

EXECUTIVE SUMMARY

1 INTRODUCTION

The invisibility of groundwater and the unique nature of aquifers make it extremely difficult to manage and control groundwater resources. One method to overcome these difficulties is to represent waterlevels in observation boreholes graphically by contour maps. This approach has the advantage that it allows one to visualize the trends in the data.

An important aspect in groundwater is the management of the resource. Mathematical models are often used for this purpose. However, to apply these models, values for variables are often needed at points where no measurements were taken, which require reliable estimation techniques.

The packages TRICON and BAYES (or TRIPOL as it is now referred to, because it includes three different interpolation methods) were originally developed for the contouring and interpolation of geohydrological data. However, there is nothing in the programs that would prevent a potential user applying them to other regional variables.

2 PURPOSE OF THE PROJECT

The packages TRICON and BAYES were developed on a personal computer as part of the project: *A Comparative Study of Two- and Three-dimensional Groundwater Models*, between the Water Research Commission and the Institute for Groundwater Studies, that ended in December 1991. The main properties of these packages, which are described in the reports by Buys *et al.* (1992) and Van Sandwyk *et al.* (1992), respectively, are briefly as follows:

To draw accurate and aesthetically acceptable contour maps of a regionalized variable - that is a variable that varies in space.

To estimate values of a regionalized variable, and its associated error, at points where no measurements are available.

Both these packages were developed on IBM-compatible personal computers under the DOS operating system, because of the widespread use of these machines in South Africa. However, towards the end of the project, it became clear that the maximum of 640 Kb memory, available on these machines under the DOS operating system, limits the application of both packages considerably (Buys *et al.*, 1992). A research proposal '*Conversion of the Software Packages TRICON and BAYES from Personal Computers to Machines using the UNIX operating System*', was therefore put before the Water Research Commission. The purpose of this project, as stated in the terms of reference, is as follows:

(a) To convert the present research package BAYES to a commercial package, (b) to convert the two packages, TRICON and BAYES, developed for personal computers, that use the DOS operating system to machines that use the UNIX operating system and (c) to incorporate them in the GIS system, presently developed at the Institute for Groundwater Studies, with funds from the Water Research Commission.

The proposal was accepted by the Commission and work on the project began in January 1993. The present report describes the work carried out under this project, which ended in December 1993.

3 STRUCTURE OF THE REPORT

The work on this project was undertaken in different phases, which will be discussed in Sections 2 to 7 of this report. The phases were:

- (a) Conversion of program TRICON to the SUN workstation, so that it can run under the UNIX operating system.
- (b) Combine the BAYES program with the program KRIGING, developed by Prof. G.J. van Tonder at the Institute for Groundwater Studies, into a package called TRIPOL that includes three different interpolation methods: (i) the classical Distance Weighting Method, (ii) Kriging and (iii) Bayesian Estimates. A facility for the computation of semi-variograms and the fitting of a theoretical semi-variogram to the semi-variogram values, needed by the Kriging and Bayes methods, were also included.
- (c) Develop user friendly interfaces for the DOS version of TRIPOL and the UNIX and SUN versions of both TRICON and TRIPOL.
- (d) Replace the DOS graphic library, PLOT88, presently used on DOS machines, with a Postscript library.
- (e) Incorporation of TRICON into the GIS system, presently developed at the Institute for Groundwater Studies.
- (f) The User Manual for TRICON was adapted for the UNIX version and a User Manual for TRIPOL was written from scratch. The User Manuals are included in Appendix A and B of this report.

4 SUMMARY AND CONCLUSIONS

TRICON and TRIPOL have been used extensively by the geohydrology students at the Institute for Groundwater Studies, since the second half of 1993. The UNIX versions of both packages proved to be very valuable for the handling of large data sets, required by numerical models.

The rapid development of IBM compatible personal computers in terms of speed and memory, however, increased the demand for DOS versions of TRICON and TRIPOL that require more memory than the basic 640 Kb available under current DOS versions. This problem may be solved in the near future with the publication of a linker, called BLINKER, by BLINK Inc.

CONVERSION OF THE SOFTWARE PACKAGES TRICON AND BAYES FROM PERSONAL COMPUTERS TO MACHINES USING THE UNIX OPERATING SYSTEM

1 INTRODUCTION

The packages TRICON and BAYES (or TRIPOL, so-called because it includes three different interpolation methods) were originally developed for the contouring and interpolation of geohydrological data. However, there is nothing in the programs that prevents a potential user applying them to other regional variables - that is variables that vary in space.

Regionalized variables are usually associated with very large areas. Therefore, it is practically impossible to measure them at all points of interest - least at points where their values may coincide with prescribed contour values or pre-defined nodes in a simulation problem. The variable is, consequently, mostly known at a small number of points (considerably less than needed to generate smooth contour lines or coinciding with each node of the mesh) scattered throughout the domain.

There are two methods that can be used to circumvent the discretization of arbitrary spaced points: (a) use an irregular triangular finite element mesh for contouring, and (b) interpolate or extrapolate the measured values, if values are needed at points where no measurements were taken. TRICON and TRIPOL do just that.

2 PROGRAM TRICON

TRICON is a graphical package that can be used to contour a regionalized variable with known discontinuities (Buys *et al*, 1992). However, it can also be used for interpolation of the variable to a regular rectangular grid, as well as to draw maps of any specified geographic information about a region and to represent groundwater velocities graphically.

TRICON uses a triangular irregular mesh, constructed between the actual data points, for contouring, interpolation and velocity computation. It constructs a Deluanay triangulation between the actual data points, but it can also be used to triangulate points on a square grid.

Contour lines, constructed by TRICON, are consistent and reflect changing roughness of the terrain. Contouring with TRICON is fast and provides piecewise linear, or smoothed, contours. The smoothing of contour lines can be controlled by the user to avoid intersecting contour lines.

Separation of the triangulating and contouring steps makes it possible to compute various sets of contour lines for the same set of data points, without reconstructing the triangulation. Using piecewise linear contours is a good way of checking for erroneous points, and to see if the expected trends are present. Contours are smoothed, using curve fitting techniques, but extensive smoothing is not done because this may lead to inconsistent contours.

TRICON incorporates discontinuities in the triangulation by *partially* subdividing the region

into subregions, with the discontinuities as boundaries, while the terrain around the discontinuity is still viewed as a whole. Contour lines are interrupted where they cross the discontinuity, without increasing the computer time needed to compute the contours.

3 PROGRAM TRIPOL

TRIPOL is an interpolation program that estimates values for random variables from a given set of regionalized variables, that is variables distributed in space (and/or time). Variables encountered in environmental sciences such as geohydrology, geology, weather forecasting etc., are all regionalized variables.

TRIPOL includes the following:

- Computation of a semi-variogram for a given set of regionalized variables (data points);
- Fitting a mathematical function to the semi-variogram;
- Estimating values for any set of random variables from the given set of data points.

TRIPOL implements three interpolation methods, namely:

- Distance Weighting;
- Kriging;
- Bayesian Estimates.

The interpolation procedures do not only yield an estimate of the random variable, but also the error in the estimate.

The Distance Weighting method is a classical method that is based on the assumption that the variable of interest can be represented by a smooth function, and its use is consequently limited.

The Kriging method describes the spatial variability of environmental variables by representing them with random functions. This approach has the advantage that it allows one to describe an environmental variable in statistical terms, through the Theory of Regional Variables. The best known estimation methods, based on this approach, is Ordinary Kriging, or *Kriging* as it is conventionally known and Universal Kriging.

The Bayes method is a versatile procedure for estimation of groundwater levels (Van Sandwyk *et al*, 1992). The method has the advantage that one can use any expert knowledge about a given regionalized variable as a qualified guess. For example, a useful qualified guess for the groundwater level is the topography. Unfortunately, difficulties can be experienced in establishing a suitable qualified guess for some regionalized variables. It is therefore recommended that this method be used only when the user can establish a suitable qualified guess for the base variable, otherwise it may be better to use Kriging.

Because of the nature of Kriging and Bayesian Kriging, a semi-variogram, computed from the regionalized variables or data points, is needed to estimate the manner in which the mean value of the variable varies over the region. The computation of a semi-variogram for a given set of regionalized variables (data points) was therefore also built into the program, as well as a facility to fit a mathematical function to the semi-variogram.

Drawings created by TRIPOL can be drawn on the screen or a Laser Jet printer. Alternatively, a Postscript file or HPGL (Hewlett Packard Graphic Language) file, can be created which can be imported into a word processor.

4 USER INTERFACES FOR DOS, UNIX AND OPEN WINDOWS

The SUN versions of both programs were written on a SUN SPARC station II, that uses the SUN-OS 4.1.1 operating system based on Unix, and the OPEN WINDOWS 3.1 window manager based on the X window system.

The X Window System is an industry-standard software system that allows programmers to develop portable graphical user interfaces. X Windows is available on most Unix systems, like the SUN, IBM, HP and DEC workstations. The most widely used low-level interface to X is the standard C language library known as Xlib. Xlib defines an extensive set of functions that provide complete access and control over the display, windows, and input devices linked to the computer.

Although programmers can use Xlib to build applications, most prefer to use one of the higher level toolkits designed for use with X Windows, for example, the standard X or Xview toolkits.

The standard X toolkit consists of two parts: a layer known as the Xt Intrinsics, and a set of user interface components known as widgets. Applications based on the X toolkit, can use either the widget set OPEN LOOK (also known as OLIT), developed by AT&T and Sun Microsystems, or MOTIF, developed by the Open Software Foundation. They are both written in C and are built on top of Xlib.

The graphical user interfaces (GUT's) of TRIPOL and TRICON use the OLIT toolkit (Young *et al*, 1992), since it is available on all SUN workstations. It implements user interface components like scroll bars, menus and buttons, as well as graphics for drawing maps and graphs in a graphic window. However there is today a trend to shift towards Motif. Sun has already announced that they will move to Motif. An implementation of Motif exists already for the majority of workstations (HP, IBM, DEC, ...). It may therefore be useful to transfer the GUT's of TRIPOL and TRICON to Motif later.

Both programs can, however, already be used on other workstations, since the Unix versions run in any Unix shell, but it is much more aesthetically acceptable using OPEN LOOK.

The DOS version of TRIPOL was originally developed in FORTRAN. I decided to keep it that way and to develop a user interface that uses the Microsoft FORTRAN graphic library. The Unix and SUN versions of TRIPOL were, however, successfully linked with the C and X libraries.

5 GRAPHIC LIBRARY

The PC version of TRICON was originally developed in C and uses the PLOT88 graphics library, from PLOTWORKS Inc., to create drawings. This library has the advantage that it includes a wide variety of drivers for various printers and can also create HPGL (Hewlett Packard Graphic Language) and Postscript files for importing graphs into word processors,

like Word for Windows or Mac. The only disadvantage is that royalties must be paid for programs that include the PLOT88 library, when they are sold. An agreement has been reached with PLOTWORKS that only a small amount of \$10 have to be paid on each package, if TRICON is distributed at \$100 only.

Although the drawings on the Sun version can be previewed in a graphics window, the SUN and Unix versions use a Postscript Library that was assembled from public software, to create hard copies. It frees these versions from any obligations to software developers, and makes it very versatile for use on other workstations. Without this library, it would not be possible to port the programs to other Unix machines, since PLOTT88 is only available on Sun workstations.

6 GGIS

GGIS is an interface between the geographic information system ARC INFO and the HYDROCOM data base, developed for use on SUN workstations, by the Institute for Groundwater Studies.

The SUN version of TRICON was adapted to receive input directly from the GGIS system, through temporary files. TRICON is then automatically initiated from GGIS. All the facilities of TRICON can still be used to create and view drawings, whereafter the drawings can be exported to GGIS, for incorporation in the ARC INFO system.

7 COMMERCIALIZATION

The Institute for Groundwater Studies regularly receives requests for commercial versions of both programs. Since a complete user manual for both programs is now available, the software is available through the Institute for Groundwater Studies at a small administration fee. A review of the PC version of TRICON has been published in an issue of the international journal, *Geographical Systems*.

8 CONCLUSIONS

The packages TRICON and TRIPOL are particularly useful for the contouring and interpolation of any set of values, associated with a two-dimensional regionalized variable. Although the packages may not satisfy the needs of all users, experience has shown that it is very versatile and user friendly. It also allowed scientists at the Institute for Groundwater Studies and other institutions to solve problems that were previously thought to be intractable. This applies in particular to groundwater pollution studies and phenomena where accurate contours and estimations are needed.

9 RECOMMENDATIONS

The Unix and Sun version of TRICON and TRIPOL can now be used for very large data sets, but the demands for DOS versions that can utilize more memory than the basic 640 Kb memory, that can be addressed by current DOS versions, still remains. These demands are also increasing because of the fast development of IBM compatible personal computers in terms of