 2 MB RAM is required unless the user has an operating system that uses virtual memory. A hard disk with a minimum space of 10 MB is also required for each application of the model. The model is provided with executable code as well as the source FORTRAN code.

4) Availability:

The model and documentation can be obtained by contacting:

Water Quality & Contaminant Branch, Environmental Laboratory,
Waterways Experimental Station,
US Army Corps of Engineers,
3909 Halls Ferry Road,
Vicksburg MS 39180-6199
Telephone (601) 634 3785

The computer code and documentation can be copied without restriction.

4.1) Costs:

Cost Category: 1 – free of charge

5) Assessment:

In South Africa, the model has not been used for water quality assessment. More emphasis has been placed on the use of the two-dimensional version of the model CE-QUAL-W2

5.1) Level of competency required:

R1 requires the user to be familiar with FORTRAN, compilers, data infilling procedures, meteorological data, hydrology and system operation information, water quality simulation and model interpretation, water chemistry, and limnology.

Training: The US Corps of Engineers run annual training workshops for the use of the model. Contact the Waterways Experimental Station for more information, or browse the web for advertisements of training sessions.

Grading: High level of user competency required.

5.2) Keywords for task-based search:

Reservoir, hydrodynamics, water quality, one-dimensional, eutrophication, dissolved oxygen, sediments, mixing conditions, metals, nutrients, suspended solids, TDS, reservoir operation, impact assessment

5.3) Application algorithms and main mathematical limitations:

The model uses a one-dimensional description of the water body as a fixed number of layers. All variation in the longitudinal axis of the impoundment is averaged. The model adjusts the thickness of the layers to account for periods of high inflow or outflow.

A number of utilities are provided with the model these include pre-processors, that assist the user in the construction of the input data set. Two graphic utilities and a statistics package for comparing measured and simulated results.

One of the main assumptions in the use of the model is that a water body can be represented in one-dimension. The model represents a water body as a vertical series of well mixed horizontal layers. This assumes that:

- The longitudinal gradients in quality and temperature are small compared with the vertical gradients;
- All inflows are dispersed through the vertical layers; and
- The model predictions are probably the most representative of the conditions at the deepest part of the water body.

The model uses the conservation of mass where changes are brought about by inflows, chemical and biological reactions within the water body, and removal of matter at the outflow. The model provides a simplification of the ecological processes by lumping the main functional groups (phytoplankton, zooplankton and fish) thus competition between groups is not considered. Under anaerobic conditions, the model provides a simplified version of the different chemical interactions.

5.4) How widely is the model used and how well is it established in the industry:

The model has been extensively used in the United States by the US Corps of Engineers. Evaluation and development of the model involved the use of the DeGray Lake and the Eau Galle Reservoir data sets. In South Africa, the two-dimensional version of the model has been used.

5.5) Related References:

WES (1986). CE-QUAL-R1 : A numerical one-dimensional model of reservoir water quality: users manual, US Army Engineer Waterways Experimental Station (WES), Environmental Laboratory, PO Box 631, Vicksburg, MS, United States. Report E-82-1.

Wurbs, R.A. (1995). Water management models, a guide to software, Prentice Hall PTR, Englewood Cliffs, New Jersey 07632.

5.6) Links to other Organizations:

National Nutrient Assessment Strategy: An Overview of Available Endpoints and Assessment Tools. Models and methods for catchments, rivers, reservoirs and estuaries
URL: www.epa.gov/owowwtr1/NPS/proceedings/overview.html

Pollution Prevention and Abatement Handbook. World Bank, 1997.
URL: http://www-esd.worldbank.org/pph/part2/Water1.htm

The staff at P2T maintain a large library of environmental modeling software that we use on client projects.
URL: http://204.194.169.125/html/models.html

Lake and Reservoir Management Proceedings of the Third Annual Conference. EPA 440/5/84-001 United States Environmental Protection Agency.
URL: www.nalms.org/bkstore/1984epa1.htm

5.7) Range of Applications:

Water quality problems that can be addressed include:
- Prediction and analysis of thermal stratification;
- Anoxic conditions (and associated impact on water quality);
- Algal blooms;
- Growth of algae and macrophytes;
- Location of selective withdrawal points and their dimensions;
- Land use change upstream of the impoundment;
- Effects of storm events; and
- Changes in reservoir operation.

6) Case Studies:

R1 has been used in several applications run by the Waterways Experimental Station, refer to their web site:

http://www.wes.army.mil/EL/elpubs/apcrp.html

Case Study: Evaluation of a Water Quality Model (CE-**QUAL-R1**) Using Data from a Small Wisconsin Reservoir.

By: Wlosinski, J.H.; Collins, C.D., Environmental Laboratory, Waterways Experiment Station, Vicksburg, Ms, Usa.

Source: *Ecological Modelling (Amsterdam)*, Vol 29, No 1-4, P 303-313 (11 Pages)

Publication Date: 1985

Descriptor(s): Water Quality Models; Model Evaluation; Field Tests; Reservoirs; Water Temperature; Vertical Distribution; Chlorophyll A; Nitrite Nitrogen; Nitrate Nitrogen; Phytoplankton; Concentration Gradients; Forecasting; Inflow; Discharge; Eutrophication

MODEL: **CE-QUAL-W2**

EVALUATED BY: **Dr. Andrew Bath, Ninham Shand,**
ftp://ftp.shands.co.za, bath@iafrica.com

1) Description:

CE-QUAL-W2 is a two-dimensional (2-D), laterally averaged, hydrodynamic and water quality simulation model. The model (referred to as W2) is based on the assumption that the water body shows maximum variation in water quality along its length and depth. Therefore, the model is suited to relatively long and narrow water bodies that show water quality gradients in the longitudinal and vertical directions. The model has been developed and applied to reservoirs, lakes, rivers, and estuaries. The two-dimensional model simulates the vertical and longitudinal distributions of thermal energy (water temperature) and selected biological and chemical constituents in a water body with time.

The original version of the model was known as *LARM* (Laterally Averaged Reservoir Model) and developed in 1975 by Edinger and Buchak. The first application of the model was on a reservoir with a single main branch. Modifications to the model allowed for multiple branches and the ability to handle estuarine boundary conditions. The revised version of the model was known as *GLVHT* (Generalised Longitudinal-Vertical Hydrodynamics and Transport model). Water quality simulation capabilities were added by the Water Quality Modelling Group at the US Army Engineer Waterways Experimental Station in Vicksburg, Mississippi and was known as *CE-QUAL-W2* Version 1. Considerable modifications were made to the model to improve the structure of the code and decrease the data storage requirements. These modifications resulted in Version 2 of the model. The latest enhancements to the model include: dynamic adjustment of the time step, selective withdrawal algorithm, higher order transport scheme, and improved volume balance and mass balance algorithms (Cole, 1993; Cole and Buchak, 1993, Cole, 1996).

2) Data requirements:

The time varying (daily) input requirements include: temperature, quality and flow of the inflowing rivers, starting conditions in the reservoir, meteorological data, inflow and outflow data.

3) Computer requirements:

Software:
The source code provided is written in FORTRAN 77. This code has to be compiled for each application. W2 has been developed for personal computer (PC) application, operating under DOS. The user requires a 32 bit FORTRAN compiler with a DOS extender that will use the PC's protected mode. In the South African applications, the model is compiled using the Lahey FORTRAN F77L3 compiler with DOS extension and optimized for use on a 80486 / Pentium PC.

Hardware:
The minimum configuration is a 80486 personal computer equipped with a mathematical co-processor. The model requires a minimum of four megabytes of memory with between ten and fifteen megabytes of hard disk space. Ideally, W2 should be run on a Pentium with clock speed greater than 100 MHtz.

4) Availability:

The model and documentation can be obtained by contacting:

Water Quality & Contaminant Branch, Environmental Laboratory,
Waterways Experimental Station,
US Army Corps of Engineers,
3909 Halls Ferry Road,
Vicksburg MS 39180-6199
Telephone (601) 634 3785

The computer code and documentation can be copied without restriction.

4.1) Costs

The model is supplied free of charge (Category 1). The cost of using W2 lies in the time spent setting up the model input files and configuring the model for a particular reservoir. Also, in the purchase of the visualization software which costs around US$1000.

5) Assessment:

W2 has been successfully used in USA and RSA for numerous applications in the field of water resource and quality management. The model requires a high level of computer literacy (see 5.1).

5.1) Level of competency required:

W2 requires the user to be familiar with FORTRAN, compilers, data infilling procedures, meteorological data, hydrology and system operation information, water quality simulation and model interpretation, water chemistry, and limnology.

Training:
The US Corps of Engineers run training workshops for the use of the model. Contact the Waterways Experimental Station for more information. Routine training workshops are run in the US, refer to: http://www.ce.pdx.edu/~wellsS/w2/

Grading:
High level of user competency required.

5.2) Keywords:

Reservoir, hydrodynamics, water quality, two-dimensional, eutrophication, dissolved oxygen, sediments, mixing conditions, metals, nutrients, TDS.

5.3) Algorithms and mathematical limitations:

Model capabilities include:

- The hydrodynamic routines predict the water surface elevations, velocities and temperatures. The heat exchange routine, in contrast to other hydrodynamic models, has modest input requirements.
- The water quality algorithms allow the simulation of up to 21 water quality constituents in addition to water temperature.
- The model has been modified so that simulations can be run over long time periods, which can extend up to ten years (to assess trends in water quality).
- The ability of the model to simulate upstream and downstream head boundary conditions allows the use of the model for estuaries, or reservoirs in which the inflow volumes are unknown.
- The branching algorithm allows the model to be used in reservoirs, which have a complex layout such as dendritic reservoirs, or estuaries with multiple freshwater inflows. The selective withdrawal algorithm calculates the vertical extent of the withdrawal zone based on outflow velocity and water density.
- The water body may be configured using segments of unequal length and layers of unequal thickness. The model adjusts the location of the surface layer and upstream segment to account for a rising or falling water level.
- The model uses a variable time step algorithm, which ensures numerical stability even during extreme hydrological inflow events.

Model limitations include

- The lateral averaging assumes that the variations in water velocity, water temperature and constituents across the width of a water body are negligible. In South Africa, this "limitation" has not influenced the simulation capabilities of the model.
- The availability of input data: This is often a constraint in the use of a hydrodynamic model where insufficient data are available for calibration. Experience gained in the use of the model and the development of advanced data infilling methods have meant the model can be used in comparatively "data scarce" applications (Bath *et al.*, 1998).

Model Enhancements:

It has been recognised that internal recycling of nutrients in a reservoir plays a major role in water quality. Therefore the latest enhancements being made to the model include refinement of the process descriptions for the sediments. The model is under constant development by the US Army Corps of Engineers, thus the latest routines are constantly being tested and incorporated into the model (Cole, 1995; Cole, 1996). As part of a South African research project, a graphical interactive post-processor was developed for W2. This software has greatly enhanced the use of the model in water quality studies (Görgens *et al.*, 1993; Bath *et al.*, 1998). Edinger and Associates have developed a complete set of pre and post processors for W2 which are available at cost. Their contact web site is http://www.jeeai.com

5.4) How widely used:

In **South Africa**, *W2* has been used to provide information for the management of water resources and detailed water quality assessment. These applications are summarized in the case studies.

In the **United States**, *W2* has been used in numerous applications for reservoirs, by way of example these include the following.

5.5) References:

Bath, A.J. & Timm, D.T. (1993). Hydrodynamic simulation of the water quality in reservoirs of Southern Africa, Proceedings of the eighteenth ICOLD conference, Durban, South Africa, p.625-633.

Bath, A.J., De Smidt, K.O., Görgens, A.H.M., & Larsen, E.J. (1998). Applicability of hydrodynamic reservoir models for water quality management in stratified water bodies in South Africa: Application of *DYRESM* and *CE-QUAL-W2*. Report by Ninham Shand Inc. to the Water Research Commission, Pretoria. Report in press.

Bath, A.J. & Quibell, G (1998). Application of a hydrodynamic model in the testing of system operating rules for the upper Vaal River, paper presented at the IAWQ conference in Vancouver, 1998.

Cole, T.M. (1993). Personal communication, Environmental Laboratory, US Army Corps of Engineers, Waterways Experimental Station, Vicksburg, MS.

Cole, T.M. (1994). User guide to *CE–QUAL–W2*. Instruction report, US Army Engineer, Waterways Experimental Station, Vicksburg, Mississippi, USA.

Cole, T.M. (1995). Personal communication, Environmental Laboratory, US Army Corps of Engineers, Waterways Experimental Station, Vicksburg, MS.

Cole, T.M. (1996). Personal communication, Environmental Laboratory, US Army Corps of Engineers, Waterways Experimental Station, Vicksburg, MS.

Cole, T.M. & Buchak, E.M. (1993). *CE-QUAL-W2*: A two-dimensional, laterally averaged, hydrodynamic and water quality model. User Manual, Environmental Laboratory, US Army Corps of Engineers, Waterways Experimental Station, Vicksburg, MS. Instruction report number ITL-93, September 1993.

Görgens, A.H.M., Bath, A.J., Venter, A., de Smidt, K. & Marais, G.v.R. (1993). Applicability of hydrodynamic reservoir models for water quality management in stratified water bodies in South Africa. Report by Ninham Shand Inc. and the University of Cape Town to the Water Research Commission, Pretoria. Report number 304/1/93.

Ninham Shand (1998). Water Quality - Application of daily water quality model, Amatole Water Resources System Analysis, Phase Two, Report for the Directorate of Project Planning, Department of Water Affairs and Forestry.

NS (1989). Laing Dam: Application of a hydrodynamic model for planning purposes, Report to the Department of Water Affairs, Project Planning Division by Ninham Shand Inc., report number NS 1521/4705.

NS (1993a). Amatole Water Resource System Analysis: Volume 13 - Water Quality Study, DWAF by Ninham Shand Inc. Report number PR 000/00/1393

NS (1993b). Water Quality Characterization of B500 Catchment. Pre-feasibility Study of the Olifants-Sand Transfer Scheme, for the Department of Water Affairs and Forestry, A.B.Ottermann, Ninham Shand Inc, 1993

NS (1996). Mearns Dam Modelling Study: Hydrodynamic water quality assessment, Report to Umgeni Water by Ninham Shand Pty Ltd.

NS (1998). Amatole Water Resource System Analysis: Phase 2: Volume 3 - Water Quality: Application of the daily reservoir model, for the Chief Directorate Project Planning, Department of Water Affairs and Forestry, by Ninham Shand Pty Ltd.

5.6) Links to other Organizations:

- Ninham Shand Consulting Engineers, PO Box 1347, Cape Town 8000, telephone 021 245588 fax 021 245588, email nscpt@shands.co.za
- John Edinger and Associates, specialist hydrodynamic modelling consultants: http://www.jeeai.com/
- Water Quality & Contaminant Branch, Environmental Laboratory, Waterways Experimental Station, US Army Corps of Engineers, 3909 Halls Ferry Road, Vicksburg MS 39180-6199, Telephone (601) 634 3785, Source code: Ftp://134.164.208.85
- Post processor: www.loginetics.com/agpm.html
- Post processor developed by Ninham Shand is available by contacting: abath@shands.co.za
- Post processor: 204.194.169.125/html/w2_post.html
- Post processor: www.ffts.com/agpm.html
- General information: http://dino.wiz.uni-kassel.de/model_db/mdb/w2.html
- General information: http://www.jeeai.com/cequalw2p2.htm
- Software information: www.wes.army.mil/el/elmodels/w2info.html
- Control file information: http://www.coe.uncc.edu/~jdbowen/eget3000/1997/content1.html
- RSA application example: http://www-wrc.ccwr.ac.za/sanciahs/bath.htm
- Estuarine application: www.coe.uncc.edu/~jdbowen/neem/w2_info.html
- Training workshops: http://www.ce.pdx.edu/~wellsS/w2/

5.7) Range of applications:

- Wasteload allocation

- *Point and diffuse source assessment*
- Mixing conditions in rivers, impoundments and estuaries
- Assessment of withdrawal structure design and location
- System operation
- System operating rules
- Nutrient and sediment interaction
- Selective withdrawal

6) Case Studies:

W2 is provided with documentation and a selection of case studies from the US. One of the most detailed case studies in South Africa is described in Görgens *et al.*, 1993 and Bath *et al.*, 1998. In South Africa, *W2* has been used to provide information for the management of water resources and detailed water quality assessment. These applications are summarized below.

Inanda Dam, Mgeni River, South Africa: The bulk supply reservoir experiences extended periods of stratification, sediment release of contaminants, and high algal growth. These factors have affected the treatment of water for domestic supply. The nutrient/algal interactions of Inanda Dam were simulated to provide information on: algal dynamics, draw off depth, sediment interactions, reservoir draw-down, reservoir hydrodynamics, and the phosphorus regime of the reservoir (Bath, *et al.*, 1998).

Witbank Dam, South Africa: The impoundment receives runoff from mining and rural areas with the result that the TDS and sulphate concentration of the water body has increased to a point where it exceeds the user requirements for power generation. The study uses an integrated river routing model linked to W2 to predict the influence of scheduled releases from the mining areas and support the scheduling of these releases to minimize the impact on the quality of Witbank Dam.

Vaal Barrage, Vaal River, South Africa: The salinity of the water body is governed to a large extent by saline tributary inflows and low salinity releases from the Vaal Dam. The hydrodynamic and salinity behaviour of the Barrage was simulated to provide information on the influence of freshening releases, optimization of releases, and diversion canal options (Bath, *et al.*, 1998).

Vaal Barrage, Vaal River, South Africa: The calibrated version of the model was used to provide detailed information to guide the operation of the water body and minimize the water quality impacts on water treatment and downstream water users (Bath & Quibell, 1998; http://www-wrc.ccwr.ac.za/sanciahs/bath.htm).

Roodeplaat Dam, Pienaars River, South Africa: The reservoir shows pronounced thermal and chemical stratification for almost nine months each year. The model was used to simulate the thermal stratification and dissolved oxygen regime of Roodeplaat Dam. This information was then used to assess the influence of destratification on the nutrient/ algal regime of the impoundment (Bath, *et al.*, 1998).

Rooipoort Dam, Olifants River, South Africa: A reservoir is proposed to be constructed on the Olifants River at Rooipoort to supply potable water to

Pietersburg, in the Northern Province. The model was used to provide preliminary information on the thermal stratification, hydrodynamic response, and salinity gradients within the reservoir. The information provided by the model was used to identify key water quality issues which include: location of the off-take tower, draw off depth, preliminary water treatment process design, and management guidelines for the upstream catchment (NS, 1993b; Bath, *et al.*, 1998).

Laing Dam, Buffalo River, South Africa: During periods of low flow, Laing Dam receives drainage of high salinity from point and non-point sources. This gives rise to elevated salinity and density stratification within the reservoir. A simulation was performed successfully to determine the influence of low salinity transfers from the Kubusi River catchment on the receiving water quality behaviour of Laing Dam (NS, 1993a; NS, 1998).

Mearns Dam, Mooi River, South Africa: It is proposed that an impoundment be built on the Mooi River to divert water into the Mgeni River system. The model was used to investigate the time varying water quality in the impoundment, the influence of the hydrodynamic mixing conditions in the impoundment, and the impact on downstream water quality (NS, 1996).

Fika Patso Dam, Nomahadi River, South Africa: W2 was calibrated for the bulk supply impoundment to provide detailed information on the possible influence of water quality on the treatment for potable use. The impoundment is one of the highest bulk supply impoundments in South Africa (situated just under 2000 metre above sea level). The model provided information, which was used in the design of the water treatment works, operation of the impoundment, and in the development of a management guide for the upstream catchment (Bath & Timm, 1993).

Swartwater Dam, Metsi Matso River, South Africa: Swartwater Dam is a highly eutrophic bulk supply impoundment. The water quality has become so degraded that the water treatment works was unable to meet the quality requirements for domestic use. W2 was used to guide the operation of the impoundment, and also in the development of a management guide for the upstream catchment (Bath & Timm, 1993).

Wriggleswade, Nahoon and Bridle Drift Dams, South Africa: The model has been used to investigate the eutrophication and hydrodynamic response of these bulk supply impoundments serving the water supply to the greater East London area (NS, 1998).

In the United States, *W2* has been used in numerous applications for reservoirs, by way of example these are described in some detail on the web site: http://www.jeeai.com/cequalw2p4.htm
Examples include:

Degray Lake is a reservoir with a single branch configuration and the model is used to simulate and demonstrate the full water quality capabilities of the model.

The *Neuse Estuary* Eutrophication Model is an application of W2. For use in the Neuse Estuary, the model features have been extended to estimate model

uncertainties, and a system for graphically displaying the data has been added. Information on these developments is found at: http://www.coe.uncc.edu/~jdbowen/neem/w2_info.html

JST Dam is situated on the Savannah River between Georgia and South Carolina. The model is used to examine the influence of pump storage on the water quality response of the reservoir.

Thames River Estuary is situated on the East Coast of the United States and the model is used to simulate temperature, salinity, water flow velocities, and water surface elevations of the estuary. The model is used to analyze the release of compensation releases on the water quality of the estuary.

Cumberland River near Nashville is modelled to demonstrate the simulation of BOD and dissolved oxygen.

MODEL: **Daily Flow Modelling (DAYFLOW)**

EVALUATED BY: **Dr W V Pitman, Stewart Scott Inc.**
model@ssi.co.za

1. Description

The program HDYP16 was developed in 1976 to simulate daily streamflow. Development of the daily model followed that of the monthly simulation model MORSIM, which underwent several enhancements. The most recent update is known as WRSM90. The daily salt washoff model developed by Herold (NACL1) uses an adaptation of HDYP16 to generate daily catchment runoff, to which water quality routines have been added. Apart from this development HDYP16 remained in its original form virtually since inception. A daily version of WRSM90 would have been the most logical development of HDYP16 but lack of funds has hampered this option. Accordingly, DAYFLOW was developed to incorporate many of the features of WRSM90 as an interim step. Unlike WRSM90 it does not have the capability to simulate a complex network in a single run. However, it is possible to handle a fairly complex network by simulating a number of simpler networks that can be linked.

DAYFLOW is a batch file that allows the user to run any of the following three programs:

- HDYP16 Updated daily rainfall-runoff simulation model
- SCPLOT Plotting of various graphs depicting monthly flow
- DAYPLOT Plotting of graphs depicting daily flow

HDYP16 models a simple network comprising runoff, channel, reservoir and irrigation modules. The reservoir and irrigation modules are optional. An upstream input is also optional and can be used to add in flows from another network or e.g. from return flows.

SCPLOT is virtually identical to the plotting routine used in WRSM90, with the choice of seven different graphs to compare the observed and simulated monthly streamflow.

DAYPLOT allows the user to select one year at a time. It then plots (on a logarithmic scale) the observed and simulated daily flows as well as the duration curves for that year.

2. Data requirements

The model normally uses both daily and monthly time series of rainfall appropriate to the catchment to be modelled. The monthly time series, produced by HDYP08, is identical to the rainfall input to WRSM90. The monthly rainfalls are disaggregated to daily falls on the basis of a record at a single rainfall station chosen for its location plus length and reliability of record. This approach avoids the complications of averaging daily records, where recording errors are more of a problem than for

monthly records. However, it is possible to run the model without the time series of monthly rainfall.

The model also requires mean monthly evaporations and appropriate factors to convert these (usually Symons pan for catchments and reservoirs; A-pan for irrigation lands) to potential evaporation rates. If the model is used in calibration mode the observed monthly and daily streamflow records at gauging points in the system must be provided.

The runoff module also requires initial estimates of the rainfall-runoff parameters. These may be changed in the course of each run. Land-use effects are modelled by inputting appropriate areas of afforestation and irrigation plus combined full supply areas and capacities of reservoirs in the system. These data can be set at a particular level of development or allowed to change with time, according to historical developments in the catchment. Files of monthly abstraction (run-of-river or from dams) and return flow can also be incorporated. Monthly volumes are converted automatically into mean daily rates.

2.1 Inventory of data sources

Monthly and daily rainfall and monthly evaporation data can be obtained directly from the South African Weather Bureau or the Computing Centre for Water Research (CCWR). The CCWR also supplies monthly and daily streamflow data but this information can also be obtained from the Department of Water Affairs & Forestry (Directorate: Hydrology). Information on water abstractions and return flows is usually obtained from the authority in question. DWAF is also the main source of information on major dams and large water supply schemes, including water for irrigation.

3. Computer requirements

The suite of programs can run on virtually any PC that is supplied with HERCULES or EGA/VGA graphics cards for the plotting programs. However run times will be very slow on older (pre-486) machines.

4. Availability

DAYFLOW can be obtained from:

Stewart Scott Incorporated
PO Box 784506
Sandton 2146
South Africa

Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email ssisan@ssi.co.za

4.1 Cost

Cost Category 4: DAYFLOW was developed for in-house use and no arrangements have been made (as yet) for sale and distribution of the software.

5. Assessments

5.1 Level of competency required

DAYFLOW is relatively simple to use once all the input files have been set up correctly. However, the user should have at least a basic grounding in hydrology and some knowledge of statistics. The user should also be aware of the kind of errors that may be encountered when dealing with hydrological data. Any user familiar with WRSM90 should have no problems in running DAYFLOW.

5.2 Keywords for task-based research

Water resources, simulation, rainfall-runoff, modelling, hydrology, model calibration.

5.3 Application algorithms and main mathematical limitations

Although the basic time step is one day the model reduces the time step to one hour whenever rainfall occurs. Two of the model parameters are used to estimate the duration of the rainfall (to the nearest hour) and the temporal distribution of the rain is governed by a built-in function. Since the distribution of daily rainfall is based on the observed pattern at a single gauge, large catchments should preferably be sub-divided into smaller units for modelling purposes. This approach is recommended because daily rainfall is subject to much greater spatial variability than is the case for monthly rainfall.

5.4 How widely is the model used and how well is it established in the industry

DAYFLOW has – to date – been used in only one important project (see Case Study). However, the rainfall-runoff component of the model has been employed in a number of studies as part of the NACL1 daily washoff model.

5.5 Related references

PITMAN, W V (1976). *A mathematical model for generating daily river flow from meteorological data in South Africa.* Report No. 2/76, Hydrological Research Unit, University of the Witwatersrand, Johannesburg, South Africa.

5.6 Links to organisations

Enquiries on DAYFLOW can be directed to Stewart Scott Inc.
PO Box 784506
Sandton 2146
South Africa
Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email ssisan@ssi.co.za

5.7 Range of applications

DAYFLOW is designed primarily for calibrating the daily rainfall-runoff module (HDYP16) against observed daily, monthly and annual streamflow. The model can then be employed to generate time series of streamflow appropriate to given levels of catchment development, including the natural condition. It has a limited ability for simulating the performance of reservoirs and run-of-river abstractions.

6. Case study

DAYFLOW has been used in the project: "The Hydrologic and Hydraulic Study of the Behaviour of the Nyl River Floodplain", undertaken on behalf of the Department of Water Affairs and Forestry. The daily model was calibrated on ten gauged catchments that feed the floodplain. The performance of the daily model was compared with that of WRSM90. The performance of both models was similar with respect to the simulation of annual flows but the daily model was found to be superior in the generation of monthly flows. Further tests on the daily model's ability to simulate daily flows included ranked annual maxima and the frequency of flows above a threshold. It was concluded that the model's performance was satisfactory, notwithstanding the shortcomings in the distribution of rainfall gauges.

MODEL: **DYRESM**

EVALUATED BY: Dr. Andrew Bath, Ninham Shand,
ftp://ftp.shands.co.za, bath@iafrica.com

1) Description:

DYRESM-1D is a one-dimensional hydrodynamic reservoir simulation model for the prediction of the vertical temperature and salinity distribution in small to medium size lakes and reservoirs. The model uses a one-dimensional Lagrangian layer structure, which allows for varying layer thickness and the model design is based on parameterisations of the individual processes that contribute to the hydrodynamics of a water body. The processes included in the basic *DYRESM* model are:

- Surface heat, mass and momentum exchanges
- Surface mixed layer deepening
- **Inflow**
- Outflow
- Mixing in the hypolimnion

A more detailed description of the *DYRESM-1D* model is given in Görgens *et al.* (1993).

DYRESM-2D is a quasi two-dimensional hydrodynamic reservoir simulation model (Hocking and Patterson, 1991). It represents the reservoir being modelled by a two-dimensional 'wedge' similar to that used by *CE-QUAL-W2*, however, *DYRESM-2D* uses a Lagrangian layer structure in which each layer is divided into 'parcels'. These parcels are only changed when layers are combined or split, or when parcels become too large or too small. This approach reduces the computation time required when compared with models, which use a fixed grid such as *CE-QUAL-W2*.

This basic *DYRESM* model structure has formed the background to a number of specialist developments and applications. These are described below (Patterson, *pers. comm.*, 1995).

Large Lake version:
A version for application in a limited sense to large lakes, in which Coriolis influences are important. In this version, simulations of the profile averaged over the inertial period were calculated by modifying the shear production algorithm to account for rotational effects. This model also incorporated a bottom mixed layer with the energy production arising from a bottom current. This was specifically for application in Lake Erie, but was also incorporated into the dissolved oxygen version of the model.

Dissolved oxygen (DO) version:
A version of the model, which incorporated a simple dissolved oxygen budget, was developed for Lake Erie, as a first step to demonstrate the validity of the *DYRESM* hydrodynamic module for water quality models in general. Briefly, the model incorporated equilibrium productivity-light intensity (P-I) relationships, and fixed respiration and sediment demand. The oxygen model was totally driven by the dynamics: the DO distribution in the upper mixed layer was determined by integrating the P-I curve over the exponentially decaying light field. This is an extreme simplification, but one which, in some circumstances may be appropriate for a first

model, specifically when the response time of the phytoplankton to changing light is short, compared to the circulation time. Alternatively, if attenuation depth is much greater than the mixed layer depth, the cells are circulating in an essentially constant light environment, and equilibrium productivity relationships are again relevant. *(The above simplification may well not be adequate for the correct simulation of DO in South African water bodies.)*

Ice and snow version:
To simulate cold northern lakes, ice and snow routines were added to the basic model, together with an expanded density-temperature algorithm with pressure effects, to account for the effects near 4°C. These models were based on the assumption that the heat transfer through the cover was quasi-steady: the temperature field in the ice and snow adjusted on a time scale faster than the changes to the boundary conditions, in this case the meteorological forcing. This was shown to be appropriate for all but very thick ice, and the difficulties associated with the moving boundaries at the ice-water interface were avoided. The model included the effects of partial ice cover by applying the surface forcing to only the open fraction of the surface.

Solar pond version:
A version of the model for simulating salt gradient solar ponds has been developed. This involved the incorporation of an algorithm to simulate the double diffusive instabilities, which may arise, and a much finer Lagrangian layer specification. This model has been applied successfully to solar ponds in Israel and Australia. A control system for managing the ponds, based on the simulation model, has also been designed.

Destratification version:
To simulate the effect of bubble plume aerators, a version has been constructed that includes an algorithm which simulates the effect of a bubble plume as a single buoyant plume of a density which is the mean density of the air-water mixture. A simulation of Myponga Reservoir in South Australia showed that this simple model was, in certain circumstances, successful. The assumption that a single aerator plume behaves as a simple buoyant plume with the mean density is effectively assuming that the bubbles are infinitely small; for the case of large bubbles, the fixed entrainment rate associated with buoyant plumes must be modified. For the case of a number of closely spaced aerator outlets, the model switches to a line source plume algorithm, rather than a number of separate single plume models. This model has been extensively used for the design of aerator systems and management practices.

2) Data requirements:

The model receives as input daily sequences of:

- Inflow to impoundment
- Inflow water temperature
- Inflow TDS
- Outflow data from impoundment
- Releases from impoundment
- Meteorology (short wave radiation, sunshine ratio, average daily air temperature, average daily saturated vapor pressure, average daily vapor pressure, daily wind speed, total daily rainfall)

The operation of the model is achieved using a control file that contains:
Drag coefficient, vertical transport constant, start date and end date of simulation, number of vertical layers, initial layer depth, initial salinity

Information on the impoundment includes:
Kinematic viscocity, diffusivity, wind sheltering coefficient, water level, storage volume, surface area, crest level, offtake level, reservoir length at crest level, width of wall, angle of river bed.

2.1) Data Sources:

Email address for the CWR: talianch@cwr.uwa.edu.au

Web site address for contacts and information:

www.cwr.edu.ac.au

www.cwr.uwa.edu.au/cwr/commercial/projects.html

Model applications

http://www.fwr.org/distrib/uwraa024.htm

http://www.fwr.org/distrib/uwraa034.htm

http://www.fwr.org/distrib/uwraa023.htm

http://www-wrc.ccwr.ac.za/publications/res_reports/quality.htm

http://196.21.78.64/publications/bulletin/v24_1/models.htm

3) Computer Requirements:

Hardware:
The minimum configuration is a 80486 personal computer equipped with a mathematical co-processor. The model requires a minimum of four megabytes of memory with between ten and fifteen megabytes of hard disk space. Ideally, DYRESM should be run on a Pentium with clock speed greater than 100 MHtz.

4) Availability:

The model is available from:

The Centre for Water Research
University of Western Australia
Western Australia 6009
Telephone: +61 9 380 3911
Fax: +61 9 380 1015

4.1) Costs:

Category 2 - <US$2000

5) Assessment:

As part of a WRC funded study, DYRESM was used to assess the application and capabilities of the model to provide a description of the hydrodynamics and thermal stratification in a number of South African impoundments (Görgens *et al.*, 1993). The model was then used as a follow up WRC study to assess the use of the model to design bubble plume aeration systems for reservoir destratification purposes (Bath, *et al.*, 1998). Subsequent to that investigation, information from the model was used to assess the design of destratification aeration systems for a number of reservoirs.

5.1) Level of competency required:

DYRESM requires the user to be familiar with data infilling procedures, meteorological data sets, hydrology and system operation information, water quality simulation and model interpretation, and physical limnology.

Grading: High level of user competency required.

5.2) Keywords:

One dimensional, reservoir hydrodynamics, destratification, bubble plume aeration, salinity, dissolved oxygen, Lagrangian

5.3) Application Algorithms and main mathematical limitations:

DYRESM 1-D was developed in 1978 as a one-dimensional description of the hydrodynamics of an impoundment or lake. The model was developed to simulate the vertical gradient in water temperature and salinity in small and medium sized water bodies.

The model is based on the assumption that the water body can be represented in one-dimension and that the density stratification inhibits vertical mixing while lateral and longitudinal variations in density are removed quickly by horizontal convection occurring at rates faster than the vertical advection.

The basic processes included in the model include: surface heat, mass and momentum exchanges, surface mixed layer deepening, inflow, outflow, and mixing in the hypolimnion. These processes are linked in a framework of a Lagrangian layer structure. The water body is divided into a number of horizontal layers each with a particular uniform property, and varying thickness. These layers are influenced by the magnitude of the inflow and outflow that may cause the expansion or contraction of the layer depth. Coupled with this are the processes that are responsible for the deepening of the upper mixed layer, such as convective overturn due to surface cooling, wind action, entrainment at the metalimnion, and internal seiche movement. Mixing in the hypolimnion are predominantly the result of smaller scale events and represented by eddy diffusivity (Allanson, Patterson & Imberger, 1987).

Mixing is represented by an amalgamation of layers. The model has a time step resolution of down to one minute and spatial resolution down to one centimeter. The one-dimensional model was enhanced with the inclusion of the algorithms for the simulation of bubble plume destratification (Patterson & Imberger, 1989) that allows the design and testing of destratification systems. The model was then enhanced to include: large lake simulations, solar pond modelling, ice and snow cover simulations, chemical and biological variables, and a quasi two-dimensional version (DYRESM-2D).

The strength of the model lies in the fact that the main processes do not change from one water body to the next because they describe invariant physical processes, the properties of which are defined by hydrodynamic theory (Allanson, Patterson & Imberger, 1987). Thus, the model requires minimal "calibration" for each water body.

5.4) How widely is the model used:

The model has been widely distributed both within Australia and overseas for use in teaching, research and industry in a wide variety of applications. These applications include the use of the model for reservoir management and the design of destratification systems by, amongst others, the following organisations:

- Engineering and Water Supply, Southern Australia
- Department of Water Resources, New South Wales, Australia
- Sydney Water Board, New South Wales, Australia
- Rural Water Commission, Victoria, Australia
- Murray Darling Basin Commission, Australia
- Power and Water Authority, Northern Territories, Australia
- Mt Isa Mines, Australia
- Ward and Associates, Vancouver, Canada
- Ninham Shand, South Africa

The following web site provides information on the model: www.cwr.uwa.edu.au/cwr/commercial/projects.html

In particular *DYRESM* has been used to design physical bubbler systems for, amongst others, the following reservoirs:

- **Lake Burbury, Tasmania, Australia**
- Glennies Creek Reservoir, New South Wales, Australia
- Avon Reservoir, New South Wales, Australia
- Nepean Reservoir, New South Wales, Australia
- Sugarloaf Reservoir, Victoria, Australia
- Upper Yarra Reservoir, Victoria, Australia
- Myponga Reservoir, Southern Australia
- Harding Reservoir, Western Australia
- Lan Tarn Reservoir, Taiwan
- Hollywood Reservoir, California, USA

5.5) Related References:

Allanson, B R and Jackson, P.B.N. (1983). "Limnology and fisheries potential of Lake Le Roux" South African National Scientific Programmes Report number 77, CSIR, Pretoria.

Bath, A.J., De Smidt, K.O., Görgens, A.H.M., & Larsen, E.J. (1998). Applicability of hydrodynamic reservoir models for water quality management in stratified water bodies in South Africa: Application of *DYRESM* and *CE-QUAL-W2*, Report by Ninham Shand Pty Ltd to the Water Research Commission, Pretoria. Report number: 304/2/97

Centre for Water Research, (1992). "*DYRESM* 1D user's manual, Ver. 6.75.2 DW", University of Western Australia, Nedlands, Australia.

Centre for Water Research, (1992). "2D *DYRESM* supplement to the 1D *DYRESM* user's manual (6.75.2 DW)", University of Western Australia, Nedlands, Australia.

Görgens, A.H.M., Bath, A.J., Venter, A., de Smidt, K. and Marais, G.v.R. (1993). "The applicability of hydrodynamic reservoir models for water quality management of stratified water bodies in South Africa", Report by Ninham Shand Inc. and the University of Cape Town to the Water Research Commission, Report No. 304/1/93, Pretoria, South Africa, ISBN 1 86845 004X.

Hocking, G.C. and Patterson, J.C. (1991). "Quasi-two-dimensional reservoir simulation model", ASCE Journal of Environmental Engineering, 117(5), 595-613.

Imberger, J., Patterson, J.C., Hebbert, R. and Loh, I. (1978). "Dynamics of reservoir of medium size", ASCE Journal of Hydraulic Engineering, 104(HY5), 725-743.

Imberger, J., Patterson, J.C. (1981). "A dynamic reservoir simulation model - *DYRESM* : 5", Transport Models for Inland and Coastal Waters, Academic Press, New York, 310-361.

Patterson, J.C. and Imberger, J. (1989). "Simulation of bubble plume destratification systems in reservoirs", Aquatic Sciences, 51(1), 3-18.

Robertson, D.M., Schladow, S.G. and Patterson, J.C. (1991). "Interacting bubble plumes: the effect on aerator design", Environmental Hydraulics, 1, 167-172.

Schladow, S.G. (1991). "A design methodology for bubble plume destratification systems", Environmental Hydraulics, 1, 173-178.

Schladow, S.G. and Patterson, J.C. (1991). "Bubble plumes and mixing efficiency in a stratified reservoir", Proceedings of the International Hydrology and Water Resources Symposium, Perth, Australia, 274-279.

Schladow, S.G. (1992). "Bubble plume dynamics in a stratified medium and the implications for water quality amelioration in lakes", Water Resources Research, 28(2), 313-321.

Thirion, C. and Chutter, F.M. (1993). "The use of artificial aeration in Inanda Dam as a management tool for the control of eutrophication and its effects", Hydrological Research Institute Report No. N U200/04/DPQ/0693, Department of Water Affairs and Forestry, Pretoria, South Africa.

5.6) Links to other Organizations:

Requested from CWR.

The Centre for Water Research
University of Western Australia
Western Australia 6009
Telephone: +61 9 380 3911
Fax: +61 9 380 1015
Http://www-wrc.ccwr.ac.za/publications/res_reports/quality.htm

5.7) Range of applications the model is capable of supporting:

- Thermal stratification and mixing conditions in medium/small impoundments
- Destratification assessments
- Design of bubble plume aeration systems
- Assessment of mixing conditions
- Design of outlets

6) Case Studies:

The model has also been applied to a number of lakes and reservoirs without significant change to the model structure, although in all cases the simulations have guided further development of various aspects of the model. These simulations include the following lakes and reservoirs:

- Babine Lake, Canada
- Burrunjuck Reservoir, New South Wales, Australia
- Canning Reservoir, Western Australia
- Chaffey Reservoir, New South Wales
- Char Lake, Canada
- Darwin River Reservoir, Northern Territories, Australia
- Eklutna Lake, United States of America
- Glennies Creek Reservoir, New South Wales, Australia
- Harding Reservoir, Western Australia
- Harris Reservoir, Western Australia
- Kooteney Lake, Canada
- Lake Argyle, Western Australia
- Lake Constance, Germany
- Lake Erie, Canada
- Lake Geneva, Switzerland
- Lake Le Roux (Van der Kloof Dam), South Africa
- Lake Lugano, Italy
- Lake Mendota, USA
- Manton River Reservoir, Northern Territories, Australia

- Mt Bold, Southern Australia
- Myponga Reservoir, Southern Australia
- Wellington Reservoir, Western Australia

See Section 5.6 (Links to web sites) for the various applications.

MODEL: **FLUX, BATHTUB, PROFILE - Simplified Procedures for Eutrophication Assessment and Prediction**

EVALUATED BY: Nico Rossouw, Environment and Forestry Technology, CSIR
Email: nrossouw@csir.co.za

1) Description:

The simplified procedures for eutrophication assessment and prediction were developed by Dr W. W. Walker for the US Army Corps of Engineers, Waterways Experiment Station. It consists of three interrelated programs, FLUX, PROFILE and BATHTUB. All three programs can be used in a stand-alone mode.

FLUX is a program designed to calculate stream loading (mass discharges) from sampled concentration data and continuous flow data (for example daily flow records). The program has five methods for estimating loads and potential errors are quantified. Graphic and tabular displays allow model users to evaluate the input data and calculation results. Mass loads, and associated error statistics (CV) are provided as input to BATHTUB.

PROFILE is designed to facilitate analysis and reduction of in-lake water quality data. Algorithms are included for calculating the hypolimnetic oxygen depletion rates and estimation of area-weighted, surface-layer mean concentrations of nutrients and other eutrophication related variables.

BATHTUB is a program with a series of empirical eutrophication models for morphologically complex lakes and reservoirs. The program performs steady-state water and nutrient balance calculations in a spatially segmented hydraulic network, which accounts for advection and diffusion transport and nutrient sedimentation. Eutrophication related water quality constituents (total phosphorus, total nitrogen, chlorophyll-a, transparency and hypolimnetic oxygen depletion) are predicted using empirical relationships derived for the assessment of reservoir data.

FLUX has been used most often in South Africa and was be evaluated in this review.

2) Data requirements:

Data requirements the FLUX model:

- The FLUX model requires flow data in cubic hectometres/year (10^6 m^3/year) and water quality data (milligrams/cubic metre - mg/m^3). A facility is provided in the program to convert flows, eg. from cubic metres/second (m^3/s) to the required units, or to convert water quality, eg. from milligrams/litre to the required units. Different conversion factors are provided in the back of the manual.
- Continuous daily river flow data: Units: cubic hectometres/year (10^6/year)
- River water quality data: Units: milligrams/cubic metre (mg/m^3)

The PROFILE program requires vertical profiles of water quality data collected at one or more sample stations throughout the period of interest.

The BATHTUB model requires information describing watershed characteristics, water and nutrient loads, and lake or reservoir morphology.

2.1) Inventory of data sources:

Continuous river flow data: Directorate of Hydrology, Department of Water Affairs & Forestry
River water quality data: Directorate of Hydrology, Department of Water Affairs & Forestry

Any other data sources can be used where flow data is collected on a continuous basis and grab chemical samples are collected on a less frequent basis.

3) Computer requirements:

Personal computer, MS DOS

4) Availability:

Can be downloaded from the Waterways Experiment Station web site: http://www.wes.army.mil/el/elmodels/index.html

Contact person (USA):
Dr Robert H Kennedy
Environmental Laboratory
US Amy Engineer Waterways Experiment Station
3909 Halls Ferry Road
Vickburg, MS 39180
Email: kennedr@ex1.wes.army.mil

Technical support (South Africa):
Nico Rossouw
Environmentek, CSIR
PO Box 395
Pretoria 0001
Tel: 012 841 4576
Fax: 012 841 2506
Email: nrossouw@csir.co.za

4.1) Costs:

This model is available free of charge

5) Assessment:

5.1) Level of competency required:

The user should be technically competent to manipulate flow and water quality data obtained from various sources. Model input data can be provided in ASCII or Lotus-123 Release 2.x (*.WK1) file format and the user should be competent to create these type of files.

The model user should also have an understanding of statistics and the concepts of constituent loading.

5.2) Keywords for task-based search:

Data analysis, empirical models, eutrophication, nutrient loading, reservoirs, water quality

5.3) Application algorithms and main mathematical limitations:

FLUX program input data limitations:
Number of paired flow and water quality concentration values: 500
Number of flow data values: 7000

BATHTUB applications are limited to steady-state evaluations of relationships between nutrient loading, transparency

5.4) How widely is the model used and how well is it established in the industry:

In South Africa, the FLUX model has been used in a number of studies in South Africa to calculate mass loadings:

CSIR (1997). Baseline Water Quality and Aquatic Communities Studies. Phase 1B. Volume 2 - Technical Report. LHDA Contract 1007. Report to the Lesotho Highlands Development Authority.

Grobler, D.C. and Rossouw, J.N. (1988). Nonpoint source derived phosphorus export from sensitive catchments in South Africa. Report to the Department of Water Affairs & Forestry, Pretoria.

Examples of the application of the BATHTUB model in the USA can be found in:

Ernst, M. R., Frossard, W. and Mancini, J.L. (1994). Two Eutrophication Models make the Grade. Water Environment and Technology, November, 15-16.

Kennedy, R. H., 1995. Application of the BATHTUB Model to Selected Southeastern Reservoirs. Technical Report EL-95-14, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

5.5) Related References:

Walker, W.W. (1996). Simplified Procedures for Eutrophication Assessment and Prediction: User manual. US Army Corps of Engineers, Waterways Experiment Station. Instruction Report W-96-2

Walker, W.W. (1985). Empirical Methods for Predicting Eutrophication in Impoundments; Report 3, Phase III: Model Refinements. Technical Report E-81-9, US Army Engineer Waterways Experiment Station, Vickburg, MS.

Walker, W.W. (1985). Empirical Methods for Predicting Eutrophication in Impoundments; Report 3, Phase III: Applications Manual. Technical Report E-81-9, US Army Engineer Waterways Experiment Station, Vickburg, MS.

5.6) Links to organisations:

http://www.wes.army.mil/el/elmodels/index.html

5.7) Range of applications:

- Computation of mass loading
- Relationships between flow and concentration

6) Case study:

Accurate estimates of nutrient loads on water bodies are essential to understand the functioning of catchment-river-reservoir systems and to predict their response to natural and man-made phenomena. Sources of phosphorus are usually classified as either point or nonpoint (diffuse) sources. In several of the designated sensitive catchments in South Africa nonpoint source derived phosphorus loads make up a significant part of the total phosphorus load on reservoirs. To be able to justify decisions related to the enforcement of a phosphorus standard it was imperative that the best possible estimates of nonpoint source derived phosphorus loads be obtained and that their impacts on the eutrophication of reservoirs be understood and compared to that of point sources when considering point source control measures.

A monthly model was developed which simulated nonpoint source derived total phosphorus (TP) export as a function of monthly runoff and TP export parameters which had to be estimated for different catchments. The FLUX software was used extensively to obtain the best possible estimates, based on available data, of the TP export parameters for all the designated sensitive catchments. Estimating the parameters for the nonpoint source derived TP export model required four important steps:

1. For each sensitive catchment, gauging stations were identified for which both discharge and TP concentration data were available and which were not significantly affected by point sources.
2. Appropriate methods for estimating TP flux at the gauging stations were developed using the FLUX software. For rivers characterized by highly variable discharge, such as most rivers in South Africa, flux: discharge regression models proved to be the most appropriate for estimating pollutant fluxes.

3. Monthly TP loads and flows were calculated using FLUX. The monthly flows and TP loads were then converted to export and runoff data by dividing through the respective catchment areas.
4. The runoff and TP export data thus obtained were used to estimate the TP export parameters for the nonpoint source derived TP export model by means of a nonlinear regression procedure.

Grobler, D.C. and Rossouw, J.N. (1988). Nonpoint source derived phosphorus export from sensitive catchments in South Africa. Report to the Department of Water Affairs & Forestry, Pretoria.

MODEL: **Catchment Rainfall Program (HDYP08)**

EVALUATED BY: **Dr W V Pitman, Stewart Scott Inc.**
model@ssi.co.za

1. Description

HDYP08 is essentially a pre-processor for the rainfall-runoff simulation model WRSM90. It averages monthly rainfalls obtained from records at any selected number of rainfall stations. The individual record periods do not have to be coincident but it is recommended that the rainfall data be fairly evenly distributed in space and time. Output from the program takes the form of averaged monthly rainfalls expressed as percentages of MAP (mean annual precipitation).

2. Data requirements

The primary input to HDYP08 comprises monthly records of rainfall at a selected number of stations. Breaks in record (entire years only) can be accommodated by the use of headers at the start of each record section, giving the ensuing record period and the MAP. The MAP is, however, applicable to the entire record. Missing or incomplete monthly records must be in-filled. Alternatively, the entire year must be discarded. The individual records should be checked for stationarity and any other errors before being used.

2.1 Inventory of data sources

Monthly rainfall data can be obtained directly from the South African Weather Bureau or from the Computing Centre for Water Research. The Surface Water Resources of South Africa 1990 database has (on CD-ROM) over 2500 in-filled rainfall records at a selection of stations distributed throughout South Africa. These records are up to September 1990 only.

3. Computer requirements

HDYP08 can run on any PC but will obviously run faster on more modern machines. The PC must have a HERCULES, EGA\VGA or CGA graphics card in order to view the program's graphical output on the screen.

4. Availability

HDYP08 can be obtained from:

Stewart Scott Incorporated
PO Box 784506
Sandton 2146
South Africa

Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email ssisan@ssi.co.za

4.1 Costs

Cost Category 1: HDYP08 is supplied free of charge to purchasers of WRSM90.

5.1 Assessments

5.1 Level of competency required

HDYP08 is very easy to run as the user responds to a simple set of requests. However, the user must be aware of problems associated with the measurement and capture of rainfall data so that the program inputs and outputs can verified.

5.2 Keywords for task-based research

Rainfall, catchment rainfall, rainfall-runoff, hydrology.

5.3 Application algorithms and main mathematical limitations

Monthly rainfalls at each station are converted to percentages of local MAP. The percentages are then averaged to obtain the catchment rainfall – also as a percentage of MAP. These percentages are converted to rainfall depths (in mm) in WRSM90 by applying the MAP of the catchment to be modelled. The use of MAP as a weighting factor helps to minimise bias, where there is a significant variation in MAP among the stations. It is also important, however, to select stations that provide a reasonably consistent spatial and temporal spread.

5.4 How widely used is the model and how well is it established in the industry

Since HDYP08 is an essential pre-processor for WRSM90 (and its predecessors), it is just as widely used and established in the industry.

5.5 Related references

MIDGLEY, D C, PITMAN, W V & MIDDLETON, B J (1994). *Surface Water Resources of South Africa 1990 – User's Manual.* Water Research Commission Report No. 298/1/94, Pretoria, South Africa.

PITMAN, W V (1973). *A mathematical model for generating monthly river flows from meteorological data in South Africa.* Report No. 2/73, Hydrological Research Unit, University of the Witwatersrand, Johannesburg, South Africa.

PITMAN, W V and KAKEBEEKE, J P (1991). *WRSM90 User's Guide.* Stewart Scott Inc, Sandton, South Africa.

5.6 Links to organisations

Enquiries on HDYP08 can be directed to Stewart Scott Inc.
PO Box 784506
Sandton 2146
South Africa
Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email ssisan@ssi.co.za

5.7 Range of applications

HDYP08 was designed specifically to provide time series of catchment rainfall to be used in the rainfall-runoff simulation model WRSM90. The program can also be used to depict the temporal variation of rainfall (monthly and annual) for any designated area covered by a suitable network of rain gauges. The program output gives, at a glance, the severity and duration of wet and dry periods that have occurred since rainfall measurements commenced.

6. Case study

HDYP08 was used in conjunction with WRSM90 to facilitate model calibration and subsequent streamflow generation in the Surface Water Resources of South Africa 1990 (WR90) study (Midgley *et al.*, 1994). HDYP08 was used to create monthly rainfalls for about 450 sub-catchments covering the whole of South Africa, Lesotho and Swaziland.

MODEL: **HEC River Analysis System (HEC-RAS)**

EVALUATED BY: Dr W V Pitman, Stewart Scott Inc.
Email: model@ssi.co.za

1. Description:

HEC-RAS assesses water levels and velocities in open channel river systems. It has the ability to model:

- Steady flow water surface profiles
- Branched or looped channel networks
- Bridges, culverts, weirs and spills
- Subcritical, supercritical or mixed flow regimes

HEC-RAS has a user-friendly graphical user interface with full reporting and graphics facilities. It can produce graphics of river system schematics, X-Y-Z perspective plots and cross-section profiles.

2. Data requirements:

Geometric data is required in the form of connectivity information for the stream system, cross-section data and hydraulic structure data (bridges, culverts, weirs, etc.). The first step is to draw the river system schematic, with an identifier for each reach and junction. After the river schematic is drawn the cross-section and hydraulic structure data can be entered. Data for each cross-section comprises pairs of station (distance) and elevation readings, plus additional data including reach length, left and right bank stations, Manning's n for main channel, left overbank and right overbank, plus contraction and expansion coefficients. Once the cross-section data are entered, details of any hydraulic structures can be added.

Once the geometric data are entered the flow and/or sediment data can be entered, depending on the type of analysis to be performed. Several profiles can be calculated by entering different data for each profile. Finally, boundary conditions are required in order to perform the calculations. If a subcritical analysis is to be performed, then the downstream boundary conditions are required. If a supercritical analysis is to be performed, then the upstream boundary conditions are required. If a mixed flow regime is to be performed, then both upstream and downstream boundary conditions are required.

2.1 Inventory of data sources:

Where available, detailed contour plans of the river reach to be modelled (including the adjacent floodplain) can be used to provide geometric information. If this information is not available it will be necessary to survey a number of pre-selected cross-sections to describe the geometry. Details of hydraulic structures will also have to be surveyed, unless suitable as-built drawings are available.

3. Computer requirements:

The minimum requirements to run HEC-RAS are as follows:

- Any IBM or compatible machine with an 80386 processor
- A hard disk with at least 2.5 Mb of free disk space
- 4 Mb of free extended memory (RAM)
- MS-DOS version 3.3 or later
- MS Windows version 3.1 or later, in enhanced mode

4. Availability:

HEC-RAS can be obtained from:
Bullen Consultants Ltd.
Bradford, BD1 3AZ,
United Kingdom.
Telephone 01274 370410
Facsimile 01274 734447

4.1 Costs

Single user (program disks, manual and licence)	£350 + VAT
Additional copies (with manual)	£150 + VAT
Additional copies (without manual)	£100 + VAT
Corporate (10 user) package	£700 + VAT
Additional copies of manual	£25 + VAT

5. Assessment

5.1 Level of competency required

Although HEC-RAS is user friendly it is considered essential that the user has a sound understanding of open channel hydraulics, in order to make a sensible selection of cross-sections and to interpret correctly the program outputs.

5.2 Keywords for task-based research

Open-channel hydraulics, water surface profiles, steady flow, subcritical flow, supercritical flow, mixed flow regimes, channel stability.

5.3 Application algorithms and mathematical limitations

The user manual includes a hydraulic reference manual describing the theory and data requirements for the hydraulic calculations performed by HEC-RAS. Equations are presented along with the assumptions used in their derivation. Discussions are provided on how to estimate model parameters, as well as guidelines on various modelling approaches.

The basic computational procedure is based on the solution of the one-dimensional energy equation. Energy losses are evaluated by friction (Manning's equation) and contraction/expansion (coefficients multiplied by change in velocity head). The momentum equation is utilised in situations where the water surface profile is rapidly varied. These situations include mixed flow regime calculations (i.e. hydraulic jumps), hydraulics of bridges and evaluating profiles at river confluences.

5.4 How widely is the model used and how well established is it in the industry

The original computer program HEC-2, Water Surface Profiles, originated from a step-backwater program written as early as 1964. This early version was revised in 1966 and released by the Hydrologic Engineering Centre (HEC) in the USA. Since then the program has been revised several times and HEC-RAS, first released in 1995, represents the latest version. HEC-RAS (and its earlier derivatives) has been widely used in the USA but the extent of its use in South Africa is not known.

5.5 Related references

BARKAU, R L (1992). *UNET One-dimensional Unsteady Flow Through a Full Network of Open Channels.* Computer Program, St. Louis, MO, USA.

FEDERAL HIGHWAY ADMINISTRATION (1978). *Hydraulics of Bridge Waterways,* Hydraulic Design Series No. 1, by Joseph Bradley, US Department of Transportation, 2nd Edition, revised March 1978, Washington, DC, USA.

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HYDROLOGIC ENGINEERING CENTRE (1991). *HEC-2, Water Surface Profiles,* User's Manual, US Army Corps of Engineers, Davis, CA, USA.

HYDROLOGIC ENGINEERING CENTRE (1993). *UNET, One-Dimensional Unsteady Flow Through a Full Network of Open Channels.* User's Manual, US Army Corps of Engineers, Davis, CA, USA.

HYDROLOGIC ENGINEERING CENTRE (1994). HECDSS, User's Guide and Utility Programs Manual, US Army Corps of Engineers, Davis, CA, USA.

5.6 Links to organisations

HEC-RAS (and its earlier derivatives) has been developed by:

US Army Corps of Engineers
Hydrologic Engineering Centre
609 Second Street
Davis, CA 95616
USA
Telephone (916) 756-1104
Facsimile (916) 756-8250

5.7 Range of applications

Typical applications for HEC-RAS include the following:

- Assessment of watercourse hydraulic capacity
- Sizing of culverts
- River channel design and modification
- Flooding assessments
- Assessment of channel stability
- Design of river temporary works (coffer dams, diversion channels)

6. Case study

The author of this submission is not aware of any case studies undertaken in the USA, of which there must be several. With regard to South African experience, HEC-RAS was used in a study to determine the effectiveness of various remedial measures to reduce flooding in Newcastle, Kwa-Zulu Natal, which straddles the Ncandu River. Verification data was sparse but the model did yield a similar pattern of flooding to that experienced during the worst flood on record (February 1975) when simulating the 50-year flood. Results of the modelling exercise helped to identify the most cost-effective measures for the alleviation of flooding.

Model: **Hydrological Simulation Program Fortran (HSPF)**
Evaluated by: **Dr MC Dent, Computing Centre for Water Research**
dent@aqua.ccwr.ac.za

1) Description:

The Hydrological Simulation Program—FORTRAN (HSPF) is a comprehensive package for simulation of watershed hydrology and water quality for both conventional and toxic organic pollutants. HSPF incorporates the watershed scale ARM and NPS models into a basin-scale analysis framework that includes fate and transport in one-dimensional stream channels. It is the only comprehensive model of watershed hydrology and water quality that allows the integrated simulation of land and soil contaminant runoff processes with instream hydraulic, water temperature, sediment transport, nutrient, and sediment-chemical interactions. The runoff quality capabilities include both simple relationships (i.e. empirical buildup/washoff, constant concentrations) and detailed soil process options (i.e., leaching, sorption, soil attenuation and soil nutrient transformations).

The result of this simulation is a time history of the runoff flow rate, sediment load, nutrient, pesticide, and/or user-specified pollutant concentrations, along with a time history of water quantity and quality at any point in a watershed. HSPF simulates three sediment types (sand, silt, and clay) in addition to a single, organic chemical and transformation products of that chemical. The instream nutrient processes include DO, BOD, nitrogen and phosphorus reactions, pH, phytoplankton, zooplankton, and benthic algae.

The organic chemical transfer and reaction processes included are hydrolysis, oxidation, photolysis, bio-degradation, a volatilization, and sorption. Sorption is modelled as a first-order kinetic process in which the user must specify a desorption rate and an equilibrium partition coefficient for each of the three solid types. Resuspension and settling of silts and clays (cohesive solids) are defined in terms of shear stress at the sediment-water interface. For sands, the capacity of the system to transport sand at a particular flow is calculated and resuspension or settling is defined by the difference between the sand in suspension and the capacity. Calibration of the model requires data for each of the three solids types. Benthic exchange is modelled as sorption/desorption and desorption/scour with surficial benthic sediments. Underlying sediment and pore water are not modelled.

2) Data requirements:

The data required by the model is dependent on the range of simulations required. The data requirements can be small and simple or extensive and complex. Please see the section, which outlines the range of simulations that the model can perform. This will give an idea as to the data required.

2.1) Inventory of data sources:

The data for the model is varied depending on what options one invokes. The primary data sources would be the SA Weather Bureau (Climatic data), DWA&F

(streamflow and water quality data, catchment boundary and rivers spatial data), ISC&W of the ARC (land type data and land use data).

3) Computer requirements:

The Fortran source code is supplied and the system can run on almost all platforms from the smallest PC to the largest super computer using *inter alia* UNIX, DOS, WINDOWS95 and other platforms. The power of the computer naturally affects the run time.

4) Availability:

The HSPF model is in the public domain and can be downloaded free of charge from the US EPA web site.

4.1) Costs:

Cost Category 1: Free. It is in the public domain.

5) Assessment:

The following quote is by Dr R.C. Russo, Director, Environmental Research Laboratory, Athens, Georgia in the foreword to the HSPF User's Manual for Release 11.

> *" HSPF is thought to be the most accurate and appropriate management tool presently available for the continuous simulation of hydrology and water quality in watersheds."*

5.1) Level of competency required:

The fundamental determinant of the levels of competency required are those of the potential users' knowledge of the real world system that he/she is trying to model. If one has the scientific knowledge of the systems that one is modelling then the competency required to run the model is trivial by comparison. However, if one does not know the science behind the systems that one is modelling then any model is difficult and should not be used.

HSPF is designed to accommodate a wide range of competencies.

5.2) Keywords:

Integrated, water resources, simulation, modelling, hydrological modelling, water quality modelling, conflict resolution,

5.3) Application algorithms and main mathematical limitations:

The model operates at a user specified time step. The range is from 1 minute to 1 day, 19 time steps are available. The spatial and temporal scale must however be matched realistically. This naturally requires the model user to be fully aware of the scientific systems being modelled.

No extra libraries or packages such as NAG or SAS are required. Ancillary programs such as ANNIE and IOWDM are available free from the EPA and the USGS and these are highly recommended for time series data manipulation and display.

5.4) How widely is the model used and how well is it established in the industry:

The model is extensively used in the USA. See the section on the case studies, above. In South Africa use is also growing (see case studies section) and is set to increase rapidly with the installed modelling system requirements which will be necessary in order to manage water resources in an integrated manner under the new water law.

5.5) Related References:

- Ball, J.E., M.J. White, G.de R. Innes, and L. Chen. 1993. Application of HSPF on the Upper Nepean Catchment. Hydrology and Water Resources Symposium, Newcastle, New South Wales, Australia. June 30-July 2, 1993. pp. 343-348.
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- Johanson, R.C. and J.L. Kittle. 1983. "Design, Programming and Maintenance of HSPF", Journal of Technical Topics in Civil Engineering, Vol. 109, No. 1
- Larouche, A., J. Gallichand, R. Lagace, and A. Pesant. 1996. Simulating Atrazine Transport with HSPF in an Agricultural Watershed. ASCE J. Env. Engr., Vol. 122(7):622-630.
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- Linker, L.C., C.G. Stigall, C.H. Chang, and A.S. Donigian. 1996. Aquatic Accounting: Chesapeake Bay Watershed Model Quantifies Nutrient Loads. Water Env. & Tech. Vol. 8(1):48-52.
- Scheckenberger, R.B. and A.S. Kennedy. 1994. The Use of HSP-F in Subwatershed Planning, In: Current Practices in Modelling the Management of Stormwater Impacts. W. James (ed). Lewis Publishers, Boca Raton, FL. p. 175-187.

- Smith, R.H., S.N. Sahoo, and L.W. Moore. 1992. GIS Based Synthetic Watershed Sediment Routing Model. In: Proceedings of Water Resources sessions at Water Forum '92. Baltimore, Maryland. August 2-6, 1992. p. 200-207.
- Snohomish County Surface Water Management. 1993. North Creek Watershed Management Plan, Public Hearing Draft. Everett, WA.
- Snohomish County Surface Water Management. 1994. Swamp Creek Watershed Management Plan, Public Hearing Draft. Everett, WA.
- Xie, J.D.M. and W. James. 1993. Modelling Solar Thermal Enrichment of Urban Stormwater. In: Current Practices in Modelling the Management of Stormwater Impacts. W. James (ed). Lewis Publishers, Boca Raton, FL. p. 205-217.
- Yang, J.C., H.P. Lee, and J.H. Chang. 1992. Pollutant Transport Modelling for a Complex River System, In: Computer Techniques and Applications. Hydraulic Engineering Software IV. Computational Mechanics and Publications. Southampton, England, and Elsevier Applied Science, London, England. p. 49-60.

5.6) Links to organisations:

HSPF was developed and is maintained under contract to the EPA. The EPA funds continual updates, maintenance and advice on the model and there is an active HSPF user group on the Internet. The model is currently in version 11 and version 12 is due shortly. In South Africa the Computing Centre for Water Research has knowledge of the model. Several consulting and research groups are also building up knowledge on the model as they use it in various situations.

5.7) Range of applications:

- integrated water resources simulation modelling.
- hydrological modelling.
- instream water quality modelling.
    - conservative constituents including sulphate and flouride
    - water temperature
    - sediment transport
    - DO & BOD
    - hydrolysis
    - oxidation
    - photolysis
    - volatilisation
    - generalised first order decay
    - advection of adsorbed suspended material
    - nitrogen
    - phosphorous
    - plankton
    - carbon
    - carbon dioxide and total inorganic carbon
    - acid mine drainage
    - alkalinity
    - lethality analysis

- non-point and point sources water quality modelling
- conflict resolution,
- urban runoff modelling
- complex networking of flows in catchments
- linking simulation modelling systems

6) Case studies:

In South Africa the model is being used on the Sabie, Mooi (Gauteng), Umkomaas, Olifants, Umgeni and Amatola Rivers by consultants and researchers.

In Australia its most well known application is for the Sydney Water Board on the Hawksbury-Nepean catchments feeding Sydney and where it was linked to TIDEWAY, CMSS and MIKE11.

In the USA the bibliography of case studies is extensive. The records of one consultant list approximately 180 case studies from his and other consulting firms and university researchers.

MODEL: **IMPAQ (Impoundment/river management and planning assessment tool for water quality simulation)**

EVALUATED BY: *Dr. Andrew Bath, Ninham Shand*
ftp://ftp.shands.co.za, bath@iafrica.com

1) Description:

IMPAQ (**I**mpoundment/ river **m**anagement and **p**lanning **a**ssessment tool for water **q**uality simulation) was developed as part of numerous water resource system analysis studies for the Department of Water Affairs and Forestry (Directorate of project Planning). The model was developed so that it could import monthly hydrology from the *Water Resource Yield Model* and then simulate water quality at various points in a river system. IMPAQ was used to fine-tune system operating rules and also assess the impact of contaminant sources (point and diffuse).

In 1992, the first version of the model simulated conservative constituents (TDS) in impoundments. Later enhancements included the simulation of whole catchments (washoff, rivers, and reservoirs) and conservative and non-conservative constituents. The current version of IMPAQ simulates: soluble phosphorus SP, particulate phosphorus PP, total phosphorus TP, suspended solids SS, E.coli, and algae (expressed as chlorophyll-a).

The hydrology input to the model is from the *Water Resource Yield Model* but can also input flow sequences from other sources. The conceptual design of the model allows a catchment system to be represented as a washoff module, river transport module, reservoir module and modules representing point sources and urban washoff. The modular design was adopted to allow the model to be applied to a wide variety of rivers in South Africa.

IMPAQ software suite includes a variety of graphical interfaces to allow the user to present the model output in a variety of different ways. Simple time output plots can be generated showing measured and simulated results. These plots can be custom designed to suit the needs of the user. In addition, model output can be viewed using the GIS map utility so that the user can examine the spatial variation in water quality. The latest output graphics allow the user to view the mass loading inputs from point and diffuse sources, and the option to adjust point source loads.

The model has been developed so that it can be used to:

- Run different hydrological sequences and then to assess the differences in water quality;
- Modify point source loading and assess the changes in quality of the rivers and reservoirs;
- Assess the input loading rates from point and nonpoint sources; and
- Assess and fine-tune system operating rules.

2) Data requirements:

Hydrology: Monthly sequences of: river flow, river withdrawal, point source discharge, urban runoff, reservoir withdrawal, reservoir spillage, evaporation and

precipitation. The model was developed to be run in conjunction with the *Water Resources Yield Model*.

Water Quality: Monthly sequences of the variables listed above for rivers, and point sources. Data sequences are also created for as many points in the rivers and impoundments for calibration of the model.

2.1) Inventory of data sources:

For more information on the software please contact:

Dr Andrew Bath or Mr André Greyling
Ninham Shand (Pty) Ltd, PO Box 1347, Cape Town 8000
Email: nscpt@shands.co.za

3) Computer requirements:

The software has been developed to operate on personal computer:

Hardware requirements:	Pentium
Hard drive requirements:	20 MB
Clock speed	>100 MHz
Operating System	Windows 95
Additional drive	CD-ROM

4) Availability:

The model is available from: Dr Mike Shand or Dr André Görgens
Ninham Shand Pty Ltd
PO Box 1347
Cape Town 8000
Email: nscpt@shands.co.za

The software is provided on CD-ROM.

4.1) Costs:

Free (excluding the cost of the media and postage). It is recommended that the first time users undergo training, which will be at their cost.

5) Assessment:

Mgeni River, KwaZulu Natal: The early version of the model was used to assess the impact of different operating rules on the water quality response of the bulk supply impoundments on the Mgeni River. The model was also used to assess the impact of future changes in point and diffuse loading to the Duzi River and response of Inanda Dam. The simulations included the conservative and non-conservative constituents (phosphorus, suspended solids, and coliform bacteria).

Upper Kei River Basin, Eastern Cape: The early version was used to determine the TDS of the Kei River and assess the influence of water resource developments.

Buffalo River, Nahoon River, Kubusi River, Qgunube River, Eastern Cape: The latest version of the model was configured for the rivers in the Amatole Water Supply Area. The model was used to fine tune system operating rules, and assess the impact of contaminant sources on the fitness for use of the water. The model was used to simulate both conservative and non-conservative constituents. The level of expertise is high. The Water Resources Yield model was configured and run to provide hydrological input sequences. The calibration of the model required detailed work to use all available measured data to calibrate the washoff, rivers and impoundments.

5.1) Level of Competency required:

High: the model requires configuration of the monthly hydrology, which could entail the use of the Water Resources Yield Model, or some other monthly time step hydrology. The water quality modules require the generation of monthly time sequences of water quality data for the point sources, and calibration of the washoff, river transport and impoundment modules. It must be noted that the calibration of the washoff module requires a good understanding of the diffuse washoff modelling principles, and the understanding of the water quality response of the river system (*i.e.* data are essential for calibration).

5.2) Keywords

Whole catchment model, Conservative and non-conservative constituents, Water Resources Yield Model, System Analysis, System operating rules, Mixed reactor modelling, TDS, soluble phosphorus, particulate phosphorus, total phosphorus, suspended solids, algae, *E. coli*

5.3) Application algorithms and main mathematical limitations:

Catchment washoff module:

- TDS: can be derived from WQT model or simulated using flow-TDS function
- SP: loading function approach
- **PP: loading function approach**
- SS: loading function approach
- *E. coli*: loading function approach

River transport module (cascade of mixed reactors)

- TDS: mass balance
- SP: modified mass balance using adsorption/desorption isotherm
- PP: modified mass balance with sedimentation and remobilization
- Algae: growth limitation as a function of SP, light and season (surrogate for water temperature)
- SS: modified mass balance with sedimentation and remobilization
- *E. coli*: first order decay (with seasonal switching function)

Impoundment module (mixed reactor)

- TDS: conventional mass balance
- SP: modified mass balance using sedimentation and hypolimnetic release from sediments during overturn
- PP: modified mass balance with sedimentation
- Algae: growth limitation as a function of SP, light and season (surrogate for water temperature)
- SS: modified mass balance with first order sedimentation
- *E. coli*: first order decay (with seasonal switching function)

Point source module

All variables generated by the user as a monthly flow and concentration sequence for the variables: TDS, SP, PP, SS, and *E. coli*.

5.4) How widely is the model used:

The model has been applied to the following river systems in South Africa:

- Mgeni River, KwaZulu Natal
- Upper Kei River Basin, Eastern Cape
- Qgunube River, Eastern Cape
- Nahoon River, Eastern Cape
- Buffalo River, Eastern Cape
- Kubusi River, Eastern Cape

5.5) Related References:

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Quibell, G van Vliet H, & van der Merwe, W (1997) Characterising cause effect relationships in support of catchment water quality management, Water SA, 23, 3, 193 - 199.

Baxter-Potter, WR and MW Gilliland (1988) "Bacterial pollution in runoff from agricultural lands," *Journal of Environmental Quality*, 17(1):27-34.

Gilliland, MW and WR Baxter Potter (1987) "A Geographic Information System to Predict Nonpoint Source Pollution Potential," *Water Resources Bulletin*, 23(2): 281-291.

Haith, DA (1985) "An event based procedure for estimating monthly sediment yields," *Transactions of the ASAE*. Vol 28(6): 1916-1920.

Haith, DA & LL Shoemaker (1987) "Generalized Watershed Loading Functions for Streamflow Nutrients," *Water Resources Bulletin*, 23(3):471-478.

McElroy, AD, SY Chiu, JW Nebgen, A. Aleti & FW Bennett (1976) *Loading Functions for the Assessment of Water Pollution from Nonpoint Sources*, EPA report number 600/2-76-151.

Mills, WB, DB Porcella, MJ Ungs, SA Gherini, KV Summers, L. Mok, GL Rupp, GL Bowie & DA Haith (1985) *Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants in Surface and Ground Water*, EPA report number 600/6-85/002, Athens, GA.

Pegram, GC, AB Ottermann, S Terry and AJ Bath (1996) "Assessment of *E.coli* contamination to support water quality management," paper presented at the *Vic Falls Conference on Aquatic Systems*, July 1996, SASAQS.

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Rooseboom, A., Verster, E., Zietsman, H.L. and Lotriet, HH (1992) *The development of a new sediment yield map of southern Africa*. WRC Report No. 297/2/92

Schulze, RE (1995) *Hydrology and Agrohydrology: A text to accompany the ACRU 3.00 agrohydrological modelling system*. WRC Report TT69/95. Pretoria.

Smithen, J and RE Schulze (1995) *ACRU Agrohydrological Modelling System: User Manual Version 3.00*. WRC Report TT70/95. Pretoria.

Taylor, A W and Kunishi M (1971) Phosphate Equilibria on Stream Sediment and soil in a Watershed Draining an Agricultural Region. J. Agr. Food Chem. 19, no5, 827-831.

5.6) Links to other Organizations

DWAF web site: www.dwaf.gov.za
Ninham Shand web site: www.shands.co.za

5.7) Range of Applications:

- Optimization of system operating rules
- Assessment of point source impacts
- Assessment of diffuse source impacts
- Assessment of water quality management priorities based on source loadings and response of water bodies.

6) Case Studies:

The model has been configured and calibrated for the Amatole Water Supply system that includes the rivers listed below.

- Buffalo River, Eastern Cape
- Kubusi River, Eastern Cape
- Qgunube River, Eastern Cape
- Nahoon River, Eastern Cape

During the development phase, the model was applied to:

- Mgeni River, KwaZulu Natal
- Upper Kei River, Eastern Cape

MODEL: **MINEQL⁺ 4.0 Geochemical Speciation Programme**

EVALUATED BY: Ms. S. Wadley, Department of Chemical Engineering, University of Natal, Durban, Email: Wadley@eng.und.ac.za
And
Dr. Rudy Boer, Pulles Howard & De Lange Inc.
Email: rudy@phd.co.za

1) Description:

MINEQL⁺ (Westall et al., 1976) and its precursor, REDEQL (Morel and Morgan, 1972), were developed to solve mass balance expressions using equilibrium constants WATEQ3 (Ball et al., 1981) addressed the same problem through minimization of Gibbs Free Energy. The use of Gibbs Free Energy or equilibrium constants are both valid approaches, however WATEQ3 greatly advanced research in chemical speciation through providing a comprehensive and up-to-date thermodynamic database. Recently efforts were made to combine the database of WATEQ3 and the numerical structure of MINEQL (MINTEQA1; Brown and Allison, 1987).

MINEQL⁺ is an interactive data management system for chemical equilibrium modelling, which uses the original MINEQL program as an underlying numerical engine (Schecher and McAvoy, 1992). The fundamental structure of MINEQL has not been altered except with regard to input / output protocol. The result is an integrated software package that has a solid theoretical foundation superimposed on advanced data management tools.

A summary of MINEQL⁺ software attributes includes:

- A spatial user interface;
- On-line help screens;
- MINTEQA1 thermodynamic data with additional data from the original MINEQL database;
- Advanced relational database techniques for scanning thermodynamical data managing and output data;
- A relational spreadsheet editor for creating, altering, or deleting chemical species input;
- A multi-run manager for processing field monitoring data, creating synthetic titrations or performing sensitivity analysis;
- A utility for creating and accessing a personal thermodynamic database;
- An object-oriented database tool for managing model output;
- On-line DOS utilities;
- Extensive error checking.

In addition the software allows options for temperature and ionic strength correction. Version 3.0 of MINEQL⁺ also supports:

- Graphical display of output data as X-Y plots or bar charts;
- Support for graphical output to video displays and printers;
- A wide variety of surface complexation models including the Triple Layer Model, the Generalized Two-Layer Model (plus a specific instance for FeOH solids), and the Constant Capacitance Model;

- An updated thermodynamic database for adsorption of anions and cations on to FeOH surfaces;
- An improved user interface for many file maintenance functions.

The thermodynamic database used by MINEQL* contains the entire database from the US EPA model MINTEQA2 plus data for chemical components that the EPA did not include, so all calculations will produce results compatible with EPA specifications.

2) Data requirements:

The data needed to run MINEQL* are similar to that required for MINTEQA2. It generally consists of a chemical analysis of the water sample to be modeled giving total dissolved concentrations for the components of interest, and other relevant measurements for the system like the pH, pe, and/or the partial pressure of one or more gases. Measured values for pH and/or pe may be specified as invariant in the model, or MINEQL* can be used to calculate equilibrium values. In addition, a measured amount of a mineral may be specified as initially present in the system and subject to dissolution if equilibrium conditions warrant; or, a mineral may be specified as definitely present at equilibrium and not subject to complete dissolution.

The MINTEQA2 database contains 61 inorganic and 28 organic components. Special purpose components for adsorption sites, electrostatic potentials, and dissolved organic matter are included. The chemical components include major ions commonly found in natural aqueous systems (Ca, Fe, S, etc.), trace metal/metalloids of environmental concern (Ag, As, Ba, Cd, Cr, Cu, Hg, Ni, Pb, Sb, Se, Tl, and Zn), other metals, and organic ligands significant in metal complexing. The thermodynamic database contains over 1400 species each involving two or more components. There are also databases containing metal oxide surface complexation constants and complexation constants for a humic material distribution model for metal complexation with dissolved organic matter.

If suitable data is not present in the database for the system of interest, then additional data must be added by editing the relevant databases.

3) Computer requirements:

A pentium PC is recommended to run the software. MINEQL* runs on Windows 3.1/95/NT. MINEQL* version 4.0 requires at least 4 MB of RAM and 2.5 MB of bardisk space. Additional disk space is required to accommodate output data. 10 MB is recommended for average applications. A 3.5 inch disk drive is required to install the software. The use of the model does not require any programming. MINEQL* Version 4.0 is written to operate under Windows 3.1, 95 or NT. The previous version, Version 3.0, is DOS based.

4) Availability:

MINEQL* is copyrighted and all rights are reserved by William Schecher and Environmental Research Software. Under this copyright, Environmental Research Software supports the wide distribution and use of MINEQL* for research and

classroom applications. Persons who copy or distribute MINEQL$^+$ must do so at no profit. The software is available from:
Dr. William D. Schecher,
Environmental Research Software,
16 Middle St.,
Hallowell, ME 04347,
Tel: (091) (207) 622-3340,
Fax: 091-207-622-3340,
Email: ersoftwr@agate.net
Web Page: http://www.agate.net/~ersoftwr/mineql.html

4.1) Costs:

Cost Category 2: < US$2000

5) Assessment:

MINEQL$^+$ is a geochemical model capable of calculating equilibrium aqueous speciation, adsorption, gas phase partitioning, solid phase saturation states, and precipitation-dissolution of metals. MINEQL$^+$ can solve a broad range of chemical equilibrium problems.

The standard features present in MINEQL$^+$ include creation of aqueous system with acid/base, redox, or precipitation reactions, management of multiple calculations, extraction of output data from any perspective, performance of synthetic titrations, processing of field data or any data in text format, and running of sensitivity analyses.

No programming is required to run MINEQL$^+$. In the simplest case, the user just selects chemical components from a menu and inputs certain other data pertaining to the system. The software then scans the thermodynamic database and runs the calculation. MINEQL$^+$ Version 4.0 also enables the user to take control of the reaction data, create a personal thermodynamic database, perform synthetic titrations and automatically process multiple samples (such as field data).

New features in Version 4.0 (not present in version 3.0):

- The model allows either fixing the pH or calculating the pH. The pH can be calculated assuming electroneutrality of the solution or using the total proton concentration.
- The model enables setting of the P_{CO2}, total carbonate, or estimation of the total carbonate
- using pH and alkalinity.
- The model allows setting of the pe or P_{02} directly.
- Ionic strength can be set at a fixed value or be calculated from dissolved species.
- The output contains pseudo-species for the total dissolved concentration, the total adsorbed concentration, and the total dissolved minus the total adsorbed.
- The output can be summarized in a number of special reports that perform additional data extraction or additional calculations on the output data. Reports include:
- Alkalinity Reports to provide output on total alkalinity, pH and a breakdown of

major alkalinity sources.
  - Totals Report to provide a compilation of total dissolved forms.
  - Saturation Index Report to provide the SI values for every solid in the system.
  - Ion Balance Report to provide a complete summary of charge discrepancy for all samples. (This is useful for determining if all ions have been measured in a sample, or if there is significant analytical error.)
  - Summary Report to provide a compilation of all species output for a single run.
- Numerical procedures have been improved to solve problems with a very high number of solids and to provide stable starting places for all calculations.
- The model has a bulk solids mover which allows moving of solid species as a group or individually.
- Several output tables or graphs can be opened at once.
- The progression of software tools that are needed to solve a chemical equilibrium problem is automated. This is a helpful feature for new users and it can be controlled by setting user preferences.
- Personal thermodynamic data can be read by MINEQL$^+$ just like the default data, or the default data can be by-passed altogether.
- There are cut and paste features, which allow transference of the data to other software using the Windows clipboard.
- The system of managing multiple runs to help generate synthetic titrations or perform sensitivity analyses. This tool also provides the means to run data from other software, so field data, laboratory samples can be automatically processed, or output from other models can be processed.
- Input parameters that can be varied include: the total concentration of every component, the log K and enthalpy of every species, temperature and, if surface models are used, surface area.

5.1) Level of competency required:

The fundamental determinant of the levels of competency required are those of the potential users knowledge of the real world system that he/she is trying to model. If one has the scientific knowledge of the systems that one is modelling then the competency required to run the model is trivial by comparison. However, if one does not know the science behind the systems that one is modelling then any model is difficult and should not be used.

5.2) Keywords for task-based search:

MINEQL, MINEQL$^+$, water chemistry modelling, aquatic systems, chemical speciation, geochemistry, pollution

5.3) Application algorithms and main mathematical limitations:

The model operates at a one-month time step. The spatial and temporal scale must however be matched realistically. This naturally requires the model user to be fully aware of the scientific systems being modelled.

5.4) How widely is the model used and how well is it established in the industry:

Combinations of the following types of reactions proceeding in a system can be modelled:

- acid/base reactions
- complexation reactions
- precipitation/dissolution reactions
- oxidation/reduction (redox) reactions
- adsorption/desorption reactions
- gas absorption reactions

The program was originally designed to be a research tool but it is currently used in over 500 colleges and universities world-wide as an aid in teaching aquatic chemistry.

5.5) Related References:

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5.6) Links to organisations:

Web Page: http://www.agate.net/~ersoftwr/mineql.html

5.7) Range of applications:

Combinations of the following types of reactions proceeding in a system can be modelled:

- acid/base reactions
- complexation reactions
- precipitation/dissolution reactions
- oxidation/reduction (redox) reactions
- adsorption/desorption reactions
- gas absorption reactions

6) Case study:

Example: Control of pe with Dissolved O_2

The System: The upper waters of a lake contain a total of $2x10^{-4}$ moles/l of S (either as SO_4 or S^{2-} complexes). The pH of the water is 5.34 and the system is in equilibrium with dissolved oxygen ($P_{O2} = 10^{-0.7}$). The concentration of Fe (II or III) is negligible.

The Goal: Calculate the pe and equilibrium concentrations of SO_4^{2-} and HS^-.

The Method: Step 1. This system will use dissolved O_2, rather than pe, to control e^-. Select the components, scan the thermodynamic database and bring up the Fixed Solids editor. This time, remove the pe "species" from the list of Fixed Solids by moving the cursor to its location on screen and pressing Del.

The Log K value listed for 02 (g) is -83.12. This is the negative pe° for the half reaction:

$$O_2(g) + 4H^+ + 4e^- = 2H_2O; \qquad pe^{\circ} = 83.12$$

You need to correct the Log K value to include the effect of P_{O2}:

$$Log\ K = -(pe^{\circ} + LogP_{O2})$$

or

Log K = -[83.12 + (-0.7)] = -82.42

Step 2. Change the Log K value of 02 (g) to -82.42. Make sure that the Log K of pH is 5.34. Change the total concentrations of both SO4(2-) and HS(-) to 1 $x10^{-4}$ (the initial concentration of the sulphur components is not important so long as they add up to $2x10^{-4}$). Run the calculation.

The Output: All of the sulphur is as SO_4^{2-} ($2x10^{-4}$ M) in this system as shown in the S1.SO(2-)/SPEC/RUN1 view. If you want to know the pe of the final solution, open the SI.e(-)/SPEC/RUN1 view and find the Log C value for e(-) (ID = 1, Type = 6). This is the negative pe; in this case pe = 15.3.

MODEL: **MINTEQA2 Version 3.11 (1991) and MINTEQAK**

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1) Description:

MINTEQA2 is a geochemical equilibrium speciation model written by the US EPA. It is capable of computing equilibria between dissolved species in dilute aqueous solutions and adsorbed, solid and gas phases in laboratory or natural aquatic systems. MINTEQA2 is an update of MINTEQ that was developed by combining the fundamental mathematical structure of MINEQL with the thermodynamic database of WATEQ3. MINTEQA2 is MS DOS based.

MINTEQA2 can be used to calculate the mass distribution between the dissolved, adsorbed, and multiple solid phases under a variety of conditions including a gas phase with constant partial pressure. Calculations can be carried out to take into account the pH, ionic strength, temperature and redox potential of the system.

The program has an extensive database of thermodynamic data pertaining to reactions leading to complex formation, mineral dissolution/precipitation, gas absorption and redox reactions. MINTEQA2 has seven adsorption models, including simple adsorption isotherm models, cation exchange equilibria and surface complexation models.

MINTEQA2 is accompanied by the interactive program called PRODEFA2, which is used to create input files to describe the problem. Using PRODEFA2 the user can access species available in MINTEQA2 thermodynamic database and define other aqueous, solid, and/or adsorption species not present in the database.

The results from a MINTEQA2 calculation are given as an output file, which can be viewed using any text editor. MINTEQA2 can generate reports at any of three levels of detail. Reported parameters include the concentrations of all species in the system and saturation states of all solids. Multiple output files can be created for similar problems where one of the input concentrations or activities is varied systematically using the sweep option.

A related code, MINTEQAK, has been written by the Colorado School of Mines to model geochemical and biogeochemical processes in wetlands and reactors to treat acid drainage. It is based on the MINTEQA2 code with extensive modification to model the change in composition of aqueous flow as it traverses a wetland or reactor system. The code allows modeling of an anaerobic wetland/reactor, an aerobic wetland, or an anaerobic wetland/ reactor in series with an aerobic wetland. Modeled processes include dissolution of limestone, ion exchange, microbial sulfate reduction, denitrification, adsorption, precipitation of solids, and dilution by precipitation.

2) Data requirements:

The data needed to run MINTEQA2 generally consists of a chemical analysis of the water sample to be modeled giving total dissolved concentrations for the components of interest, and other relevant measurements for the system like the pH, pe, and/or the partial pressure of one or more gases. Measured values for pH and/or pe may be specified as invariant in the model, or MINTEQA2 can be used to calculate equilibrium values. In addition, a measured amount of a mineral may be specified as initially present in the system and subject to dissolution if equilibrium conditions warrant; or, a mineral may be specified as definitely present at equilibrium and not subject to complete dissolution.

The MINTEQA2 database contains 61 inorganic and 28 organic components. Special purpose components for adsorption sites, electrostatic potentials, and dissolved organic matter are included. The chemical components include major ions commonly found in natural aqueous systems (Ca, Fe, S, etc.), trace metal/metalloids of environmental concern (Ag, As, Ba, Cd, Cr, Cu, Hg, Ni, Pb, Sb, Se, Tl, and Zn), other metals, and organic ligands significant in metal complexing. The thermodynamic database contains over 1400 species each involving two or more components. There are also databases containing metal oxide surface complexation constants and complexation constants for a humic material distribution model for metal complexation with dissolved organic matter.

If suitable data is not present in the database for the system of interest, then additional data must be added either via PRODEFA2 or by editing the relevant databases.

2.1) Inventory of data sources:

General thermodynamic data:

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- Bard A.J., Parsons R. and Jordan J., 1985, Standard Potentials in Aqueous Solution, Marcel Dekker Inc., New York, ISBN 0-8247-7291-1.
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- Martell A.E. and Smith R.M., 1974, Critical Stability Constants, Volume 1, Amino Acids, Plenum Press, New York.
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- Perrin D.D., 1965, Dissociation Constants of Organic Bases in Aqueous Solutions, London, Butterworths.
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- Perrin D.D., 1982, Ionisation Constants of Inorganic Acids and Bases in Aqueous Solutions, 2nd Edition, IUPAC Chemical Data Series, No. 29, Pergamon Press, Oxford.
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- Woods T.L. and Garrels R.M., 1987, Thermodynamic Values at Low Temperature for Natural Inorganic Materials; An Uncritical Summary, Oxford University Press, Oxford.

3) Computer requirements:

For the microcomputer version:

- Fully IBM compatible 80286, 80386, 80486, or 80586 MS or PC DOS version 3.30 or higher 640k base (low end), memory and 2.0m bytes of free disk space.
- Diskette Drive: Required for diskette installation only.
- Hard Disk Drive: 20m byte drive recommended (minimum) with 2.0m bytes free (minimum).
- Run time size: Up to approximately 2.0m bytes plus space for user input data files, output, and temporary files produced by model system.
- Numerical Coprocessor: Optional.
- \CONFIG.SYS Statements:

BREAK=ON
BUFFERS=20 or BUFFERS=32
FILES=20
DEVICE=C:\ANSI.SYS
SHELL=C:\COMMAND.COM C:\
/e:512/p

To modify the source code a Fortran compiler is required, however this is not needed to run the software. There is also a version of the software for UNIX computers.

MINTEQAK is a public domain program distributed on a DOS-formatted disk, containing source code, executable image, and data sets. The documentation includes an IGWMC prepared file with installation instructions.

4) Availability:

U.S. EPA, Environmental Research Laboratory (ERL), College Station Road, Athens, GA 30613-0801, USA. Email: ceam@epamail.epa.gov

The microcomputer version can be downloaded from:

ftp://ftp.epa.gov/epa_ceam/DOS/MINTEQ/INSTALMT.EXE

The manual can be downloaded from:
ftp://ftp.epa.gov/epa_ceam/DOS/MINTEQ/INSTALTD.EXE

The software for the microcomputer and manual (in WordPerfect format) can also be downloaded from the CCWR computer in South Africa:
ftp://ftp.ccwr.ac.za/pub/minteqa2/minteqa2.zip

MINTEQAK is available from the author:

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Colorado School of Mines
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USA
Tel: (303) 273-3617
Fax: (303) 273-3629
Email: rklusman@mines.edu

A description of MINTEQAK can be found at :
http://igwmc.mines.colorado.edu%3A3851/0/software/igwmcsoft/hydrogeo/minteqak.htm

4.1) Costs:

MINTEQA2 and its associated documentation are downloadable free of charge from the Internet.

MINTEQAK currently costs US$95

5) Assessment:

The MINTEQA2 user should have a scientific or engineering background. At least one year of chemistry is required. Additional experience with thermodynamics is helpful, especially if it becomes necessary to add data to the database.

1. The model is purely an equilibrium model hence it cannot be used to evaluate systems with significant kinetic constraints. Examples:
   - i) **Although a particular solid may precipitate given sufficient time, this precipitation may not be observed during the time the system is observed.**
   - ii) Some redox reactions are very slow so that the redox state observed may not be the redox state that the model predicts.
2. The model cannot deal with a mixture of streams, but the user must sum all the conserved parameters (concentrations, not activities) before entering the data into MINTEQA2.
3. Limited sorption data is available in the database because sorption onto natural surfaces is highly site specific.

4. The nature and amount of dissolved organic matter in the system being studied is often poorly defined, hence although MINTEQA2 has a dissolved organic matter model, this may not adequately describe the system being investigated.
5. The database may not contain all the species required for the system being considered and the data could be inaccurate or not relevant to the conditions prevailing in the system.
6. Errors relating to the formation constants between metals and organic ligands are present in the thermodynamic database supplied with version 3.11 of MINTEQA2. Hence this thermodynamic data should be checked before using the model.
7. The concentrations in the MINTEQA2 output are given to four significant figures, however only one or two figures at most will be accurate. The high number of significant figures reported is necessary for error analysis.

5.1) Level of competency required:

MINTEQA2 is user friendly to the first time user due to the interactive program PRODEFA2 which is used to create the input files. An understanding of water chemistry is required to ensure appropriate use of the model.

MINTEQA2 has an extensive database, hence most first time users do not have to add their own thermodynamic data. However the range of calculations that it can perform is more limited than codes such as PHREEQE or PHREEQC. The input of data into MINTEQA2 Version 3.11 is more laborious in MINTEQA2 than in MINEQL+ Version 4.0, since MINEQL+ Version 4.0 has an interface which enables importing of input data from a spreadsheet. However MINTEQA2 is able to do all the types of calculations that MINEQL+ can do.

MINTEQA2 is a useful place to start for the person who has never done geochemical speciation modeling before. The output of MINTEQA2 is easy to read for the first time user, however due to the limited amount of data that MINTEQA2 can export to a spreadsheet, the use of this data in further calculations or the construction of graphs is more difficult than for MINEQL+. MINEQL+ has text file, spreadsheet and graphical output options.

5.2) Keywords for task-based search:

MINTEQA2, MINTEQAK, water chemistry modeling, aquatic systems, chemical speciation, geochemistry, biogeochemistry, wetlands, acid drainage, pollution

5.3) Applicable algorithms and main mathematical limitations:

MINTEQA2 expresses each species that could exist in the system in terms of a unique linear combination of a pre-defined set of components. It then formulates this multi-component chemical equilibrium problem by expressing all the equilibrium reactions that could possibly occur between these species in terms of nonlinear mass action expressions and forming linear mass balance relationships using the amounts of each component known to be present. MINTEQA2 finally solves these equations simultaneously using the iterative Newton-Raphson approximation method.

To solve a chemical equilibrium problem, MINTEQA2 uses an initial guess for the activity of each component to calculate the concentration of each species according to mass action expressions written in terms of component activities. The total mass of each component is then calculated from the concentrations of every species containing that component. The calculated total mass for each component is then compared with the known input total mass for each component.

If the calculated total mass and the known input total mass for any component differ by more than a pre-set tolerance level, a new estimate of the component activity is made and the entire procedure is repeated. The aqueous phase equilibrium composition is that set of species concentrations that gives a mass imbalance less than the tolerance level set for every component.

After equilibrating the aqueous phase, MINTEQA2 computes the saturation index for each possible solid with respect to the solution. If solid precipitation and/or dissolution is allowed in the calculation, then MINTEQA2 will use the saturation indices as a guide to add or deplete mass from the aqueous phase. The aqueous solution is then re-equilibrated.

Activity coefficients for all species are functions of solution ionic strength and vary as species distributions alter the ionic strength. Unless a fixed ionic strength is specified, MINTEQA2 calculates successive sets of activity coefficients for all solution species with each iteration. These are used to generate corrected values of the equilibrium constants that appear in the mole balance expressions. Initial activity guesses for the input components are provided in the input file for a given problem. These initial component activity guesses are used to estimate the concentrations of each dissolved species so that the solution ionic strength can be calculated. Each succeeding iteration provides improved estimates of species concentrations and activity corrections.

The activities of each charged species are calculated from the ionic strength of the solution using either the modified Debye-Hückel equation or the Davies equation. If the user selects the modified Debye-Hückel equation, it will be used for those species that have the necessary parameters in the database. For any species lacking the necessary parameters, the Davies equation will be used to estimate the activity coefficient for that species. If the user selects the Davies equation, it will be used throughout the problem because it requires no species-specific data besides charge.

Since these equations can only reliably predict ion activity coefficients for solution ionic strengths less than 0.5 mol/l, MINTEQA2 can only be used for relatively dilute systems.

MINTEQA2 uses two ways of adjusting the equilibrium constants for temperature. If the necessary data are available in the thermodynamic database, MINTEQA2 uses a power function equation. (Only 25 of the more than 1000 species in the database have these constants available.) For those species that do not have the constants needed for the above correlation, the equilibrium constant is corrected for temperature variations from 25°C by the van't Hoff equation.

The van't Hoff equation implicitly assumes that the enthalpies of reaction are independent of temperature. Hence significant errors can result at higher temperatures. Since for solids only a single K_{sp} is present in the database, this model does not allow for maximum and minimum solubilities which occurs for many solid species such as $CaSO_4$. Hence the model applies best at temperatures close to 25 °C.

MINTEQA2 makes use of the following algorithm for solving the equations relating to *the system:*

1. Make initial guess for the activity of each component.
2. Calculate the concentration of each species according to the mass action expressions (written in terms of component activities).
3. Calculate the total mass of each component from concentrations of every species containing that component.
4. Compare calculated total mass of each component with its known input total mass.
5. If calculated total mass and known input total mass for any component differ by more than pre-set tolerance, estimate the component activity again and repeat the procedure.
6. Once this tolerance is reached for all components, calculate the aqueous phase equilibrium for each species that occurs.
7. Then calculate the saturation index (SI) for each possible solid with respect to the solution.
8. For the solid with the most positive SI, calculate the amount, which would precipitate and subtract this from the concentrations of those components, which comprise the solid. (If an existing solid is found to be undersaturated with respect to the solution, do the reverse).
9. Re-equilibrate solution after mass has been added to or removed from the aqueous phase.
10. Repeat process until equilibrium is achieved, so that there are no oversaturated possible solids and no undersaturated existing solids.

5.4) How widely is the model used or how well established it is in the industry:

Used extensively around the world, but especially in the USA. The US EPA requires MINTEQA2 investigations to be undertaken by a competent person for site investigations and assessments.

5.5) Related references:

References to studies using MINTEQA2:

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References to studies using MINTEQAK:

- Klusman, R.W., D.H. Dvorak, S.L. Borek, 1993. Modeling of wetlands and reactor systems used for mine drainage treatment. Proc. American Society for Surface Mining and Reclamation. Spokane, WA, May 16-19, 1993, pp. 685-704.
- Klusman, R.W., 1993, Computer code to model constructed wetlands for aid in engineering design: Vol. 1: Application of a computer code to the modeling of biogeochemical processes operating in constructed wetlands and anaerobic reactors. U.S. Bureau of Mines, Open-file Rept. 71-93, 80 p. Vol. 2: Use of the computer code MINTEQAK for modeling geochemical processes in wetlands and reactors used to treat acid drainage. Open-file Rept. 72-93, 146 p.
- Lanphear M.E., R.W. Klusman, R.R.H. Cohen, 1995, Geochemical characterization of mine drainage sources in the Chalk Creek district, Colorado. Proc. American Society for Surface Mining and Reclamation. Gillette, WY, June 5-8, 1995, pp. 528-538.
- Ozawa, Toshisuke, R.R.H. Cohen, R.W. Klusman, 1995, Biogeochemistry and behavior of arsenic and chromium in a wet substrate, anaerobic bioreactor dominated by sulfate-reducing bacteria. Proc. American Society for Surface Mining and Reclamation. Gillette, WY, June 5-8, 1995, pp. 587-602.

5.6) General links:

Government Organisations:

United States Environmental Protection Agency, USA: Centre for Exposure Assessment Modeling (ftp://ftp.epa.gov/epa_ceam/wwwhtml/minteq.htm)

Consultancies:

- Waterloo Hydrogeologic, Inc.: Tailings Geochemistry and Solute Transport (http://www.flowpath.com/Consult/mining_tails_solute.htm
- Johnson Environmental Concepts: Geochemical Model of Water Quality in Pit Lake in Oxidized Tuff (http://johnsonenviro.com/pitlake.htm)

Universities:

- Pollution Research Group, Department of Chemical Engineering, University of Natal, South Africa: Chemical Speciation Self-Study Work Manual (ftp://www.ccwr.ac.za/pub/minteqa2/home.html)
- Department of Civil and Environmental Engineering, Old Dominion University, USA: Civil/Environmenal Model Library (http://www.cee.odu.edu/cee/model/minteq.html)
- Bayer School of Natural and Environmental Sciences, Duquesne University, USA : Environmental Chemistry Course (http://nexus.chemistry.duq.edu/snes/esm/Course_ **Material/ESM552/Download/Download.HTML)**
- Colorado School of Mines, USA: International Groundwater Modeling Center (http://igwmc.mines.colorado.edu/)

5.7) Range of applications:

Combinations of the following types of reactions proceeding in a system can be modeled:

- acid/base reactions
- complexation reactions
- precipitation/dissolution reactions
- oxidation/reduction (redox) reactions
- adsorption/desorption reactions
- gas absorption reactions

6) Case Study:

The following types of problems can be solved using MINTEQA2:

- Prediction of the distribution of species between toxic and nontoxic forms.
- Investigation of the extent of adsorption of species on naturally occurring surfaces.
- Determination of effect of acid rain on the composition of surface water and ground water, and the weathering of rocks.
- Investigation of leachates from waste disposal sites and mine dumps.
- Determining the effect of pH on the precipitation of metals in acid mine water.
- Investigation of ion exchange characteristics of soils.
- Assessment of receiving water quality.
- Determination of required dosage of water treatment chemicals, for example lime dosing for water softening and neutralisation of alkaline water with carbon dioxide.
- Predicting the conditions under which scaling of water treatment equipment such as heat exchangers, pipelines and membranes would occur.
- Determination of the effect of organic matter on metal complexation.

- Modeling of ion exchange processes.
- Determining effect of recycled water on industrial or domestic water quality.

For details on some case studies please follow this link to Chemical Speciation Self-Study Work Manual (ftp://www.ccwr.ac.za/pub/minteqa2/guide/tcont_h.html)

MODEL: **NACL01**

EVALUATED BY: Dr C E Herold, Stewart Scott Inc.
Email: model@ssi.co.za

1) Description:

NACL01 is a daily time step catchment hydro-salinity model. It combines catchment hydrology with the related salinity. NACL01 is designed to run on a PC. NACL01 is not screen-interactive, and the user needs to enter the resulting model output into processing software or other programs. Typically this model provides daily time series of catchment runoff and salinity, which is then fed as input to the channel routing model NACL02 (which is described in this Internet site).

A full description of the model is contained in the Hydrological Research Unit report No 3/81 (Herold, 1981). NACL01 writes the catchment output to as many files as there are specified sub-catchments. The model takes account of the normal rainfall runoff processes and routes the catchment salts through similar storage elements. The model accounts for both surface and sub-surface flows and storage elements, urban and rural runoff, infiltration, direct surface runoff, inter flow, percolation and groundwater flow. Salts are modelled as slowly accumulating on rural and urban surfaces, with subsequent washoff to direct runoff and infiltration during storm events. Over land routing of both water and salt is simulated.

One of the main advantages of this model is that it simulates both surface and sub-surface salt processes for urban and rural areas. NACL01 is the precursor of a more simplified monthly time step model (Herold, 1980), which in turn served as the basis for other generations of this model. This led ultimately to the interactive monthly time step WQT model described in this Internet site

2) Data requirements:

Data preparation consists of the creation of model parameter input data and the preparation of time series data files.

The following is a summary of the data requirements.

Climatic

- Daily catchment rainfall time series

Physical

- Definition of sub-catchments for which daily surface and sub-surface storage states are to be stored.
- Catchment areas (including an allowance for growth in urban and rural diffuse source inputs).

Hydrological

- Model parameter values for each defined node

Water Quality

- Model parameter values for each sub-catchment

Miscellaneous

- Starting and ending dates

2.1) Inventory of data sources:

The daily rainfall time series can be obtained from the RSA Weather Bureau. Detailed descriptions of the model parameters, their initial selection and how best to adjust them are contained in HRU Report 3/81 (Herold, 1981a).

3) Computer requirements:

The WQT model runs under DOS (MS-DOS version 3.0 or higher). The program will run on any PC from XT upwards. The computer on which NACL01 is installed should have a minimum of 640 kb of RAM.

4) Availability:

The NACL01 model was originally developed as part of a RSA Water Research Commission project. As such it is freely available. Initial contact can be made with Dr Herold at:

Stewart Scott Incorporated
PO Box 784506
Sandton 2146
South Africa

Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email model@ssi.co.za

4.1) Costs:

Since the original NACL01 model was developed as part of a RSA Water Research Commission project, it is freely available, save for the cost of making copies, post and packaging.

5) Assessment:

NACL01 has been used in a number of detailed studies. These include the RSA Department of Water Affairs Vaal River Salinity Study and the Vaal River System Analysis Update Study. It has also been used as part of an environmental impact assessment for the Blesbokspruit, which includes the sensitive Blesbokspruit wetland (a designated RAMSAR convention site).

A version of NACL01 was also adapted to simulate the long-term effect of atmospheric deposition on catchment washoff (Herold *et al*, 1997). This version of the model simulates the relationship between salt (total dissolved salts) and sulphate and takes account of sulphate deposition, adsorption and desorption processes. This application also converts NACL01 from a lumped parameter model to a distributed parameter model to take account of the multiplicity of soils found in the study catchment.

5.1) Level of competency required:

Use of the model requires a good understanding of the physical system being modelled. This presupposes a sound knowledge of hydrological and water quality principals. General computer literacy is also required to run the models. Program NACL01 is relatively easy to run. However, in most instances it is necessary to feed the output from this model into the channel routing program NACL02, which requires a higher level of expertise to operate.

5.2) Keywords for task-based search:

Salinity, total dissolved salts, TDS, catchment washoff, surface and sub-surface, urban, rural, calibration, starting values, documented, wash off, surface water, simulation, daily, sulphate deposition.

5.3) Application algorithms and main mathematical limitations:

The model operates at a daily time step. Model algorithms are contained in HRU Report No. 3/81 (Herold, 1981a).

The main limitation of the NACL01 model is that it is not screen interactive. The input data files have to be pre-prepared before running the model.

5.4) How widely is the model used and how well is it established in the industry:

The model is somewhat specialised, since there is not a great call for daily time step modelling in the RSA.

5.5) Related References:

Herold CE (1980). A model to compute on a monthly basis diffuse salt loads associated with runoff. Report No. 1/80, Hydrological Research Unit, University of the Witwatersrand, Johannesburg, March 1980.

Herold CE (1981a). A model to simulate daily river flows and associated diffuse-source conservative pollutants. Report No. 3/81, Hydrological Research Unit, University of the Witwatersrand, Johannesburg, March 1981.

Herold CE (1981b). A model to simulate the monthly water and salt balance in the Vaal River water supply system. Report No. 4/81, Hydrological Research Unit, University of the Witwatersrand, Johannesburg, March 1981.

Herold CE and Kakebeeke JP, (1991). Monthly time step hydro-salinity system simulation model. Report P C000/00/9390, Vaal River Water Quality Management Study. Stewart Sviridov and Oliver report to Directorate of Planning, Department of Water Affairs, Pretoria.

Herold CE, Taviv I and Pitman WV (1997). Modelling the long term effect of atmospheric deposition on the salinity of catchment runoff with special reference to the Vaal Dam catchment. WRC Report No. 697/1/97. Report to RSA Water Research Commission by Stewart Scott, Sandton.

5.6) Links to organisations:

Enquiries on the NACL01 model can be directed to:

Stewart Scott Incorporated
PO Box 784506
Sandton 2146
South Africa

Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email model@ssi.co.za

5.7) Range of applications:

NACL01's purpose is to compute daily catchment runoff volumes and associated salt concentrations. The model takes account of the gradual accumulation of salts on the catchment surface and in the sub-surface storages and the subsequent release of the salts during rainfall events. Both water and salts are routed to evapo-transpiration loss, direct runoff, infiltration to the soil moisture, inter-flow, percolation to the groundwater and groundwater flow to the surface water system. Both urban (paved) and rural catchment areas are modelled. The output from NACL01 usually provides input to program NACL02 (the channel routing model).

Various applications of the model are given above in 5) Assessment.

6) Case study:

NACL01 (in conjunction with NACL02) has been applied to simulate daily stream flow and salinity for 12 sub-catchments of the Vaal Barrage catchment. The initial model development and application was carried out as part of a RSA Water Research Commission study of the Pretoria-Witwatersrand-Vereeniging area. The

Vaal Barrage is defined as the incremental Vaal River catchment between Vaal Dam and Vaal Barrage. This dynamic catchment is the most highly developed region in Southern Africa, which at the time of the model development accounted for about 60% of the GNP of the RSA. This area includes the sensitive Blesbokspruit wetland area (which is a designated RAMSAR convention site), several large industries and underground gold mines and a number of Local Authorities (including Johannesburg's southern waste water treatment works, which constitute the largest effluent source in the RSA). Details of the original work carried out for this catchment are contained in HRU Report No. 3/81 (Herold, 1981a). The calibrated model was used to carry out detailed testing of various water quality management options. It was also used to patch missing records. The patched data was then used to compute monthly records, which were then entered as input data for a more simplified monthly time step model (Herold, 1980 and Herold, 1981b).

This model was subsequently used in a number of studies carried out on behalf of the RSA Department of Water Affairs to test the impact of numerous management options for the highly saline Gauteng-Vaal River system. At a later stage the original monthly model was replaced by WQT, a modular, screen-interactive model (described elsewhere in this Internet site). This was done as part of the Department of Water Affairs Vaal River System Analysis study.

The NACL01 model was also adapted to simulate the long-term impact of atmospheric deposition on sulphate and total dissolved solids levels in the runoff from the Vaal Dam catchment (see section 5 - Assessment).

MODEL: **NACL02**

EVALUATED BY: Dr C E Herold, Stewart Scott Inc.
Email: model@ssi.co.za

2) Description:

NACL02 is a daily time step model for routing flow and salt through a river system. The model is written in FORTAN and runs on a PC. This model is not screen-interactive. The output from the catchment model NACL01 (which is described in this Internet site) is part of the input to this model.

A full description of NACL02 is contained in the Hydrological Research Unit report No 3/81 (Herold, 1981a). NACL02 routes catchment runoff and salt load through a series of connected river reaches. These reaches can be defined as normal river channels or dams. Each reach can comprise both open water surface and wetland areas. Bed losses and riparian irrigation areas are defined for each reach, along with cross sectional shape and slope. Compound channel cross sections can be specified, with different friction factors for the main channel and the side channel areas. Inputs from upstream point sources and abstractions can also be provided for each channel reach. Evaporation factors are provided for wetland and open water surface areas. Evaporation and transpiration losses from wetland areas are differentiated and track is kept of the movement of both water and salt between the central channel and the slower moving wetland area. Water and salt are transported through the central channel using a Lagrangian-type solution procedure.

This model, together with NACL01, is the precursor to a more simplified monthly time step model (Herold, 1980). The simplified monthly model in turn led to the development of other model generations (such as Herold,1981b), which led ultimately to the interactive monthly time step WQT model (described in this Internet site).

2) Data requirements:

Data preparation consists of the creation of model parameter input data and the preparation of time series data files.

The following is a summary of the data requirements.

Climatic

- Monthly rainfall time series

Physical

- Definition linkages between channel reaches
- Wetland and irrigation areas
- Mean monthly evaporation and transpiration factors
- Channel cross-section shape details
- Channel slopes

- Friction factors
- River bed losses

Hydrological

- Time series of simulated daily sub-catchment runoff
- Time series of monthly point source inputs
- Time series of monthly point abstractions

Water Quality

- Time series of monthly point source salt concentrations entering the system

Miscellaneous

- Starting and ending dates

2.1) Inventory of data sources:

The daily rainfall time series can be obtained from the RSA Weather Bureau. Detailed descriptions of the flow and water quality model parameters, their initial selection and how best to adjust them are contained in HRU Report 3/81(Herold, 1981a).

3) Computer requirements:

NACL02 runs under DOS (MS-DOS version 3.0 or higher). The program will run on any PC from XT upwards. Faster run times can obviously be achieved by more advanced computers. The computer on which NACL02 is installed should have a minimum of 640 KB of RAM.

4) Availability:

The original NACL02 model is available from the RSA Water Research Commission. As such it is available free of charge. Initial contact can be made with Dr Herold at:

Stewart Scott Incorporated
PO Box 784506
Sandton 2146
South Africa

Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email model@ssi.co.za

4.1) Costs:

NACL02 was originally developed as a WRC project. As such the original model can be obtained free of charge, save for the cost of making copies, packaging and postage.

5) Assessment:

NACL02 has been used in a number of detailed studies. These include the RSA Department of Water Affairs Vaal River Salinity Study and the Vaal River System Analysis Update Study. It has also been used as part of an environmental impact assessment for the Blesbokspruit, which includes the sensitive Blesbokspruit wetland (a designated RAMSAR convention site).

5.1) Level of competency required:

Use of the model requires a good understanding of the physical system being modelled. This presupposes a sound knowledge of hydrological and water quality principals. General computer literacy is also required. NACL02, which usually accepts the simulated catchment runoff data from NACL01 as input, has onerous data requirements. Preparation of this input data, calibration of the model and interpretation of the model results requires considerable expertise.

5.2) Keywords for task-based search:

Salinity, total dissolved salts, TDS, daily, channel and reservoir routing, point and catchment inputs, riparian irrigation, wetland, evapo-transpiration, compound channel, Lagrangian routing, channel bed losses, modelling, simulation.

5.3) Application algorithms and main mathematical limitations:

The model operates at a daily tine step. Model algorithms are contained in HRU Report No. 3/81 (Herold, 1981a).

The main limitation of the NACL02 model is that it is not screen interactive. The input data files (other than the output from the catchment washoff model, NACL01) have to be pre-prepared before running the model. The model output also has to be processed through appropriate software to obtain the requisite plots, statistics and other forms of presentation material.

5.4) How widely is the model used and how well is it established in the industry:

The model is somewhat specialised, since there is not a great call for daily time step modelling in the RSA. Specialist services are also required to run the model.

5.5) Related References:

Allen RB and Herold CE (1988). Water quality calibration model. Report P C000/00/7086, Vaal River System Analysis, BKS and Stewart, Sviridov & Oliver report to Directorate of Planning, Department of Water Affairs, Pretoria.

Herold CE (1980). A model to compute on a monthly basis diffuse salt loads associated with runoff. Report No. 1/80, Hydrological Research Unit, University of the Witwatersrand, Johannesburg, March 1980.

Herold CE (1981a). A model to simulate daily river flows and associated diffuse-source conservative pollutants. Report No. 3/81, Hydrological Research Unit, University of the Witwatersrand, Johannesburg, March 1981.

Herold CE (1981b). A model to simulate the monthly water and salt balance in the Vaal River water supply system. Report No. 4/81, Hydrological Research Unit, University of the Witwatersrand, Johannesburg, March 1981.

Herold CE and Kakebeeke JP, (1991). Monthly time step hydro-salinity system simulation model. Report P C000/00/9390, Vaal River Water Quality Management Study. Stewart Sviridov and Oliver report to Directorate of Planning, Department of Water Affairs, Pretoria.

5.6) Links to organisations:

Enquiries on the NACL02 model can be directed to:
Stewart Scott Incorporated
PO Box 784506
Sandton 2146
South Africa

Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email model@ssi.co.za

5.7) Range of applications:

NACL02's purpose is to route catchment runoff and point source inputs through a system of inter-connected river reaches. Reaches can comprise both river channels and reservoirs and can include riparian irrigation, bed losses, and wetland evaporation and transpiration. Time series of catchment runoff and associated salt concentrations are usually provided by model NACL01(described in this Internet site). Various applications of NACL02 are given above in 5) Assessment.

6) Case study:

NACL02 (in conjunction with NACL01) has been applied to simulate daily stream flow and salinity for the Vaal Barrage catchment (i.e. the incremental Vaal River catchment between Vaal Dam and Vaal Barrage). Details of the original work carried out for this catchment are contained in HRU Report No. 3/81 (Herold, 1981a). During this Water Research Commission study, the calibrated model was used to test the effectiveness of various management options.

In these studies NACL01 was used to calibrate the rainfall – runoff parameters. The output from NACL01 was then fed as input to the channel routing model, NACL02. The river system comprised of the following river elements:

- reservoir and river channel reaches;
- riparian irrigation;
- river bed losses;
- extensive wetland areas (including the Blesbokspruit RAMSAR site);
- highly saline mining point source inputs;
- numerous municipal and industrial effluent sources (including those from Johannesburg, the largest Local Authority in Southern Africa);
- significant diffuse source salt inputs (in some instances leading to a twenty-fold increase in salinity over the background contribution); and
- complex compound channel cross sections (especially in some wetland reaches).

The daily model was also used to patch missing records. The patched data was then used to compute monthly records, which in turn were used as input data for a more simplified monthly time step model (Herold, 1981b). This model was subsequently used in a number of studies carried out on behalf of the RSA Department of Water Affairs and Forestry to test the impact of numerous management options for the highly saline Gauteng-Vaal River system. At a later stage the original monthly model was replaced by WQT, a modular, screen-interactive model. This was done as part of the Department of Water Affairs Vaal River System Analysis study. The WQT model is described elsewhere in this Internet site.

MODEL: **OTEQ**

EVALUATED BY: Rob Runkel, U.S. Geological Survey

1) Description:

OTEQ is a mathematical simulation model used to characterize the fate and transport of trace metals streams and rivers. OTEQ couples the transport capabilities of OTIS (One-Dimensional Transport with Inflow and Storage) with the chemical equilibrium capabilities of MINTEQ (U.S.EPA). The coupled model considers a variety of physical and chemical processes including advection, dispersion, transient storage, the transport and deposition of water-borne solid phases, acid-base reactions, complexation, precipitation/dissolution and sorption.

The OTEQ solute transport model and related materials (data and documentation) are made available by the U.S. Geological Survey (USGS) to be used in the public interest and the advancement of science. You may, without any fee or cost, use, copy, modify, or distribute this software, and any derivative works thereof, and its supporting documentation, subject to the USGS software User's Rights Notice.

Funding for software development was provided by the USGS Toxic Substances Hydrology Program and the USGS Office of Water Quality.

2) Data requirements:

The model computes solute concentrations at user-defined times andlocations using the following user-supplied information:

a) System Configuration (Number and length of reaches)
b) upstream boundary conditions (solute concentration at x=0)
c) hydrology (flow and stream cross-sectional area)
d) mixing parameters (dispersion coefficient, transient storage parameters).

Equilibrium constants describing acid-base, complexation, precipitation/dissolution and sorption reactions are as defined within the MINTEQ database. These constants may be over-riden by user-supplied values.

2.1) Inventory of data sources:

Items a) and b) above are typically defined by the investigator. Items c) and d) are often obtained using tracer-injection methods.

3) Computer requirements:

Executable versions of the model will be available for personal computers (DOS, Win 3.1, Win 95, Win NT, Linux) and Unix workstations (Sun-OS, Sun-Solaris, IBM-AIX, DEC, DG-UX.

4) Availability:

OTEQ is not currently available for public use. A public version of OTEQ will be available after user documentation is developed.

4.1) Costs:

OTEQ is not currently available for public use. A public version of OTEQ will be available after user documentation is developed

5) Assessment:

5.1) Level of competency required:

General understanding of stream transport processes, the advection-dispersion equation, finite-difference numerical methods and equilibrium chemistry.

5.2) Keywords for task-based search:

solute transport, trace metals, streams, MINTEQ, equilibrium chemistry, sorption, precipitation/dissolution.

5.3) Application algorithms and main mathematical limitations:

Partial differential equations (PDEs) describing transport are solved using finite difference methods and the Crank-Nicolson method. The mass-balance and mass-action equations describing chemical equilibrium form a set of non-linear algebraic equations (AEs). The coupled set of PDEs and AEs are solved using sequential iteration as described by Runkel et al. (1996a).

5.4) How widely is the model used and how well is it established in the industry:

At present, the model is used exclusively within the U.S. Geological Survey (USGS). Use outside of the USGS will begin after publication of user documentation.

5.5) Related References:

Allison, J.D., D.S. Brown, and K.J. Novo-Gradac, 1991, MINTEQA2/PRODEFA2,A geochemical assessment model for environmental systems: Version 3.0 User's Manual: Rep. EPA/600/3-91/ 021, U. S. Environ. Prot. Agency, Washington, D. C.

Dzombak, D.A. and F.M.M. Morel, 1990, Surface Complexation Modeling: Hydrous Ferric Oxide: John Wiley and Sons, New York, 393 p.

Runkel, R.L., 1998, One dimensional transport with inflow and storage (OTIS): A solute transport model for streams and rivers: U.S. Geological Survey Water-Resources Investigation Report 98-4018. 73 p.

Runkel, R.L., K.E. Bencala, R.E. Broshears, and S.C. Chapra, 1996, Reactive solute transport in streams: 1. Development of an equilibrium-based model, Water Resources Research, v. 32, no. 2, p. 409-418.

5.6) Links to organisations:

http://webserver.cr.usgs.gov/oteq

5.7) Range of applications:

Broshears, R.E., R.L. Runkel and B.A. Kimball, 1995, Interpreting spatial profiles of concentration in acid mine drainage streams, in Hotchkiss, W.R., J.S. Downey, E.D. Gutentag and J.E. Moore, editors, Water Resources at Risk, Proceedings of the 1995 annual meeting of the American Institute of Hydrology, Denver, Colorado, May 14-18, 1995: American Institute of Hydrology, p. LL10-22.

Broshears, R.E., R.L. Runkel, B.A. Kimball, D.M. McKnight, and K.E. Bencala, 1996, Reactive solute transport in an acidic stream: Experimental pH increase and simulation of controls on pH, aluminum and iron: Environmental Science and Technology, v. 30, no. 10, p. 3016-3024.

Runkel, R.L., D.M. McKnight, K.E. Bencala and S.C. Chapra, 1996, Reactive solute transport in streams: 2. Simulation of a pH-modification experiment: Water Resources Research, v. 32, no. 2, p. 419-430.

6) Case study: see 5.7 above

MODEL: **OTIS**

EVALUATED BY: Rob Runkel, U.S. Geological Survey
Email: runkel@usgs.gov

1) Description:

OTIS is a mathematical simulation model used to characterize the fate and transport of water-borne solutes in streams and rivers. The governing equation underlying the model is the advection-dispersion equation with additional terms to account for transient storage, lateral inflow, first-order decay and sorption. This equation and the associated equations describing transient storage and sorption are solved using a Crank-Nicolson finite difference solution.

OTIS may be used in conjunction with data from field-scale tracer experiments to quantify the hydrologic parameters affecting solute transport. This application typically involves a trial-and-error approach wherein parameter estimates are adjusted to obtain an acceptable match between simulated and measured tracer concentrations. Additional applications include analyses of non-conservative solutes that are subject to sorption processes and/or first-order decay.

A modified version of OTIS, OTIS-P, couples the solution of the governing equation with a non-linear regression package. OTIS-P determines an 'optimal' set of parameter estimates that minimize the squared differences between the simulated and measured concentrations, thereby automating the parameter estimation process.

The OTIS solute transport model and related materials (data and documentation) are made available by the U.S. Geological Survey (USGS) to be used in the public interest and the advancement of science. You may, without any fee or cost, use, copy, modify, or distribute this software, and any derivative works thereof, and its supporting documentation, subject to the USGS software User's Rights Notice.

Funding for software development was provided by the USGS Toxic Substances Hydrology Program and the USGS Office of Water Quality.

2) Data requirements:

The model computes solute concentrations at user-defined times and locations using the following user-supplied information:

a) System Configuration (Number and length of reaches)
b) upstream boundary conditions (solute concentration at x=0)
c) hydrology (flow and stream cross-sectional area)
d) mixing parameters (dispersion coefficient, transient storage parameters).
e) first-order reaction rates and/or sorption parameters (reactive solutes only)

2.1) Inventory of data sources:

Items a) and b) above are typically defined by the investigator. Items c) and d) are often obtained using tracer-injection methods.

3) Computer requirements:

Executable versions of the model are available for personal computers (DOS, Win 3.1, Win 95, Win NT, Linux) and Unix workstations (Sun-OS, Sun-Solaris, IBM-AIX, DEC, DG-UX). Source code for compilation under other operating systems is also available.

4) Availability:

Via ftp or www: http://webserver.cr.usgs.gov/otis

4.1) Costs:

Cost Category 1: free of charge

5) Assessment:

5.1) Level of competency required:

General understanding of stream transport processes, the advection-dispersion equation, and finite-difference numerical methods.

5.2) Keywords for task-based search:

solute transport, tracer, streams, transient storage, first-order loss, sorption, parameter estimation, nonlinear regression

5.3) Application algorithms and main mathematical limitations:

Spatial derivatives in governing equations are approximated using standard finite difference methods. Resulting equations are solved using the Crank-Nicolson method as described by Runkel and Chapra (Water Resources Research, 1993, 1994). Mathematical limitations associated with solution scheme are well-documented (i.e. numerical constraints increase for highly advective systems).

5.4) How widely is the model used and how well is it established in the industry:

Established method for quantifying instream mixing based on tracer- injection data in streams and small rivers. Used extensively by stream ecologists to document stream/hyporheic zone interactions.

5.5) Related References:

Primary documentation:

Runkel, R.L., 1998, One dimensional transport with inflow and storage (OTIS): A solute transport model for streams and rivers: U.S. Geological Survey Water-Resources Investigation Report 98-4018. 73 p.

other:

Bencala, K.E., 1983, Simulation of solute transport in a mountain pool-and-rifle stream with kinetic mass transfer model for sorption, Water Resources Research, v. 19, no. 3, p. 732-738.

Bencala, K.E. and R.A. Walters, 1983, Simulation of solute transport in a mountain pool-and-rifle stream: a transient storage model, Water Resource Research, v. 19, no. 3, p. 718-724.

Broshears, R.E., K.E. Bencala, B.A. Kimball, and D.M. McKnight, 1993, Tracer-dilution experiments and solute-transport simulations for a mountain stream, Saint Kevin Gulch, Colorado, U.S. Geological Survey, Water Resource Invest., 92-4081.

Donaldson, J.R. and Tryon, P.V., 1990, User's guide to STARPAC the standards time series and regression package: Nat. Inst. Stand. Tech. Internal Report NBSIR 86-3448.

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5.6) Links to organisations:

http://webserver.cr.usgs.gov/otis

5.7) Range of applications:

Morrice, J.A., H.M. Valett, C.N. Dahm, and M.E. Campana, 1997, Alluvial Characteristics, Groundwater-surface water exchange and hydrological retention in headwater streams, Hydrological Processes, v. 11, p. 253 - 267.

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Harvey, J.W., and Fuller, C.C., 1998, Effect of enhanced manganese oxidation in the hyporheic zone on basin-scale geochemical mass balance: Water Resources Research, v. 34, no. 4, p. 623-636.

Laenen, A., and Bencala, K. E., 1997, Transient storage assessments of dye-tracer injections in the Willamette River Basin, Oregon [Abstract] : American Society of Limnology and Oceanography Annual Meeting, February 10-14, Santa Fe, NM

Runkel, R.L., McKnight, D.M., and Andrews E.D., 1998, Analysis of transient storage subject to unsteady flow: Diel flow variation in an Antarctic stream: Journal of North American Benthological Society, v. 17, no. 2, p 143-154.

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6) Case study:

see 5.7 above.

MODEL: **PHREEQC Version 1.6 (1998)**
Model type: **Geochemical Speciation**
EVALUATED BY: **Susan Wadley, University of Natal, Durban.**
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1) Description:

PHREEQC is a multipurpose geochemical program that can perform speciation, inverse, reaction-path, and one dimensional advective reaction-transport modeling. It was written by the US Geological Survey in 1995. It is derived from the Fortran program PHREEQE, but has been completely rewritten in C with the addition of many new capabilities. PHREEQC runs under DOS or Windows.

PHREEQC is based on an ion-association aqueous model and has capabilities for:
(1) Speciation and saturation-index calculations,
(2) Reaction-path and advective-transport calculations involving specified irreversible reactions, mixing of solutions, mineral and gas equilibria, surface-complexation reactions, and ion-exchange reactions, and
(3) Inverse modeling, which finds sets of mineral and gas mole transfers that account for composition differences between waters, within specified compositional uncertainties.

A Windows-based graphical user interface PHREEQC called Phreeqcl is also available. Phreeqcl provides the capability to generate and edit input data files, run simulations, and view text files containing simulation results, all within the framework of a single interface. Interactive access to all of the capabilities of PHREEQC is available with Phreeqcl. The interface is written in Visual Basic and will run on personal computers under the Windows(3.1), Windows95, and Windows NT operating systems.

A computer code called PHRQCGRF has been written to create a variety of graphs from the data generated by PHREEQC. The output data from PHREEQC may be plotted against distance, time, or other data listed in the PHREEQC selected output file, and a series of data versus distance graphs can be animated. PHRQCGRF can also extract the data of interest from the PHREEQC transport results and write the data sets to an external file.

2) Data requirements:

The data needed to run PHREEQC generally consists of a chemical analysis of the water sample to be modeled giving total dissolved concentrations for the components of interest, and other relevant measurements for the system like the pH, pe, and/or the partial pressure of one or more gases.

If suitable data is not present in one of the databases for the system of interest, then additional data must be added by editing the relevant database.

2.1) Inventory of data sources:

General thermodynamic data:

- Baes C.F., Mesmer R.E., 1976, The Hydrolysis of Cations, John Wiley and Sons Inc., New York.
- Bard A.J., Parsons R. and Jordan J., 1985, Standard Potentials in Aqueous Solution, Marcel Dekker Inc., New York, ISBN 0-8247-7291-1.
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- Charlot G., Collumeau A. and Marchon M.J.C., 1971, IUPAC Selected Constants : Oxidation-Reduction Potentials of Inorganic Substances in Aqueous Solution, Butterworths, London.
- Chase M.W., Davies C.A., Downey J.R., Frurip D.J., McDonald R.A. and Syverud A.N., 1985, The JANAF Thermochemical Tables, 3rd Edition, J. Phys. Chem. Ref. Data, Supplement No. 1 to Volume 14, American Chemical Society, Washington, D.C., 2 Volumes, 1896 pages.
- Dana E.S. and Ford W.E., 1922, A Textbook of Mineralogy, Third Edition, John Wiley and Son's Inc. London.
- Deer W.A., Howie R.A. and Zussman J., Rock Forming Minerals, Volume 1 to 5, Longmans, London.
- Garrels R.M. and Christ C.L., 1965, Minerals, Solutions and Equilibria, Harper and Row Publishers Inc., New York.
- Garrels R.M. and Christ C.L., 1965, Solutions, Minerals, and Equilibria, Freeman, Cooper and Co., San Francisco.
- Hogfeldt E., 1982, Stability Constants of Metal-Ion Complexes, Part A: Inorganic Ligands, IUPAC Chemical Data Series, No. 21, Pergamon Press, Oxford.
- Horvath A.L., 1985, Handbook of Aqueous Electrolyte Solution : Physical Properties, Estimation and Correlation Methods, Ellis Horwood Ltd, Chichester, ISBN 0-85312-894-4.
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- Martell A.E. and Smith R.M., 1974, Critical Stability Constants, Volume 1, Amino Acids, Plenum Press, New York.
- Martell A.E. and Smith R.M., 1974, Critical Stability Constants, Volume 5, First Supplement, Plenum Press, New York.
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- Oelkers E.H., Helgeson H.C., Shock E.L., Sverjensky D.A., Johnson J.W. and Pokrovskii V.A., 1995, Summary of the Apparent Standard Partial Molar Gibbs Free Energies of Formation of Aqueous Species, Minerals, and Gases at Pressures 1 to 5000 Bars and Temperatures 25 to1000 oC, J. Phys. Chem. Ref. Data, Vol. 24, No. 4, pp. 1401 - 1560.
- Perrin D.D., 1965, Dissociation Constants of Organic Bases in Aqueous Solutions, London, Butterworths.

- Perrin D.D., 1972, Dissociation Constants of Organic Bases in Aqueous Solutions: Supplement, London, Butterworths. (IUPAC Chemical Data Series No. 12, 1972, Pergamon, Oxford).
- Perrin D.D., 1979, Stability Constants of Metal-Ion Complexes, Part B: Organic Ligands, IUPAC Chemical Data Series, No. 22, Pergamon Press, Oxford.
- Perrin D.D., 1982, Ionisation Constants of Inorganic Acids and Bases in Aqueous Solutions, 2nd Edition, IUPAC Chemical Data Series, No. 29, Pergamon Press, Oxford.
- Pourbaix M., 1966, Atlas of Electrochemical Equilibria in Aqueous Solutions, Pergamon Press.
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- Smith R.M. and Martell A.E., 1974, Critical Stability Constants, Volume 2, Amines, Plenum Press, New York.
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- Wagman D.D. , Evans W.H., Parker V.B., Schumm R.H., Halow I. , Bailey S.M., Churney K.L. and Nuttall R.L., 1982, The NBS Tables of Chemical Thermodynamic Properties: Selected Values for Inorganic and C1 and C2 Organic Substances in SI Units., J. Phys. Chem. Ref. Data, Supplement No. 2 to Volume 11, pp. 394.
- Woods T.L. and Garrels R.M., 1987, Thermodynamic Values at Low Temperature for Natural Inorganic Materials; An Uncritical Summary, Oxford University Press, Oxford.

3) Computer requirements:

Versions of PHREEQC are available to run on a UNIX machine or on a PC operating under DOS. An IBM-compatible PC, 486 or higher, with math coprocessor and at least 2 MB of memory is required.

For speciation, initial exchange composition, initial surface composition, and simple mixing and chemical reaction calculations, the program will run in seconds on 486 and faster machines. Large inverse calculations may take several minutes to complete. Transport calculations may take minutes to hours depending on the number of the cells and the complexity of the chemistry that is simulated.

4) Availability:

The model can be obtained from:
U.S. Geological Survey
Hydrologic Analysis Software Support Program
437 National Center
Reston, VA 20192
E-mail: h2osoft@usgs.gov

The PHREEQC software (Version 1.6, 1998) and user's guide (in Portable Document Format and PostScript format) are available from:
http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/

An older version (Version 1.04, 1995) is available from:
http://water.usgs.gov/software/phreeqc.html

The graphical user interface, PhreeqcI (Version 1.03, 1997), is available from:
http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqci/

The software for creating graphs, PHRQCGRF, is available from:
http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phrqcgrf.

4.1) Costs

Model and documentation are downloadable free of charge from the Internet.

5) Assessment:

The features found in PHREEQC which are not found in PHREEQE include the following capabilities:

(1) Use of redox couples to distribute redox elements among their valence states in speciation calculations;
(2) Modeling of ion-exchange and surface complexation reactions;
(3) Modeling of reactions with a fixed-pressure, multicomponent gas phase;
(4) Calculation of the mass of water in the aqueous phase during reaction and transport calculations;
(5) Keeping track of the moles of minerals present in the solid phases and determine automatically the thermodynamically stable phase assemblage;
(6) Simulation of advective transport in combination with PHREEQC's reaction-modeling capability; and
(7) Doing inverse modeling calculations that allow for uncertainties in the analytical data.

The construction of the input file is improved through the use of a simplified approach to redox reactions, which includes explicit mole-balance equations for hydrogen and oxygen; the use of a revised input that is modular and completely free format; and the use of mineral names and standard chemical symbolism rather than index numbers. The use of C eliminates nearly all limitations on array sizes, including numbers of elements, aqueous species, solutions, phases, and lengths of

character strings. A new equation solver that optimizes a set of equalities subject to both equality and inequality constraints is used to determine the thermodynamically stable set of phases in equilibrium with a solution. A more complete Newton-Raphson formulation, master-species switching, and scaling of the algebraic equations reduce the number of failures of the numerical method in PHREEQC relative to PHREEQE.

This program is excellent for speciation, mixing, mineral equilibration, ion-exchange, surface complexation, and reaction modeling. It also has the capability to include any of these types of chemical calculations in a one-dimensional advective transport system. This transport capability is simple and relatively fast, so it is appropriate for initial investigations of the chemistry of a dynamic system, before effort is expended on an expensive multidimensional, multicomponent transport model. However, the program lacks true kinetics and the capability to model dispersion.

PHREEQC has the following advantages over other speciation software:

(1) The capability to estimate the diffuse-layer composition in surface complexation calculations is unique among generally available codes.
(2) The use of uncertainty in inverse modeling is unique to this code.
(3) The code may also serve well as a geochemical module for coupled reaction and transport models.

This program supersedes PHREEQE, but not PHRQPITZ, which is based on a specific interaction aqueous model. PHREEQC has all of the capabilities of WATEQ4F and the WATEQ4F database is included on the distribution disk. The use of uncertainties in inverse modeling makes it a valuable companion to the NETPATH code.

5.1) Level of competency required:

The user must be familiar with the concepts involved in geochemical speciation and should preferably have had some experience in using simpler software such as MINTEQA2 or MINEQL+.

PHREEQC has several thermodynamic databases, so the user needs to have a good idea of which of these is most suited to their application. PHREEQC is more versatile than MINTEQA2 and MINEQL+.

PHREEQC has become more user-friendly since the inclusion of the graphical user interface Phreeqcl.

5.2) Keywords:

PHREEQC, PHREEQE, PHRQPITZ, PHRQCGRF, speciation, geochemistry, advection, migration, chemical reactions, environmental transport

5.3) Applicable algorithms and main mathematical limitations:

For speciation, reactions, and transport calculations, the PHREEQC code solves a reduced set of simultaneous non-linear equations that define equilibrium between the various phases in the chemical system: water, solutes, gases, minerals, ion-exchangers and surface-complexers. Equilibrium is based on an ion-association model for the aqueous phase and mass-action equations for the minerals, gases, ion-exchangers, and surface-complexers.

The complete set of equations includes:

- A mole balance equation for each element in the system;
- Mass-action equations for each aqueous species, gas component, mineral, exchange species, and surface complex;
- An activity coefficient equation for each aqueous species;
- A charge balance-equation for the aqueous phase;
- A charge-balance or charge-potential equation for each surface complexer;
- An equation for the activity of water; and
- An equation for the ionic strength of a solution.

Subsets of this set of equations are solved for a particular geochemical calculation. The equations are solved by a modified Newton-Raphson calculation. The modification involves the use of an optimization routine based on linear programming. During the iterative Newton-Raphson process, some of the equations are included as objective functions rather than strict equalities. This approach is useful for determining the stable set of minerals and the presence or absence of a gas phase in a chemical system. It also makes the numerical algorithm more robust.

The solution to the equations provides:

- The activities and molalities of each aqueous species, and
- The moles of each mineral, gas component, exchange species, and surface species present in the system.

In inverse modeling, one aqueous solution is assumed to react with minerals and gases to produce the observed composition of a second aqueous solution. The inverse model calculates the amounts of these gases and minerals from the difference in elemental concentrations between the two aqueous solutions. It is also possible to determine mixing fractions for two or more aqueous solutions and the mole transfers of minerals necessary to produce the composition of another aqueous solution. Inverse modeling is based strictly on a mole-balance approach and does not rely on the ion-association model except to determine the total number of moles of each element and redox state in each aqueous solution. The inverse model is formulated including uncertainty in each analytical datum.

A linear set of equations is formulated including:

- Mole balance for each element and element redox state in the system,
- A charge-balance equation for each aqueous solution, and
- A water-balance equation.

In addition, inequality constraints are included to ensure that any adjustments to the analytical data are smaller than the uncertainties and to constrain the sign of mole transfers of mineral (if specified). The system of equalities and inequalities is solved by an optimization routine based on the Simplex method. An additional algorithm is used to find all sets of minerals that are feasible solutions to the inverse problems.

PHREEQC is a general geochemical program and is applicable to many hydrochemical environments. However, several limitations need to be considered:

(1) PHREEQC uses ion-association and Debye-Hückel expressions to account for the non-ideality of aqueous solutions. This type of aqueous model is adequate at low ionic strength but may break down at higher ionic strengths (in the range of seawater and above). An attempt has been made to extend the range of applicability of the aqueous model through the use of an ionic-strength term in the Debye-Hückel expressions. These terms have been fitted for the major ions using chloride mean-salt activity-coefficient data. Thus, in sodium chloride dominated systems, the model may be reliable to higher ionic strengths. For high ionic strength waters, the specific interaction approach to thermodynamic properties of aqueous solutions should be used (e.g. Pitzer equations).

(2) There is a lack of internal consistency in the data in the database for aqueous solutions. Most of the log K's and enthalpies of reaction have been taken from various literature sources. No systematic attempt has been made to determine the aqueous model that was used to develop the log K's or whether the aqueous model defined by the current database file is consistent with the original experimental data. Hence, careful selection of aqueous species and thermodynamic data is left to the users of the program.

(3) The ion exchange model assumes that the thermodynamic activity of an exchange species is equal to its equivalent fraction. Other formulations use other definitions of activity, mole fraction for example, or additional activity coefficients to convert equivalent fraction to activity. No attempt has been made to include other or more complicated exchange models. In many field studies, ion-exchange modeling requires experimental data on material from the study site for appropriate model application.

(4) PHREEQC incorporates the Dzombak and Morel diffuse double-layer and a non-electrostatic surface-complexation model. Other models, including isotherms and triple- and quadruple-layer models have not been included in PHREEQC.

(5) Theoretical problems have been found with the standard state for sorbed species in the surface-complexation modeling. Other uncertainties occur in determining the number of sites, the surface area, the composition of sorbed species, and the appropriate log K's. In many field studies, surface-complexation modeling requires experimental data on material from the study site for appropriate model application.

(6) The capability of PHREEQC to calculate the composition of the diffuse layer (-diffuse_layer option) is ad hoc and should be used only as a preliminary sensitivity analysis.

(7) PHREEQC tries to identify input errors, but it is not capable of detecting some physical impossibilities in the chemical system that is modeled. For example, PHREEQC allows a solution to be charge balanced by addition or removal of an element. If this element has no charged species or if charge

imbalance remains even after the concentration of the element has been reduced to zero, then the numerical method will appear to have failed to converge. Other physical impossibilities that have been encountered are:
i) when a base is added to attain a fixed pH, but in fact an acid is needed (or vice versa) and
ii) when noncarbonate alkalinity exceeds the total alkalinity given on input.

(8) Inclusion of uncertainties in the process of identifying inverse models is a major advance. However, the numerical method has shown some lack of robustness due to the way the solver handles small numbers. The option to change the tolerance used by the solver is an attempt to remedy this problem. In addition, the inability to include isotopic information in the modeling process is a serious limitation.

5.4) How widely the model is used:

PHREEQE was written in 1980 and has been widely. Due to its advantages over PHREEQE, PHREEQC has probably been used more than PHREEQE since its release in 1995.

5.5) Related references:

- Appelo, C.A.J, 1994, Cation and proton exchange, pH variations, and carbonate reactions in a freshening aquifer: Water Resources Research, v. 30, no. 10, p. 2793-2805.
- Appelo, C.A.J., 1994. Some calculations on multicomponent transport with cation exchange in aquifers. Ground Water, v. 32, p. 968-975.
- Appelo, C.A.J. and Beekman, H.E., 1992, Hydrochemical modeling of a seawater diffusion profile, Lake Yssel, The Netherlands. in: Water-Rock Interaction, Kharaka and Maest (eds), Balkema, Rotterdam, ISBN 90 5410 075 3, p. 205-208.
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- Parkhurst, D.L., 1997, Geochemical mole-balance modeling with uncertain data: Water Resources Research, v. 33, no. 8, p. 1957-1970.
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- Postma, D., Boesen, C., Kristiansen, H. and Larsen, F., 1991. Nitrate reduction in an unconfined sandy aquifer: water chemistry, reduction processes, and geochemical modeling. Water Resour. Res. 27, 2027-2045.
- Van Breukelen, B.M., Appelo, C.A.J., and Olsthoorn, T.N., 19xx, Hydrogeochemical transport modelling of 24 years of Rhine water infiltration in the dunes of the Amsterdam water supply: submitted to Journal of Hydrology.
- Vrabel, Joseph, and Glynn, P.D., 1998, User's guide to PHRQCGRF- A computer program for graphical interpretation of PHREEQC geochemical transport simulations: U.S. Geological Survey Open-File Report 98-281, 30 p.

5.6) Links to organizations:

US Geological Survey, USA: PHREEQC
(http://h2o.usgs.gov/software/phreeqc.html)

National Water Research Institute, Canada: Extension of
Geochemical Modelling Techniques to Brines: Coupling of the Pitzer Equation to
PHREEQE (http://gw2.cciw.ca/gwrp/abstracts/crowe-017.html)

5.7) Range of applications:

Combinations of the following types of reactions proceeding in a system can be modeled:

- acid/base reactions
- complexation reactions
- precipitation/dissolution reactions

- oxidation/reduction (redox) reactions
- adsorption/desorption reactions
- gas absorption reactions

In addition PHREEQC can do:
- reaction-path and advective-transport calculations
- inverse modeling

6) Case Study:

The PHREEQC user's guide contains the following 12 worked examples:
1. Speciation calculation (uranium in seawater)
2. Equilibrium with pure phases (temperature dependence of solubility of gypsum and anhydrite)
3. Mixing (groundwater and seawater)
4. Evaporation and homogenous redox reactions (rainwater)
5. Irreversible reactions (oxidation of pyrite)
6. Reaction-path calculations (dissolution of microcline follwed by precipiation of other phases)
7. Gas-phase calculations (evolution of a fixed-pressure multicomponent gas phase)
8. Surface complexation (sorption of zinc on hydrous iron oxides)
9. Advective transport and cation exchange (exchange of calcium for sodium and potassium in a cation exchange resin column)
10. Advective transport, cation exchange, surface complexation, and mineral equilibria
11. Inverse modeling (several examples of determining which mineral phases would, when dissolved, produce the observed quality of water in a system)
12. Inverse modeling with evaporation.

MODEL: **PMWIN (Processing MODFLOW for Windows)**

EVALUATED BY: **Gerrit van Tonder, University of the Orange Free State**
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1) Description:

Processing Modflow for Windows (PMWIN) is an integrated system for modelling that includes:

- Groundwater flow and solute transport with the USGS groundwater flow model MODFLOW (McDonald, *et al.*, 1988);
- The particle tracking model PMPATH (Chiang, *et al.*, 1994);
- The solute transport model MT3D (Zheng, 1990); and
- The parameter estimation program PEST (Doherty, *et al.*, 1994).

MODFLOW can simulate the effects of wells, rivers, drains, head-dependent boundaries, recharge and evapotranspiration. PMWIN also supports the simulation of cut-off walls and the calculation of subsidence of the ground surface due to changes of hydraulic heads.

The particle-tracking model PMPATH can be used for the delineation of catchment area or for the calculation of groundwater paths and travel times.

The MT3D transport model can be used to simulate changes in concentration of single species miscible contaminants in groundwater considering advection, dispersion and some simple chemical reactions. The chemical reactions included in the model are currently limited to equilibrium-controlled linear or non-linear sorption and first-order irreversible decay or biodegradation.

The purpose of PEST is to assist in data interpretation and in model calibration. If there are field or laboratory measurements, PEST can adjust model parameters and/or excitation data in order that the discrepancies between the pertinent model-generated numbers and the corresponding measurements are reduced to a minimum.

2) Data requirements:

1) Geometry of the underground structure
2) Hydraulic heads, hydraulic conductivities, porosity and for transient simulations: storage coefficient.
3) (only for solute transport) Concentration of groundwater, bulk density of the soil matrix, dispersivity and distribution coefficient.
4) Other hydrological information, such as river stage, rain falls, evapotranspiration, etc.

3) Computer requirements:

Hardware:

- Personal computer running Microsoft Windows 95/98 or Windows NT 3.51 or later
- 16 MB of available memory (32MB or more recommended)

- A CD-ROM drive and a hard disk
- VGA or higher-resolution monitor
- Microsoft Mouse or compatible pointing device

Software:
A FORTRAN compiler is required if you intend to modify and compile the models MODFLOW-88, MODFLOW-96, MOC3D or MT3D. For the reason of compatibility, the models must be compiled by a Lahey Fortran compiler.

4) Availability:

Scientific Software Group
P.O. Box 23041
Washington, DC 20026-3041
Tel: +1-703-620-9214
Fax: +1-703-620-6793
Web site: http://www.scisoftware.com
Email: info@scisoftware.com

4.1) Costs:

US$ 995 and US$ 495 for Universities = Cost Category 2 (< US$2000).

5) Assessment:

5.1) Level of competency required:

PMWIN is a user-friendly, windows based program. Very easy to use.

5.2) Technical keywords to be included in task-based search:

groundwater model, flow, solute transport, inverse model, automatic calibration, particle tracking, interpolation.

5.3) Range of applications for which the model is capable:

- Simulation of steady-state and transient two and three-dimensional groundwater flow and solute transport.
- Groundwater recharge, evapotranspiration and geotechnical measures, such as drainage and cut-off wall; surface water bodies, such as river, open channel and reservoirs can be simulated.

5.4) Applicable algorithms and main mathematical limitations:

Four algorithms can be used to solve the flow equations in MODFLOW:
- Strongly implicit procedure;
- Slice-successive over-relaxation approach;
- Preconditioned conjugate-gradient (Hill, 1990); and
- A direct solver using Gaussian elimination with an alternating diagonal equation numbering scheme.

The particle tracking model PMPATH uses a semi-analytical particle-tracking scheme developed by Pollock (1988) to calculate the groundwater paths and travel times. The MT3D transport model uses a mixed Eulerian-Lagrangian approach to the solution of the three-dimensional advective-dispersive-reactive transport equation. PEST uses the Levenberg-Marquardt method to solve the non-linear regression problem.

5.5) How widely is the model used or how well established is it in the industry:

There are more than 2,000 installations of PMWIN and maybe more than 10,000 installations of MODFLOW and MT3D world wide.

5.6) Related references:

- Chiang, W. H., 1994, PMPATH for Windows. User's manual. Scientific Software Group. Washington, DC.
- Doherty, J., L. Brebber and P. Whyte (1994), PEST - Model-independent parameter estimation. User's manual. Watermark Computing. Australia.
- Hill, M. C., 1990a, Preconditioned Conjugate-Gradient 2 (PCG2), A computer program for solving groundwater flow equations, U. S. Geological Survey, Denver.
- McDonald, M. C. and A. W. Harbaugh, 1988. MODFLOW, A modular three-dimensional finite difference ground-water flow model, U. S. Geological Survey, Open-file report 83-875, Chapter A1.
- Pollock, D. W. 1988. Semianalytical computation of path lines for finite difference models. Ground Water (26)6, 743-750.
- Zheng, C., 1990, MT3D, a modular three-dimensional transport model, S.S. Papadopulos & Associates, Inc., Rockville, Maryland.

5.7) General links to organisations:

http://www.scisoftware.com
http://ourworld.compuserve.com/homepages/w_h_chiang/

6) Case study:

PMWIN includes 20 examples. There are at least 100 practical applications alone in Germany and more than 20 in South Africa.

http://ourworld.compuserve.com/homepages/w_h_chiang/

MODEL: QUAL2E

EVALUATED BY: Dr. Andrew Bath, Ninham Shand,
ftp://ftp.shands.co.za, bath@iafrica.com

1) Description:

The enhanced stream water quality model (QUAL2E) is a steady state riverine quality model with some dynamic features. Steady state hydraulics (flows) are combined with water quality parameters that can optimally be steady-state or reflect daily variations in river flow.

QUAL2E has been used widely and is an accepted standard particularly for wasteload allocation studies of stream systems. QUAL2E is a one-dimensional (longitudinal) model for simulating well-mixed streams and small water bodies (Brown & Barnwell, 1987). A watercourse is represented as a series of piece-wise segments or reaches of steady flow. Flows are constant with time and uniform in each reach but can vary from reach to reach. QUAL2E allows simulation of point and diffuse loading, withdrawals, branching tributaries, and in-stream hydraulic structures. The model allows the simulation of 15 water quality constituents, including dissolved oxygen, BOD, temperature, algae (as chlorophyll-a), organic nitrogen, organic phosphorus, inorganic phosphorus, coliforms, a user-defined non-conservative constituent, and three user-define conservative constituents.

QUAL2E has the optional features for analysing the influence on water quality (dissolved oxygen and water temperature) of diurnal variation in meteorological data. Diurnal variation in dissolved oxygen caused by algal growth and respiration can also be simulated. QUAL2E can also be used to determine the flow augmentation requirements to meet any predetermined dissolved oxygen concentration.

QUAL2E-UNCAS is an enhanced version of the model that provides capabilities for uncertainty analysis. The uncertainty analysis capabilities include: sensitivity analysis with an option for factorially designed combinations of input variable perturbations, first order error analysis with output consisting of a normalized sensitivity coefficient matrix, and Monte Carlo simulation with summary statistics and frequency distributions of the output variables.

AQUAL2 is an interactive data preprocessor program for the QUAL2E and QUAL2EU models. AQUAL2 can be used to build input data files for either model. Q2PLOT is an interactive data postprocessor program for the QUAL2E and QUAL2EU models. This program can read output from either model (refer to FILE NAME AND CONTENT section) then display text and/or two-dimensional graphs on the monitor.

2) Data requirements:

The model input is in the form of a single control file with separate cards for:

- Simulation name and information
- Switches for flow augmentation
- Number of reaches and junctions

- Latitude and longitude of river
- Information on each river reach
- Reach Hydraulics
- Reach coefficients
- Reach Initial conditions
- Reach Incremental flows
- Meteorological information

2.1) Inventory of data sources:

- **FTP site: ftp.epa.gov/epa_ceam/wwwhtml/softdos.mtm**
- Documentation: www.epa.gov/QUAL2E_WINDOWS/metadata.txt.html
- Run-stream modifications: www.ence.umd.edu/~klbrubak/ence688d/QUAL2E.html
- General model information: www.dino.wiz.uni-kassel.de/model_db/mdb/qual2e.html
- Statistics for model: www.epa.gov/reports/objects/ostwater/arc...QUAL2E_WINDOWS/

3) Computer Requirements:

Hardware System:
Fully IBM compatible 80386, 80486, or 80586

Operating System:
DOS version 3.30 or higher. Properly configured, this model system should also work on hardware platforms with PC DOS or MS DOS versions 4.0x, 5.0x, or 6.x

Memory Manager:
Compatible with VDISK.SYS, QEMM386, MEM.SYS, RAMDRIVE.SYS, EMM386, CEMM, 386Max; compatible with DPMI, VCPI, and XMS standards

Random Access Memory:
(Approximate minimum free bytes needed to execute EXE files) 640k base (low end) memory, plus 4.3m bytes of free extended (XMS) memory and 7.0m bytes of free disk space; or, 1m byte of free extended (XMS) memory and 11.3m bytes disk space

Hard Disk Drive:
32m byte drive recommended (minimum) with 10.0m bytes free (minimum). Numerical Coprocessor: Required.

4) Availability:

The model is freely available from the Centre for environmental Assessment Modelling (CEAM) of the United States Environmental Protection Agency (EPA).

The FTP site is: ftp.epa.gov/epa_ceam/wwwhtml/softdos.mtm

The software may also be obtained from:

Center for Exposure Assessment Modeling (CEAM)
National Exposure Research Lab - Ecosystems Research Division
Office of Research and Development (ORD)
U.S. Environmental Protection Agency (U.S. EPA)
960 College Station Road, Athens, Georgia 30605-2700
Telephone: (706) 546-3549

It is recommended that the user obtains and reference the following document to operate and apply the QUAL2EU model system: *The Enhanced Stream Water Quality Models QUAL2E and QUAL2E-UNCAS: Documentation and User Manual EPA/600/3-87/007, May 1987 NTIS accession no. PB87 202 156.*

This document can be ordered from the National Technical Information Service (NTIS) at the address shown below. When ordering, use the NTIS accession number associated with the document. Contact NTIS for current price, and for shipping and handling charges.

National Technical Information Service (NTIS)
5285 Port Royal Road
Springfield, Virginia (VA); 22161
Telephone: (703) 487-4650

4.1) Costs:

Category: 1 – Free of charge.

5) Assessment:

Evaluation of applications:
The model has been used successfully to simulate the conservative and non-conservative behaviour of rivers in South Africa. The simulations include simulation of TDS, N, P, DO and *E. coli*. In each case the model has provided a rapid and efficient tool for the assessment of water quality.

Level of Expertise:
Low, the design of the model does not require a thorough knowledge of modelling, but does require some insight into water chemistry and aquatic biology.

Limitations:
The model is a steady state description of a river and can not account for variable flow conditions. To overcome this problem the model should be configured for high, medium and low flow conditions.

5.1) Level of competency required:

Low: The model has been developed for the user who is not familiar with other models and modelling protocols. It is essential that the user make careful reference to the user manual.

5.2) Keywords:

Steady state model, river reaches, dissolved oxygen, nitrogen, phosphorus, Monte Carlo Simulation, error analysis, flow augmentation,

5.3) Application algorithms and mathematical limitations:

Qual2e is a versatile stream water quality model and can simulate up to fifteen water quality constituents, these include: DO, BOD, water temperature, chlorophyll-a, organic N, ammonia, nitrate and nitrite, organic phosphorus, dissolved phosphorus, coliforms, non-conservative constituents and three conservative constituents. The model has been developed for dendritic streams that are well mixed. It assumes that the major transport mechanism, advection and dispersion, are significant along the main direction of flow (longitudinal axis of the stream). The model thus represents the river as a one-dimensional system. Qual2e allows for multiple waste discharges, withdrawals, tributaries, incremental inflows and outflows. Hydraulically, Qual2e is limited to the simulation of time periods during which both the stream flow in the river and input waste loads are constant. The model can not be used for periods of variable, river flow. The model represents the river as a series of reaches that have uniform hydraulic characteristics. Each reach is further divided into computational elements of equal length. The model can only support 25 reaches, a maximum of 20 elements per reach (with a total of 250 elements in all), a maximum of 7 headwater elements, 6 junction elements and 25 inputs.

5.4) How widely is the model used:

QUAL2E has been used widely and is an accepted standard particularly for wasteload allocation studies of stream systems. In South Africa, Ninham Shand has use the QUAL2E to model the Kuils River system.

In South Africa, the model has been used to assess the water quality of rivers, develop management plans and examine the operation of river systems.

Overseas, the model has been used for a very wide range of applications that include detailed assessment of waste-load allocations, and statistical assessments of rivers.

The References and links show the wide use of the model around the world.

5.5) Related References:

Alpaslan, N.; Harmancioglu, N.B.; Saner, E. (1994). Proposed management plan for the Yesilirmak River basin, Integrated River Basin Development. Proceedings of an International Conference,13 to 16 Sep 1994, Wallingford, United Kingdom, p 97-107 (11 pages)

Barnwell, T.O.; Brown, L.C.; Whittemore, R.C. (1987). **QUAL2E** - a Case Study in Water Quality Modeling Software, Conference, Systems Analysis in Water Quality Management. Symposium, London, 1987, Ed. M.b. Beck; Advances in Water Pollution Control 1987, P 377-387 (11 Pages)

Brown, L.C. and Barnwell, T.O. (1987). The Enhanced Stream Water Quality Models QUAL2E and QUAL2E-UNCAS: Documentation and User Manual EPA/600/3-87/007, May 1987. NTIS accession no. PB87 202 156

Chaudhury, R.R.; Sobrinho, J.A.H. (*); Wright, R.M.; Sreenivas, M. (1998). Dissolved oxygen modeling of the Blackstone River (northeastern United States). Water research, vol 32, no 8, p 2400-2412 (13 pages)

Cubillo, F.; Rodriguez, B.; Barnwell, T.O. Jr (1992). A system for control of river water quality for the community of Madrid using **QUAL2E**, Water Quality International '92. Proceedings of the Sixteenth Biennial Conference. Part 4, 24 to 30 May 1992, Washington DC, USA, Water science and technology, vol 26, no 7-8, p 1867-1873 (7 pages)

Ninham Shand (1993). Water quality assessment of the Kuils River, Report to the Western Cape Regional Services Council, by Ninham Shand Cape Town.

Ninham Shand (1998). Metropolitan Open Space System, Water quality assessment of the Kuils River, report to the Cape Metropolitan Council, by Ninham Shand Pty Ltd, 1998, Cape Town.

Rossouw, J.N.; Quibell, G. (1993). Simulation of nutrient and algal growth dynamics in the middle Vaal River, Proceedings of the Sixth South African National Hydrological Symposium. Hydrology in Developing Regions - The Road Ahead. Volume 2, 8 to 10 Sep 1993, Pietermaritzburg, South Africa, p 589-596 (8 pages).

Truax, D.D.; Shindala, A.; Kin, K.-R. (1992). Development of a water quality model for the upper Tennessee-Tombigbee waterway, Twenty-second Mississippi Water Resources Conference. Proceedings 14 to 15 Apr 1992Jackson, Mississippi, USA, p 14-23 (10 pages), Mississippi State University, Water Resources Research Institute, PO Drawer AD, Mississippi State, MS 39762, USA

Venter, S.N.; Steynberg, M.C.; De Wet, C.M.E.; Hohls, D.; Du Plessis, G.; Kfir, R. (1997). A situational analysis of the microbial water quality in a peri-urban catchment in South Africa, Health Related Water Microbiology 1996. Selected Proceedings of the IAWQ Eighth International Symposium, 6 to 10 Oct 1996,Mallorca, Spain, Water science and technology, vol 35, no 11-12, p 119-124 (6 pages).

Wagner, R.A.; Tisdale, T.S.; Zhang, J. (1996). A framework for phosphorus transport modeling in the Lake Okeechobee watershed, Water resources bulletin, vol 32, no 1, p 57-73 (17 pages).

5.6) Links to other Organizations:

www.hec.usace.army.mil/
www.usace.army.mil

5.7) Range of applications that the model is capable of supporting:

- Wasteload allocation
- Water quality assessment
- Point source assessment
- Diffuse source impact assessment
- Ecological - nutrient study
- Stochastic analysis of water quality (Monte Carlo Simulations)
- Simple system operation to comply with predefined water quality requirement

6) Case Studies:

Barnwell *et al.* (1987) undertook a documented case study of the model. In South Africa, the model has been used to assess water quality in the following river systems:

- Kuils River to assess the changes in quality along the length of the main channel and develop a management strategy for the lower section of the river (NS, 1993; NS, 1998).
- Mzintlava River to assess the influence of the Kokstad treated effluent on the quality of the river (DWAF, 1998)
- Vaal River system to assess the nutrient and algal growth potential of the Middle Vaal River (Rossouw & Quibell, 1993).
- Rietspruit, to assess the microbiological quality of a peri-urban catchment (Venter *et al.*, 1997)

Overseas, the model has been used to assess:

- The dissolved oxygen regime of the Blackstone River (Chaudhury et al., 1998)
- Development of a model for the Tennessee-Tombigdee Waterway (Traux et al., 1992)
- Phosphorus transport modelling in the Lake Okeechobee catchment (Wagner et al., 1996)
- Development of a catchment management plan in Turkey (Alpaslan, et al. 1994)
- System for water supply control in Madrid, Spain (Cubillo et al., 1992)

MODEL: **REMDSS - Reservoir Eutrophication Model Decision Support System**

EVALUATED BY: Nico Rossouw, Environment and Forestry Technology, CSIR, Email: nrossouw@csir.co.za

1) Description:

REMDSS - Reservoir Eutrophication Model Decision Support System, is designed to simulate the phosphorus dynamics in a reservoir. The model is mainly used to assess the impact of phosphorus control measures on eutrophication in reservoirs. The model consists of three subsystems; the first subsystem describes the relationship between phosphorus control measures in a catchment and the external loads received by a reservoir, the second subsystem describes the relationship between external phosphorus load and in the phosphorus concentrations in a reservoir and the third subsystem describes the relationship between in-lake phosphorus and indicators of algal production such as algal biomass (chlorophyll *a*).

REMDSS is a management oriented model that simulates the long-term phosphorus dynamics in a reservoir on a monthly timescale. This is a major advantage over other simpler models that assumes steady state conditions in a reservoir.

2) Data requirements:

The REMDSS model requires as input:

1. A representative time series of monthly inflows into a reservoir. This can be a historical or synthetic time series of inflows. Units (10^6 m^3/month).
2. Information on point sources of phosphate in the catchment. Data fields include point sources name, annual effluent volume (10^6 m^3/yr), TP concentration (mg/l) and % river losses between point source and the reservoir.
3. Information about the catchment such as catchment area (km^2), P export parameters, Initial TP concentration in the reservoir (□g/l) and sedimentation parameter.
4. Reservoir characteristics such as the full supply volume (10^6 m^3), dead storage volume (10^6 m^3), initial volume (10^6 m^3), reservoir volume/area parameters, mean monthly compensation releases (10^6 m^3/month), mean monthly irrigation releases (10^6 m^3/month), mean monthly rainfall (mm/month), mean monthly Symons pan evaporation (mm/month) and the monthly pan factor.

2.1) Inventory of data sources:

Monthly flow data is generally available from the Department of Water Affairs & Forestry (Directorate of Hydrology) or the WR90 Publications (Surface Water Resources if South Africa, 1990. Water Research Commission Reports 298/1/94).
Point Source data is available from local authorities or the Department of Water Affairs & Forestry (Directorate of Water Quality Management).
Catchment information are available from the WR90 publications (see above)
Reservoir information is available from the WR90 publications (see above)
Typical P export and sedimentation parameters are presented in the REMDSS Manual.

3) Computer requirements:

Personal computer, MS DOS

4) Availability:

The software and manual can be obtained from:
Nico Rossouw
Environmentek, CSIR
PO Box 395
Pretoria 0001
Tel: 012 841 4576
Fax: 012 841 2506
Email: nrossouw@csir.co.za

4.1) Costs:

The model is available free of charge.

5) Assessment:

5.1) Level of competency required:

The model user should have a basic understanding of eutrophication and simple eutrophication models.

5.2) Keywords for task-based search:

Empirical models, eutrophication, reservoirs, phosphorus, algae, chlorophyll a, water quality, eutrophication management

5.3) Application algorithms and main mathematical limitations:

The model assumes that a reservoir is fully mixed i.e. there are no horizontal or vertical gradients in the reservoir. It can therefor not simulate plug flow systems.

The REMDSS model can not be used to simulate phosphorus dynamics in a small reservoir or weir where the water residence time is less than one week.

5.4) How widely is the model used and how well is it established in the industry:

Examples where the REMDSS model has been used in South Africa to assess the impacts of eutrophication control measures, include:

Rossouw, J.N. (1988). *Evaluation of the impact of eutrophication control measures on water quality in Rietvlei Dam.* Report to the Directorate of Water Pollution Control, Department of water Affairs. Similar reports were compiled for Harbeespoort Dam, The Umgeni River System, Vaal Dam, Bloemhof Dam, and the middle Vaal River.

Grobler, D.C., Rossouw, J.N., van Eeden, O. and Oliveira, M. (1987). Decision support system for selecting eutrophication control strategies. In: Systems analysis in water quality management. Edited by Beck, M.B., Pergamon Press, Oxford.

Grobler, D.C. and Rossouw, J.N. (1989). Application of a Decision Support System to develop phosphorus control strategies for South African reservoirs. In: Water Quality Modelling, Volume IV: Decision Support Techniques for Lakes and Reservoirs. Edited by Henderson-Sellers, G. CRC Press, Boca Raton.

5.5) Related References:

Rossouw, J.N. (1990). *The Development of Management Oriented Models for Eutrophication Control*. WRC Report No 174/1/90. Water Research Commission.

Rossouw, J.N. and Kelly, H. (1989). *REMDSS - A decision support system for eutrophication control. User's manual*. Division of Water Technology, CSIR.

Rossouw, J.N. and Kelly, H. (1989). Decision Support System for Water Quality Management. SA Journal of Science, 85:415,423.

Grobler, D.C.S.D. (1985). *Management-oriented eutrophication models for South African Reservoirs*. PhD Thesis. University of the Orange Free State.

5.6) Links to organisations:

Environmentek/CSIR web site (Not on the site yet)

5.7) Range of applications:

Assessment of the impact of phosphorus control measures on eutrophication related water quality in reservoirs.

6) Case study:

The REMDSS model was applied to assess the impact of the effluent phosphate (P) standard of 1.0 mg P/L that was introduced in seven sensitive catchments to control eutrophication. The standard was implemented in the Vaal Dam, Barrage, Roodeplaat Dam and Hartbeespoort Dam catchments only. The effectiveness of standard was reviewed in 1988 for the Department of Water Affairs & Forestry based on predictions of the impact of the standard and monitoring results.

In the case of Hartbeespoort dam, REMDSS was used to predict the in-lake TP concentrations in Hartbeespoort Dam, for different time horizons, using three point source control scenarios:

- A "Do nothing" scenario which predicted the impact if the concentrations in the point source effluents were maintained at 1988 concentrations,
- A 1 mg P/l standard scenario which predicted the impact of enforcing the existing 1.0 mg P/l effluent standard on all the point sources in the catchment,

- A 0.1 mg P/l standard scenario which predicted the impact of enforcing a stricter standard of 0.1 mg P/l on all the point sources in the catchment.

From the predicted in-lake TP and chlorophyll *a* concentrations, it was concluded that:

1. The 1 mg P/l effluent standard would reduce reservoir TP and chlorophyll concentrations by about 50% but that the predicted chlorophyll concentration would still result in nuisance conditions being experienced for 50% of the time. It was recommended, that as a starting point, the 1 mg P/l standard be adhered to in the Hartbeespoort Dam catchment,
2. It was predicted that a stricter effluent standard of 0.1 mg P/l would result in chlorophyll concentrations which border on nuisance conditions. It was recommended that a stricter standard than the present 1 mg P/l standard be considered for implementation as soon as possible.

Rossouw, J.N. and Grobler, D.C. (1988). *Evaluation of the impact of eutrophication control measures on water quality in Hartbeespoort Dam*. Report to the Department of Water Affairs, Pretoria.

MODEL: **CE-QUAL-RIV1**
EVALUATED BY: *Dr. Andrew Bath, Ninham Shand*
ftp://ftp.shands.co.za, bath@iafrica.com

1) Description:

The Waterways Experimental Station model CE-QUAL-RIV1 is a fully dynamic one-dimensional flow and water quality simulation model for rivers and streams (USACE Waterways Experimental Station 1990). The original version of the model was developed at the Ohio State University for the Environmental Protection Agency (Bedford et al., 1983), primarily for predicting water quality associated with storm water runoff. The present version of the model has been modified to include control structures. The model is designed for analysing highly unsteady stream flow conditions, such as those associated with peaking hydropower tail waters. The model also allows simulation of branched river systems with multiple control structures, such as flow regulation dams, navigation locks, and impounded sections.

The model package includes two stand alone programs RIV1H and RIV1Q. These programs can be run together or separately. RIV1H performs the hydraulic routing based on a numerical solution of the full St. Venant Equations. The program solves the time and space distribution of river flow, cross-sectional area, top width and water depth. When complete, these calculations are stored for use in RIV1Q .

RIV1Q is the water quality program. The model is similar to QUAL2E in that it simulates temperature, dissolved oxygen, BOD, nutrient kinetics, iron, manganese and coliform bacteria. The difference between the models QUAL2E and CE-QUAL-RIV1 is that RIV1 is fully hydrodynamic and can simulate sharp changes in river flow and water quality constituent concentration.

2) Data requirements:

Input to RIV1Q includes four files: execution control file, main control file, time varying boundary conditions, and lateral inflows.

Input to RIV1H includes eight cards: title description, grid card, specification of constants, initial conditions, boundary conditions, time step and boundary specification information.

2.1) Inventory of data sources:

Riverine Water Quality Models. U.S. Army Corps of Engineers, Waterways Experiment Station| Environmental Laboratory
URL: http://www.wes.army.mil/el/elmodels/riveinfo.html

3) Computer requirements:

The minimum requirements to run the model include a 80486 personal computer equipped with a math coprocessor. A minimum of 2 MB RAM is required unless the user has an operating system that uses virtual memory. A hard disk with a minimum

space of 10 MB is also required for each application of the model. The model is provided with executable code as well as the source FORTRAN code.

4) Availability:

The model is available from the US Army Engineers Waterways Experimental Station (WES), or from contacting the above organization at:

Environmental Laboratory: Waterways Experimental Station
US Army Corps of Engineers
3909 Halls Ferry Road
Vicksburg MS 39180-6199

Telephone: (601) 634 3670
Fax: (601) 634 3129

The model and documentation can be obtained by contacting the above organization. The computer source code and documentation can be copied without restriction.

4.1) Costs:

Cost Category: 1 – free of charge

5) Assessment:

In South Africa, the model has been tested using the flow and quality data for the Berg River, Western Cape. No documented applications using South African data sets could be found in the literature.

5.1) Level of competency required:

High user competency: the model requires experience in:

- Development of the necessary input files (using a text editor);
- Configuration of the model for a water body;
- Water chemistry;
- Data infilling procedures to convert from discrete to daily sequence of input data;
- Assessment of model output; and
- Model output visualization

5.2) Keywords:

one-dimensional, dynamic river transport model, control structures, water temperature, BOD, TDS, dissolved oxygen, Nitrogen, Phosphorus, Iron, Manganese, Coliform bacteria

5.3) Application algorithms and main mathematical limitations:

The transport of momentum and water quality constituents during periods of unsteady flows can be marked by sharp gradients in flow, elevation, and water quality constituents. These gradients can be propagated by the flow through regions of highly variable cross-section intermittently joined by inflowing tributaries as well as point

and diffuse sources. Since the speed of the flow waves is high, water quality concentrations can be dominated by advective transport rather than biogeochemical processes and diffusion. The water quality model has to be dynamic and have the following features to be able to provide adequate simulation of the transient effects in rivers during periods of unsteady flow.

- Account for time varying flow, elevation, and water quality constituent changes resulting from unsteady flow;
- Applicable to a channel of arbitrary cross section and specified bed slope;
- Allow for a number of water quality constituents and their interactions;
- Account for lateral inputs to the main river channel; and
- Allow for hydraulic structures.

The hydrodynamic program RIV1H uses a derivation of the St. Venant Equation and includes routines for: conservation of mass, conservation of momentum, and modification of momentum and continuity. The numerical solution for flow and elevation is solved using a four point implicit method first used by Piessmann (1961) with a Newton-Raphson iteration procedure.

For constituent transport, the fourth order explicit scheme developed by Holly and Piessmann (1978) is used for the mass transport along the river.

The model is one-dimensional in the downstream direction, and is unable to simulate flows in the upstream direction (such as those in estuaries and man-made control structures).

The model has no graphical user post processor, so that the user must adapt an existing piece of code, or develop new software.

5.4) How widely is the model used:

Extensive use in the United States by the Corps of Engineers. The main applications are involved with the assessment of releases from hydro-electric schemes on the downstream river quality.

5.5) Related References:

Bedford, K.W., Sykes, R.M., & Libicki, C. (1983). Dynamic advective water quality model for rivers, Journal of Environmental Engineering Division, Amercian Society of Civil Engineers, vol 109, no.3, 1983.

Holly, F.M. and Piessmann, A. (1978). Accurate calculation of transport in two dimensions, Journal, Hydraulics Division, ASCE, vol 103, number HY11, pp1259-1277.

Piessmann, A (1961). Propagation des intumescences dans les canaux et rivieres, First congress of the calculation society of France, Grenoble, pp 433-442.

Wurbs, R.A. (1995). Water management models, a guide to software, Prentice Hall PTR, Englewood Cliffs, New Jersey 07632.

5.6) Links to Organizations:

National Nutrient Assessment Strategy: An Overview of Available Endpoints and Assessment Tools. Models and methods for catchments, rivers, reservoirs and estuaries
URL: www.epa.gov/owowwtr1/NPS/proceedings/overview.html

Pollution Prevention and Abatement Handbook, World Bank, 1997.
URL: http://www-esd.worldbank.org/pph/part2/Water1.htm

5.7) Range of applications:

The model is capable of supporting applications where the user requires information on:

- BOD;
- Water temperature;
- Dissolved oxygen;
- Nitrogen kinetics;
- Phosphorus kinetics;
- Algal growth;
- Iron and Manganese; and
- Coliform bacteria

Thus, the model can be used to assess:

- The movement of constituents along a river;
- The impact of point and diffuse sources;
- Wasteload allocations;
- Eutrophication assessment; and
- Ecological conditions in rivers and effects of upstream changes in river flow.

6) Case Studies:

The model was originally developed at Ohio State University for the US Environmental Protection Agency for predicting water quality associated with storm water runoff. The model was revised during the 1980's by Ohio State University and the USACE Waterways Experimental Station (WES). The current version has been tested and applied to numerous studies by WES in the United States.

MODEL: WASP

EVALUATED BY: ***Dr. Andrew Bath, Ninham Shand***
ftp://ftp.shands.co.za, bath@iafrica.com

1) Description:

The Water Quality Analysis Simulation Program (WASP) is maintained by the Environmental protection Agency, is a generalized modelling framework for simulating aquatic systems, including rivers, reservoirs, estuaries and coastal waters. The various versions of the model developed evolved from the original WASP (di Toro *et al.*, 1983). The current version of the program is WASP5 (Ambrose *et al.*, 1993).

WASP is designed to provide a flexible modelling system. The time varying processes of advection, point and diffuse source loading, and boundary exchange are represented in the basic program. Water quality processes are modelled in special kinetic subroutines that are either selected from a library, or supplied by the user. WASP is structured to allow easy substitution of kinetic subroutines into an overall package to form a problem specific model. A compartment modelling approach represents the aqueous system as segments, which can be arranged in one, two, or three dimensions.

WASP consists of two stand alone computer programs DYNHYD and WASP, that can be run together or separately. DYNHYD simulates the hydrodynamic movement of water, and WASP simulates the movement and interaction of contaminants within the water body. EUTRO and TOXI are sub-models, which can be incorporated within the model. The EUTRO routine is used to simulate eutrophication-related variables such as nutrients, algae, dissolved oxygen, and sediments. TOXI is used to simulate toxic substances such as metals, organics, and sediment.

Problems that have been studied using WASP include biochemical oxygen demand, dissolved oxygen dynamics, nutrients/eutrophication, bacterial contamination, and toxic chemical movement.

2) Data requirements:

The input is in a logical format divided into 10 groups, A through J:

A	-	Model Identification and Simulation Control
B	-	Exchange Coefficients
C	-	Volumes
D	-	Flows
E	-	Boundary Concentrations
F	-	Waste Loads
G	-	Environmental Parameters
H	-	Chemical Constants
I	-	Time Functions
J	-	Initial Conditions

The user defines the time step that can be from minutes to months. There is also the option of allowing the model to determine an optimum time interval.

The 8 systems for eutrophication modeling (EUTRO5) are ammonia nitrogen, nitrate nitrogen, inorganic phosphorus, phytoplankton carbon, carbonaceous BOD, dissolved oxygen, organic nitrogen, and organic phosphorus.

The 6 systems for toxicant modeling (TOXI) are chemical 1, solids fraction 1, solids fraction 2, solids fraction 3, chemical 2, and chemical 3. The model can be run in different levels of complexity. The user may choose to simulate any combination of these variables using any combination of the parameter functions and values described below.

2.1) Inventory of data sources:

FTP site for access of code and documents: ftp://ftp.epa.gov/epa_ceam/wwwhtml/wasp.htm

The URL is: http://www.epa.gov/epa_ceam/wwwhtml/products.htm

3) Computer Requirements:

Software:
The source code is written in FORTRAN 77. However, an executable file is also provided with the package. Thus, the user has the opportunity to use the executable code or make changes to the FORTRAN code and then compile the FORTRAN code. WASP has been developed for personal computer (PC) application. In the South African applications, the FORTRAN code has been compiled using the Lahey FORTRAN compiler (Görgens *et al.*, 1993).

Hardware:
The minimum configuration is a 80486 personal computer equipped with a mathematical co-processor. Ideally, WASP should be run on a Pentium with clock speed greater than 100 MHtz.

Hardware System:	Fully IBM compatible 80386 or 80486
Language:	FORTRAN 77
User Interface:	INTERACTER, version 2.0m
Operating System:	DOS version 3.30 or higher. Properly configured, the WASP model system should work on systems with PC DOS or MS DOS versions 4, 5, or 6.
DOS Extender:	Phar Lap 386/DOS-extender; bound into application EXE files with automatic virtual memory management; distributed royalty free
Memory Manager:	Compatible with VDISK.SYS, QEMM386, HIMEM.SYS, RAMDRIVE.SYS, EMM386, CEMM, 386Max; compatible with DPMI, VCPI, and XMS standards
Compiler:	Lahey FORTRAN, F77L-EM/32 version 5.01
Link Editor:	Phar Lap 386LINK version 4.1L
Storage Requirements:	(k=1,024; m=1,048,576)

RAM: (approximate minimum free bytes needed to execute EXE files) 640k base (low end) memory, and 4Mb of free extended (XMS) memory or disk space

Hard Disk Drive: (minimum) 20Mbyte drive recommended (minimum) with 6Mb free

4) Availability:

The model is available by mail at the following address

Center for Exposure Assessment Modeling (CEAM)
Environmental Research Laboratory
U.S. Environmental Protection Agency
960 College Station Road
Athens, Georgia, 30605-2720

Ordering by telephone at: (706) 546-3130, or fax at (706) 546-3340

FTP site for access of code and documents: ftp://ftp.epa.gov/epa_ceam/wwwhtml/wasp.htm

The URL is: http://www.epa.gov/epa_ceam/wwwhtml/products.htm

The latest Windows 95 version of the model has been released and includes full interactive post-processor graphics. The program is not public domain and can be obtained from: http://ascicorp.com/eed/wasp.html

4.1) Costs:

The model is supplied free of charge (Category 1). The cost of using WASP lies in the time spent setting up the model, input files and configuring the model for a particular reservoir.

5) Assessment:

WASP has been successfully used in US for numerous applications in the field of water resource and quality management. The model requires a high level of computer literacy.

5.1) Level of competency required:

WASP requires the user to be familiar with data infilling procedures, meteorological data, hydrology and system operation information, water quality simulation and model interpretation, water chemistry, and limnology. Advanced applications and changes to the code require experience in the use of text editors and compilers.

Training/ technical assistance

- For questions and/or information concerning:
- Installation and/or testing of the WASP model system and/or support programs or files, call 706/546-3524 for assistance

- WASP model system and/or program content, application, and/or theory, call 706/546-3323 for assistance
- Use of the CEAM electronic bulletin board system (BBS), contact the BBS system operator (SYSOP) at 706/546-3524
- Other environmental software products and documentation distributed through CEAM, contact the Model Distribution Coordinator at 706/546-3549
- Other support available through CEAM, contact Mr. Dermont Bouchard, CEAM Manager

Contact CEAM by mail at:

Center for Exposure Assessment Modeling (CEAM)
Environmental Research Laboratory
U.S. Environmental Protection Agency
960 College Station Road
Athens, Georgia, 30605-2720
Telephone: 706/546-3130 or fax at 706/546-3340

Alternatively, contact the CEAM BBS message menu and commands. Call the CEAM BBS 24 hours a day, 7 days a week. To access the BBS, a computer with a modem, and communication software are needed. The telephone number for the BBS is 706/546-3402. Communication parameters for the BBS are: 1200-14400 baud, 8 data bits, no parity, 1 stop bit.

Grading: High level user competency

5.2) Keywords:

River, Estuary, Reservoir, hydrodynamics, water quality, two-dimensional, eutrophication, dissolved oxygen, sediments, mixing conditions, metals, nutrients, TDS, toxics.

5.3) Algorithms and mathematical limitations:

The Toxic Chemical Model (TOXI) combines a kinetic structure adapted from the Exposure Analysis Modeling System (EXAMS) with the WASP transport structure and simple sediment balance algorithms. TOXI predicts dissolved and sorbed chemical concentrations in the bed and overlying waters.

The Eutrophication Model (EUTRO) combines a kinetic structure adapted from the Potomac Eutrophication Model with the WASP transport structure. This model predicts dissolved oxygen, carbonaceous biochemical oxygen demand, phytoplankton, carbon, chlorophyll-a, ammonia, nitrate, organic nitrogen, and orthophosphate in bed and overlying waters.

The Hydrodynamic Program (DYNHYD) is a simple link-node hydrodynamic program capable of simulating variable tidal cycles, wind, and unsteady flows. It produces an output file that supplies flows, volumes, velocities, and depths (time averaged) for the WASP modeling system.

5.4) How widely is the model used:

WASP has been successfully used in US for numerous applications in the field of water resource and quality management. The original version of WASP dates back to 1981. Various versions of the model have been applied throughout the United States. The US applications include rivers, reservoirs, estuaries and coastal areas. Problems that have been studied using WASP include biochemical oxygen demand, dissolved oxygen dynamics, nutrients/eutrophication, bacterial contamination, and toxic chemical movement. In South Africa, WASP has been used to examine the hydrodynamics of the Vaal Barrage and the water quality (nutrient and eutrophication) response of Roodeplaat Dam (Gorgens *et al.*, 1993).

5.5 Related References:

Ambrose, R.B., Wool, T.A., & Martin, J.L. (1993). The Water Quality Analysis Simulation Program, WASP5, Part A, Model Documentation, Environmental Research Laboratory, Athens, Georgia 30605.

Di Toro, D.M. et al. "Documentation for water quality analysis simulation program (WASP) and model verification program (MVP)", EPA-600/3-81-044, US Environmental Protection Agency, Duluth, Minnesota, 1983.

Görgens, A.H.M., Bath, A.J., Venter, A., de Smidt, K. & Marais, G.v.R. (1993). Applicability of hydrodynamic reservoir models for water quality management in stratified water bodies in South Africa, Report by Ninham Shand Inc. and the University of Cape Town to the Water Research Commission, Pretoria. Report number 304/1/93.

5.6) Links to other Organizations:

EPA site at: http://www.epa.gov

http://www.cee.odm.edu

http://scisoftware.com/

http://www.eos.uoguelph.ca/webfiles/james/waspreadme.html

http://www.chi.on.ca/wasp.html This site provides the manual and software

http://ascicorp.com/eed/wasp.html This site provides the latest Windows 95 version

5.7) Range of Applications the model is capable of supporting:

- Wasteload allocation

- Point source assessment
- Eutrophication response of water bodies
- Behaviour of toxic contaminants
- Mixing conditions in rivers, impoundments and estuaries
- Sediment interaction

6) Case Studies:

The model is provided with a number of example data sets, these are briefly outlined below:

- POND1.INP - Sample input data files to test the installation
- POND3SEQ.INP and demonstrate application of the TOXI model.
- SEDPOND.INP These files have also been furnished to provide
- SETPOND3.INP instruction by example. To test installation,
- TOXRIV1.INP execute the TOXI model then select these files
- TOXRIV2.INP individually as input data. These are ASCII (non-binary) text files that can be displayed on the monitor screen.
- LAKE.INP - Sample input data files to test the installation
- RIVER.INP and demonstrate application of the EUTRO model.
- T-LAKE.INP. These files have also been furnished to provide instruction by example on the use of EUTRO.
- DYNRIV.INP - Sample input data files to test the installation
- RIVERQ.INP and demonstrate application of the DYNHYD program.
- CANAL_H.INP This file has also been furnished to provide an example of the DYNHYD program.

MODEL: **WQT**

EVALUATED BY: Dr C E Herold, Stewart Scott Inc.
Email: model@ssi.co.za

3) Description:

WQT is a monthly time hydro-salinity model. It is written in modular form and combines catchment hydrology with the related salinity. This PC based model is screen-interactive, allowing the user to view statistics and plots, adjust input variables and save output files repetitively without the need to exit the program or re-read the input data.

A full description of the model is contained in the DWAF report PC000/00/9390 (Herold and Kakebeeke, 1991). The model system configuration is defined as a set of nodes (of model type SW, CR, RR, RV, DC or JN as defined below) linked together by flow links called routes. Brief descriptions of each module are given below.

*Catchment salt washoff (**SW**):* This module simulates the water and salt balance of a catchment.

*Channel reach (**CR**):* This module simulates the movement of water and salt through a channel reach, which can include a wetland area and riparian irrigation.

*Irrigation (**RR**):* This module simulates the water and salt balance of an irrigated area, which can either be riparian and dependent on a CR module, or an independently supplied irrigation scheme.

*Reservoir (**RV**):* This module simulates the water and salt balance of a reservoir, which can be a dam or a natural lake.

*Demand centre (**DC**):* This module simulates monthly effluent return flow volumes and TDS concentrations from a demand centre for which a file of monthly water requirements has been specified.

*Junction (**JN**):* The purpose of this module is simply to mix the inputs from up to five flow routes before redistributing them up to five downstream routes.

The model can handle complex river systems, including salinity feedback loops whereby part of the water supply to a demand centre can be abstracted from a reservoir that receives effluent from the same demand centre.

An important advantage of the model is that it was designed to be fully compatible with the water resource system simulation models that are used extensively by the Republic of South Africa (RSA) Department of Water Affairs and Forestry (DWAF). WQT also allows for the simulation of a feedback effect, whereby salt concentrations build up after being fed back into the upstream system of demand centres, rivers and wetlands.

The sub-models that require calibration are the catchment salt wash-off (SW) and irrigation (RR) modules. The model parameters and the function of each are fully described in the DWAF: Planning reports P C000/00/7086 (BKS and Stewart, Sviridov & Oliver, 1988) and P C000/00/9490 (Stewart, Sviridov & Oliver, 1990b).

2) Data requirements:

Data preparation consists of two main parts: creating model parameter input files and preparing the time series data files. Detailed descriptions of the preparation of both of these file types are provided in the RSA DWAF: Planning report no. P C000/00/9290 (Stewart, Sviridov & Oliver, 1990a).

Input data is required for each of the six modules listed in section 1. In addition information is required on the system structure (i.e. how the nodes and routes connect) and the solution order. The following is a summary of the data requirements.

Climatic

- Monthly rainfall time series

Physical

- Definition linkages between model nodes and routes
- Definitions of routes at which output information is to be stored
- Catchment areas (including an allowance for growth in urban and rural diffuse source inputs)
- Wetland areas (including an allowance for changes at different dates)
- Irrigation areas (including an allowance for changes at different dates)
- Channel reach details (including an allowance for river losses)
- Reservoir details (including multiple commissioning dates and dam sizing)
- Demand centre details (including optional desalination plant details and growth factors)
- Junction node details

Hydrological

- Model parameter values for each defined node
- Time series of simulated or constructed monthly catchment runoff
- Time series of observed monthly flows at observation points
- Time series of monthly point source flows entering the system
- Time series of monthly point abstraction volumes

- Time series of monthly demands on demand centres

Water Quality

- Model parameter values for each defined node
- Time series of observed monthly salt concentrations at observation points
- Time series of monthly point source salt concentrations entering the system
- Time series of monthly salt loads added to demand centre return flows

Miscellaneous

- Solution order for nodes
- Starting and ending dates

2.1) Inventory of data sources:

Most of the monthly rainfall, runoff, flow, abstraction and return flow time series are created as part of the hydrological modelling process. A detailed description of sources for this type of data is included in the write up of the WRSM90 hydrological model (a description of which is included in this Internet site). In addition it is necessary to create monthly time series files of monthly salt concentrations. The raw water quality data required to construct monthly salinity time series input data for southern African can be obtained from the Hydrological Information System (HIS) or from the relevant Regional Offices of the RSA Department of Water Affairs and Forestry.

RSA DWAF: Planning report no. PC000/00/9490 (Stewart, Sviridov & Oliver, 1990c) gives comprehensive guidelines on the initial selection of variable values and how best to adjust them to improve the fit between the model and observed results.

3) Computer requirements:

The WQT model runs under DOS (MS-DOS version 3.0 or higher). The program will run on any PC from XT upwards. Faster run times can obviously be achieved by more advanced computers. The computer on which WQT is installed should have a minimum of 640 kB of RAM. Although the on screen graphics are designed for colour plots, even black and white monitors can be accommodated.

4) Availability:

The WQT model was originally a joint development of Stewart Scott and Acres (under the auspices of BKS Inc.), as part of a RSA Department of Water Affairs study. As such it will be necessary to obtain the permission of the interested parties to make use of the model. Initial contact can be made with Dr Herold at:

Stewart Scott Incorporated
PO Box 784506
Sandton 2146
South Africa

Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email model@ssi.co.za

4.1) Costs:

The cost of the model has not been defined. For bone fide DWAF users the model could be proved free of charge.

5) Assessment:

The model has been used in a number of river system analyses carried out on behalf of the RSA Department of Water Affairs and Forestry. These include the Vaal, Orange and Crocodile Rivers (which together constitute a large proportion of the surface water resources of the country). The model has also been used on the Waterval, Free State Goldfields, Blesbok and Mooi River Situation Assessment studies, and the development of a Water Management Plan for the Free State Goldfields catchment. Smaller studies include hydro-salinity modelling of the Molopo River system.

5.1) Level of competency required:

Use of the model requires a good understanding of the physical system being modelled. This presupposes a sound knowledge of hydrological and water quality principals. General computer literacy is also required to run the models. The user should also have the ability to obtain and process the requisite data sets used as input to the model.

5.2) Keywords for task-based search:

Salinity, total dissolved salts, TDS, water resources, integrated, modular, modelling, calibration, wash off, surface water, reservoir, system, simulation, monthly, feed-back, return flow, catchment, routing, irrigation, bed loss, wetland, evapotranspiration, demand centre, junction node.

5.3) Application algorithms and main mathematical limitations:

The model operates at a monthly tine step. Model algorithms are contained in the RSA DWAF reports P C000/00/9390 (Herold and Kakebeeke, 1991) and P C000/00/7086 (BKS and Stewart, Sviridov & Oliver, 1988).

The main limitation of the WQT model is that it can only accommodate systems large enough to fill the on-line memory of a DOS operating system (i.e. less that 640 k). This allows the processing of quite large systems. Other versions of the model have been developed to accommodate much larger systems, such as the Unix based system described in DWAF PC000/00/9490 (Stewart, Sviridov & Oliver, 1990b).

5.4) How widely is the model used and how well is it established in the industry:

The model is extensively used in South Africa, particularly by the Department of Water Affairs and Forestry.

5.5) Related References:

Allen RB and Herold CE (1988). Water quality calibration model. Report P C000/00/7086, Vaal River System Analysis, BKS and Stewart, Sviridov & Oliver report to Directorate of Planning, Department if Water Affairs, Pretoria.

Kakebeeke JP (1990). Documentation of data input module of monthly time step catchment hydro-salinity model. Report P C000/00/9290, Vaal River Water Quality Management Study. Stewart Sviridov and Oliver report to Directorate of Planning, Department if Water Affairs, Pretoria.

Herold CE and Kakebeeke JP, (1991). Monthly time step hydro-salinity system simulation model. Report P C000/00/9390, Vaal River Water Quality Management Study. Stewart Sviridov and Oliver report to Directorate of Planning, Department if Water Affairs, Pretoria.

Herold CE (1990). Calibration procedures for the monthly time step hydro-salinity model. Report P C000/00/9490, Vaal River Water Quality Management Study. Stewart Sviridov and Oliver report to Directorate of Planning, Department if Water Affairs, Pretoria.

5.6) Links to organisations:

Enquiries on the WQT model can be directed to:

Stewart Scott Incorporated
PO Box 784506
Sandton 2146
South Africa

Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email model@ssi.co.za

5.7) Range of applications:

WQT is designed for calibrating simulated water quality data against that observed. It is also used to simulate the effect of water quality options. This is done by generating monthly flow and salinity time series appropriate to given levels of catchment development and defined system operating rules.

6) Case study:

The WQT model was initially developed to facilitate salinity modelling for the Vaal River System Analysis study, and other system analyses that were to follow. This

model was specifically designed to fit with the system water resources models currently used by the South African Department of Water Affairs and Forestry. As such it integrates both water resources and water quality modelling and planning options. WQT has become the model of choice for simulating salinity in river systems in South Africa, undertaken on behalf of the Department of Water Affairs and Forestry.

Studies carried out using this model include:

- RSA DWAF Vaal River Salinity Study
- RSA DWAF Water Quality Situation Assessments:
  - Waterval River
  - Blesbokspruit
  - Mooi River
  - Free State Goldfields
  - Klip River (in progress)

- RSA Free State Goldfields Water Management Plan
- RSA Molopo River hydro-salinity study
- RSA DWAF System Analysis Studies:
  - Vaal River (2 studies: to end of 1984 and 1995 hydrological years)
  - Orange River (including Fish-Sundays catchments)
  - Crocodile River.

Typically it is necessary to first construct a layout of the river system. This is followed by preparation of the monthly time series input, output and observation point data files. Usually application of the model is preceded by naturalisation of the catchment hydrology. This should automatically lead to the creation of all of the requisite monthly flow time series. The RSA DWAF Regional Offices, water boards and local point source effluent contributors (such as local authorities, mines and industries) are the best sources of time series of salinity data for point inputs to the system. The RSA DWAF Regional Office and Directorate of Hydrology's HIS data base and water boards are often good sources of in-stream flow and water quality data that can be used for calibrating the WQT model at observation points.

The next step is to prepare the sub-module parameter files, followed by calibration of the model for observed historical conditions. Model output can then be used to produce time series plots and duration curves (cumulative frequency) at selected key points in the system. These can be used to assess historical salinity trends and seasonality, and compare the results with hydrological changes and water quality objectives. This is usually done as part of a water quality situation assessment. Thereafter the model can be used to simulate the effect of proposed management changes on surface water quality. For example, the effect of expected growth in water demand, new points of discharge, new dams or new uses of raw water or effluent could be tested. Versions of the model also exist that can be used to test different reservoir draft rules or the option of blending diverse sources of water to achieve a desired supply water quality.

MODEL: **Water Resources Simulation Model 1990 (WRSM90)**

EVALUATED BY: **Dr W V Pitman, Stewart Scott Inc.**
model@ssi.co.za

1. Description

The program MORSIM was written in 1973 to model runoff from a catchment. This model and the theory behind it is described in Hydrological Research Unit (HRU) Report No. 2/73 (Pitman, 1973). After HRU Report No. 2/73 was published, program MORSIM was enhanced and became known as HDYP09. This model was used in the 1981 appraisal of South Africa's surface water resources (Midgley *et al.*, 1981). The computer model WRSM90 is a refinement and enhancement of HDYP09. WRSM90 has a number of distinct advantages over its predecessors. It has graphics capabilities and features a more modular approach. These features greatly enhance the versatility and adaptability of the model. A number of new features are also incorporated.

WRSM90 is of a modular construction, with four different types of module (runoff, reservoir, irrigation and channel) linked by means of arcs or routes. The arcs represent lines along which water flows, such as river reaches. Most hydrological systems can be represented by means of the four types of module, linked using arcs.

Operation of WRSM90 is facilitated by a main menu that gives a number of options to the user, including running the simulation, viewing observed and modelled flow statistics and graphs, changing model parameters and writing results to output devices. The model stores all information internally, so that any number of runs can be undertaken without terminating the program. This facility, in conjunction with the ability to examine several streamflow gauging points in a system, speeds up the calibration process considerably. The model also provides the user with on-line guidance on parameter adjustments to arrive at a satisfactory calibration.

2. Data requirements

The primary input to WRSM90 comprises one or more time series of monthly catchment rainfall, expressed as percentages of catchment mean annual precipitation (MAP). The pre-processing program HDYP08, which works with rainfall records at one or more stations, generates these files. The model also requires mean monthly evaporations and appropriate factors to convert these (usually Symons pan for catchments and reservoirs; A-pan for irrigation lands) to potential evaporation rates. If the model is used in calibration mode the observed monthly streamflow records at gauging points in the system must be provided.

The runoff module also requires initial estimates of the rainfall-runoff parameters. These may be changed in the course of each run. Land-use effects are modelled by inputting appropriate areas of afforestation and irrigation plus full supply areas and capacities of reservoirs in the system. These data can be set at a particular level of development or allowed to change with time, according to historical developments in the catchment. Files of monthly abstraction (run-of-river or from dams) and return flow can also be incorporated.

in the catchment. Files of monthly abstraction (run-of-river or from dams) and return flow can also be incorporated.

The model requires a network file that informs the computer exactly how the modules are linked and in what order the modules must be solved. It is also used to denote the routes for which observed flows are available (to enable calibration of the runoff modules to be achieved) and which routes are to be reported in the summary file (for checking purposes).

2.1 Inventory of data sources

Monthly rainfall and evaporation data can be obtained directly from the South African Weather Bureau or the Computing Centre for Water Research (CCWR). The CCWR also supplies monthly streamflow data but this information can also be obtained from the Department of Water Affairs & Forestry (Directorate: Hydrology). Information on water abstractions and return flows is usually obtained from the authority in question. DWAF is also the main source of information on major dams and large water supply schemes, including water for irrigation.

3. Computer requirements

WRSM90 runs under DOS (MS-DOS version 3.0 or higher). The program will run on any PC from XT upwards but the execution time on the old machines will be very much slower than on 486s and Pentiums. The computer on which WRSM90 is installed should have a minimum of 640 kb of RAM. The program takes up slightly less than 494 kb of RAM, which allows a number of TSR (Terminate and Stay Resident) programs to remain in memory. Alternatively, it can run on a network if the space available for applications is more than 494 kb.

4. Availability

WRSM90 can be obtained from:

Stewart Scott Incorporated
PO Box 784506
Sandton 2146
South Africa

Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email ssisan@ssi.co.za

4.2 Costs

Cost Category 2: The cost of WRSM90 is R2100, including VAT @ 14%. A discount of 50% is available to academic institutions.

5. Assessments

The following is a quote from the report: Southern African "FRIEND" – The Application of Rainfall-Runoff Models in the SADC Region (WRC Report 235/1/97).

"The monthly time step Pitman Model has been applied extensively within South Africa and has also been applied in Swaziland, Lesotho, Botswana, Zambia and Namibia. It is accessible as part of several software packages that have been designed with efficient application in mind and was therefore the logical choice for the coarser time-step model to be used."

5.1 Level of competency required

Although WRSM90 is relatively simple to use once the network has been set up correctly, the user needs at least a basic grounding in hydrology. The user should also have an understanding of statistics and should be aware of the kind of errors that can be encountered when dealing with hydrological data. The program does have extensive error checking procedures that report inconsistencies in setting up the network and the various data files.

5.2 Keywords for task-based research

Water resources, simulation, rainfall-runoff, modelling, hydrology, model calibration.

5.3 Application algorithms and main mathematical limitations

The model works with monthly data throughout but a quarter-month time step is used in the rainfall-runoff calculations if the runoff module. The relatively coarse solution time step, coupled with the absence of information on the temporal distribution within each month, may lead to inaccurate results for specific months. The time step also requires that certain limits be placed on some of the parameters to ensure model stability.

5.4 How widely is the model used and how well is it established in the industry

WRSM90 has become the de-facto model for water resources studies undertaken on behalf the South African Department of Water Affairs and Forestry (DWAF). Listed below are of some of the more important catchments studied using WRSM90 and its predecessor, HDYP09.

- Limpopo, Sand, Luvuvhu, Letaba, Lephalala, Olifants (Mpumalanga & W Cape), Crocodile (North West Province & Mpumulanga), Mogalakwena, Sabie, Vaal, Orange, Breede, Berg, Kei, Mgeni, Thukela, Mvoti, Mhlatuze and Komati.

5.5 Related references

MIDGLEY, D C, PITMAN, W V & MIDDLETON, B J (1981). *Surface Water Resources of South Africa.* Report Nos. 8 – 13 / 81, Hydrological Research Unit, University of the Witwatersrand, Johannesburg, South Africa.

MIDGLEY, D C, PITMAN, W V & MIDDLETON, B J (1994). *Surface Water Resources of South Africa 1990 – User's Manual.* Water Research Commission Report No. 298/1/94, Pretoria, South Africa.

PITMAN, W V (1973). *A mathematical model for generating monthly river flows from meteorological data in South Africa.* Report No. 2/73, Hydrological Research Unit, University of the Witwatersrand, Johannesburg, South Africa.

PITMAN, W V and KAKEBEEKE, J P (1991). *WRSM90 User's Guide.* Stewart Scott Inc, Sandton, South Africa.

5.6 Links to organisations

Enquiries on WRSM90 can be directed to one of the following organisations:

Stewart Scott Inc.
PO Box 784506
Sandton 2146
South Africa
Telephone +27 11 780-0611
Facsimile +27 11 780-0649
Email ssisan@ssi.co.za

or

Water Research Commission
P O Box 824, Pretoria, 0001
Tel (012) 330-0340
Fax (012) 330-1935

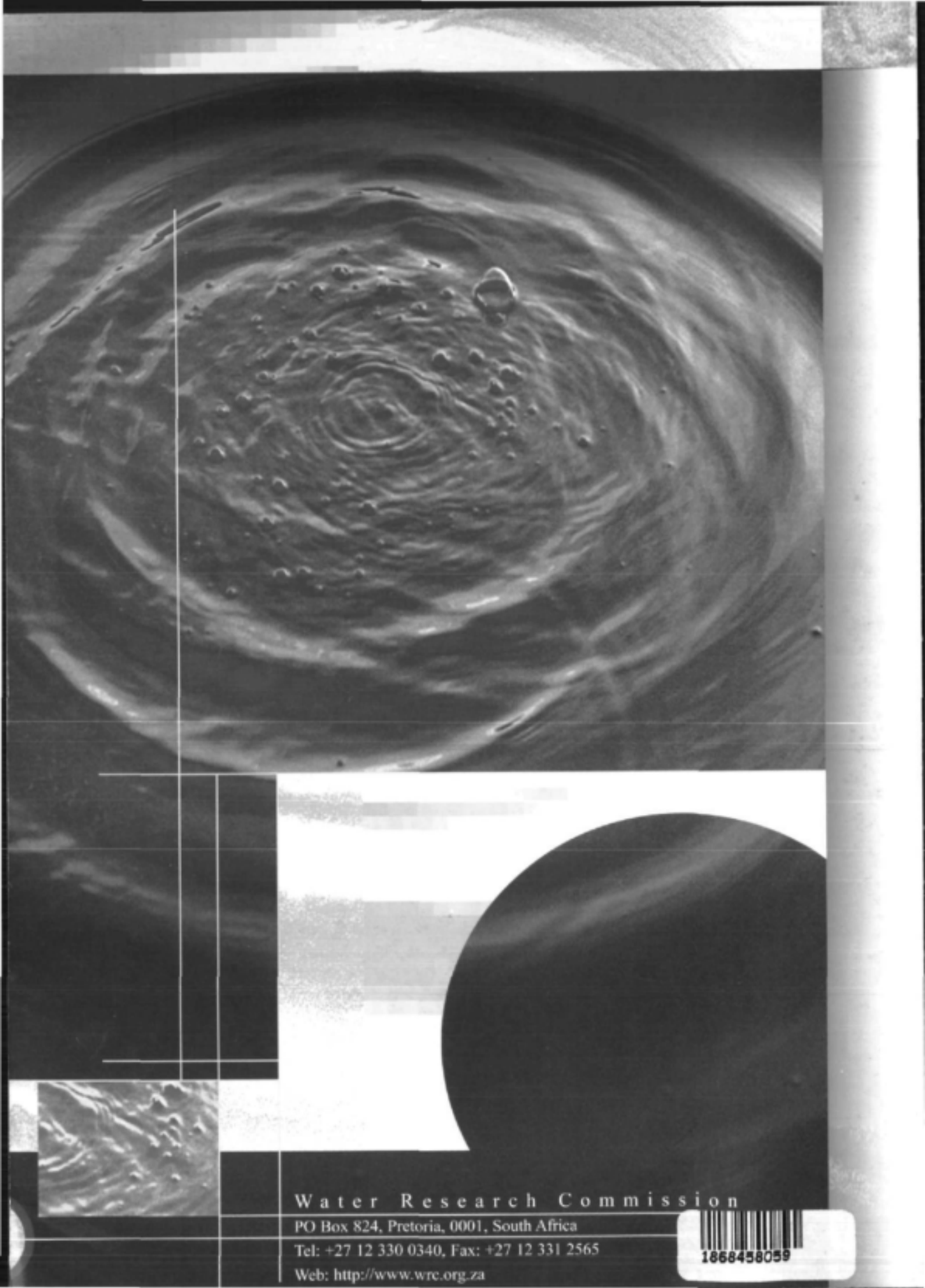
5.7 Range of applications

WRSM90 is designed primarily for calibrating the rainfall-runoff module against observed streamflows. The model can then be employed to generate time series of streamflow appropriate to given levels of catchment, including the natural condition. It has a limited ability for testing the performance of reservoirs but cannot simulate a system of reservoirs with linked operating rules.

6. Case study

WRSM90 was initially developed for the express purpose of streamlining the streamflow modelling component of the Surface Water Resources of South Africa 1990 (WR90) study (Midgley *et al*, 1994). This major study involved the calibration on 573 streamflow records and the subsequent generation of 70-year time series of natural hydrology on 1941 catchments, covering the whole of South Africa.

Since then WRSM90 has become the de-facto hydrological model for catchment and system analysis studies in South Africa, undertaken on behalf of the Department of Water Affairs and Forestry.



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