ADDENDUM TO THE WHPA CODE VERSION 2.0 USER'S GUIDE: IMPLEMENTATION OF HYDRAULIC HEAD COMPUTATION AND DISPLAY INTO THE WHPA CODE

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TABLE OF CONTENTS

LIST OF FIGURES

1.0 INTRODUCTION

This document is an addendum to the Version 2.0 WHPA Code User's Guide (Blandford and Huyakorn, 1991).   WHPA is a user-friendly microcomputer model developed by the U.S. Environmental Protection agency (EPA) to assist State and local technical staff with the delineation of wellhead protection areas (WHPAs) as mandated by the 1986 Amendments to the Safe Drinking Water Act. Previous versions of the WHPA code (2.1 or less) have the capability to delineate time-related, steady-state, or hybrid capture zones using ground-water flow pathline delineation techniques. To determine pathlines and times of travel, ground-water flow velocities and some physical aquifer properties are required.   Since ground-water flow velocities are a function of the difference in hydraulic head (or potentials), rather than the head values themselves, it is not necessary to determine hydraulic heads in order to determine pathlines and capture zones.

Calculation of the hydraulic head values, however, can be useful for visualization and model calibration purposes, and in some cases may serve as a "reality check" for a simulation scenario. For these reasons, options to compute hydraulic head fields were implemented into the RESSQC, MWCAP, and semi-analytical GPTRAC modules of the WHPA code. The purpose of this addendum is to document the implementation and proper application of the new options. Chapter 2 outlines the implemented changes in the preprocessor and postprocessor modules. presents several demonstration and verification examples. and provides some rules of thumb for model calibration. For interested readers, the mathematical formulations are presented in Chapter 3.

This latest version of the WHPA code (2.2) is entirely compatible with previous versions (2.0 or 2. 1) in that existing input and output files may be utilized without modification.

2.0 IMPLEMENTATION OF HYDRAULIC HEAD CALCULATIONS

2.1   Preprocessor Amendments and Input Items

The RESSQC, MWCAP, and GPTRAC preprocessors were amended slightly to read in new input data required to perform the head calculations. On the first input screen for RESSQC and MWCAP, and on the second input screen of GPTRAC, users are now prompted for the following input item:

<div align="center">

Perform Hydraulic Head Calculation:

(O = no, 1 = yes)

</div>

The default input is O, for not calculating hydraulic heads.   If a 1 is entered here, the following input screen will appear

---

<div align="center">

MWCAP

UNIFORM GRID INFORMATION FOR PLOTTING HYDRAULIC HEAD

Number of Grid Columns: 50

Number of Grid Rows: 50

REFERENCE HEAD INFORMATION

X-Coordinate of Reference Head (ft):

Y-Coordinate of Reference Head (ft): 2000.00

Reference Head (ft): 100.00

Note: The reference point may not be a well location!

</div>

< Enter> = select value   < Esc > = options menu   < F1 > = DOS shell

This menu prompts for five new input items required for the calculation of hydraulic heads.

The first two input items are the number of grid rows and columns: these values are required because the hydraulic head values are computed at the nodal points of a grid that has uniform spacings in the x- and y-directions. For the RESSQC and MWCAP modules, the product of the number of rows and columns must be less than or equal to 5,625, which is equivalent 75 rows and 75 columns if the length of the problem domain is equal in the x- and y-directions. For the GPTRAC module, the number of rows and columns must be 53 or less (the smaller grid size is to save computational space, since GPTRAC is substantially larger than the other code modules. The number of rows and columns are used in conjunction with the problem boundaries to determine the grid spacings in the x- and y-directions (DX and DY) using

$$DX = \frac{(XMAX - XMIN)}{(no.\ of\ columns)} \tag{2.1}$$

$$DY = \frac{(YMAX - YMIN)}{(no.\ of\ rows)} \tag{2.2}$$

As a final note, the hydraulic head values are computed at the center of each grid block, rather than at the intersection of gridlines, which is equivalent to the block-centered finite difference grid used in numerical modeling.

The remaining three input items are required to evaluate an integration constant that appears in the analytical equations for hydraulic head (see Chapter 3). These items are an x-coordinate. a y-coordinate, and the (observed) value of hydraulic head at the specified location. These values define what is called the reference point and reference head, respectively. When the head field is solved for in the code, the solution will be constrained to match the input hydraulic head at the reference point. There is no rigorous procedure for selecting the reference point, and in practice it may lie anywhere except at a well location (it can even be outside of the model domain as defined in WHPA). There are, however, some general guidelines that may be offered:

1)   If the simulation involves a stream boundary, the head (water surface elevation) in the stream at a point should *always* be used as the reference head. If ambient ground-water flow is directly towards or away from a stream, the head in the stream will be a constant. If ambient flow is prescribed at an angle to the stream, the head along the stream will vary according to the magnitude of the ambient flow component along the stream and the influence of nearby wells.   A reference point and head that reflects the situation of interest should be selected.

2)   For other cases, such as one or more pumping wells in uniform ambient flow, selection of the reference point and head is not as straightforward. It is probably best for most WHPA delineation applications to select a reference point at some distance from the active wells such that the drawdown due to wells at that point is expected to be small. The head value might be indicative of the ambient flow condition, or it might be an observed value if reasonably accurate hydraulic head data is available (either in the form of a contour map or field data).

3)   If the unconfined aquifer option in GPTRAC is utilized, the reference point and head should be indicative of the ambient flow condition outside the specified radius of influence of each well.

The examples provided in Section 2.3 may clarify this discussion somewhat. For certain problems it is possible the several reference points and heads may be selected on a trial basis until a reasonable (desired) result is obtained. For those interested in a more detailed discussion. Strack (1989) is one of the few authors who discusses the selection of constants for various analytical solutions in detail.

2.1   Displaying the Results

The postprocessor (GRAF module) of the WHPA code has been amended to permit the contouring of hydraulic head values. If hydraulic head values are generated during a simulation,

4

the necessary grid data and the head values are written to the default plotting file WHPA.PLT: this new information is placed below the pathline and capture zone data, if any. A new command line item, (T)ype, has been added to the GRAF module displays. When this option is selected by typing T or t, the following menu will appear:

```
          P L O T    T Y P E


       pathlines/capture zones only

       hydraulic heads only

       both


       [↑ ↓] = move cursor    < Enter > = select option
```

from which the desired plotting option is selected using the arrow keys (to move between options) and the Enter key (to select an option). The default option is to plot pathlines only, so even if hydraulic heads were computed during a simulation, they will not be contoured and plotted unless the (T)ype selection is utilized.

If a contour plot of hydraulic heads is selected, the following menu will appear

```
          CONTOUR INTERVAL SPECIFICATION


          Minimum Head Value [ft]: 95.92

          Maximum Head Value [ft]: 101.46

          Contour Interval [ft]: 0.00

       Label Contour Lines?[Y/N]: N
```

in which the minimum contour level, the maximum contour level, and the increment may be specified. A maximum of 50 contouring increments is permitted (if more than 50 are specified, only the first 50 will be used). For convenience, the lowest and highest calculated hydraulic head values for the current plotting file are displayed. Other plotting items, such as (M)ap Scale, (H)ard Copy, etc., operate in an identical fashion to previous versions of the code; the only limitation is that contour lines may not be saved in an ARC-INFO file format.

Finally, it should be noted that the contouring routine implemented in WHPA (modified from Harbaugh, 1990) is relatively unrefined. Although the delineated contours are accurate and generally smooth, graphical options such as the placement of-contour labels are limited. For this reason, when any of the WHPA code modules are utilized to compute hydraulic heads, the head values and nodal locations are written to the default file SURF. DAT, as well as the file WHPA.PLT. The SURF.DAT file consists of three columns of data (an x-coordinate, a y-coordinate, and the associated head value); this file format is compatible with the SURFER (Golden Software, Golden, CO) and other available contouring packages. Users may consider these specialty contouring packages if sophisticated graphical manipulations are desired.

2.3   Examples and Verification

In this section, several example and verification problems are presented. Most of these problems can be reproduced using any of the WHPA code computation modules (except MONTEC).

The first two problems involve the delineation of capture zones and the computation of hydraulic head fields for a single well in a uniform ambient ground-water flow field. The first problem (Figure 2.1) was taken from Haitjema and Strack (1993), and the second problem (Figure 2.2) was taken from Javandel et al. (1989). Note that in the first problem a confined aquifer of unit thickness was simulated (the original problem was presented for an unconfined aquifer), and a recharge well that was originally in the second problem was deleted. The input parameters for these examples are listed at the bottom of the figures.

6

Figure 2.1   Verification example 1: single pumping well in a uniform ambient flow field in a confined aquifer.
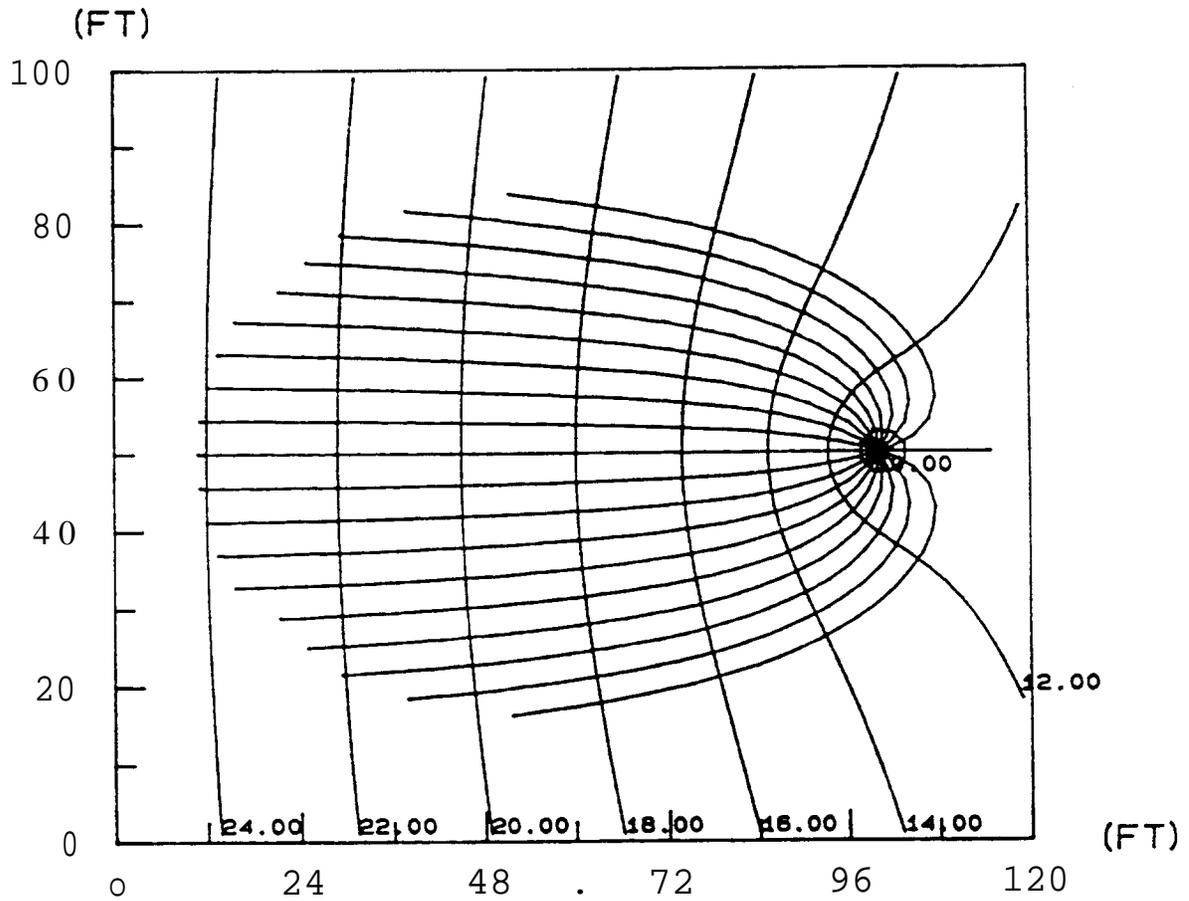
Simulation Options	Aquifer Parameters	Well No. 1
Units = ft and days	T = 1.0	X = 100
XMIN = 0.0 XMAX = 120	b = 1.0	Y = 50
YMIN = 0.0 YMAX = 100	i = 0.1	Q = 9.425
Step Length = 1	α = 0.0	No. of Pathlines = 20
No. of pumping wells = 1	θ = 0.3	Time = 180
XREF = 140	No Boundary	
YREF = 50	NCOLS = 50	
HREF = 10.0	NROWS = 50	

7
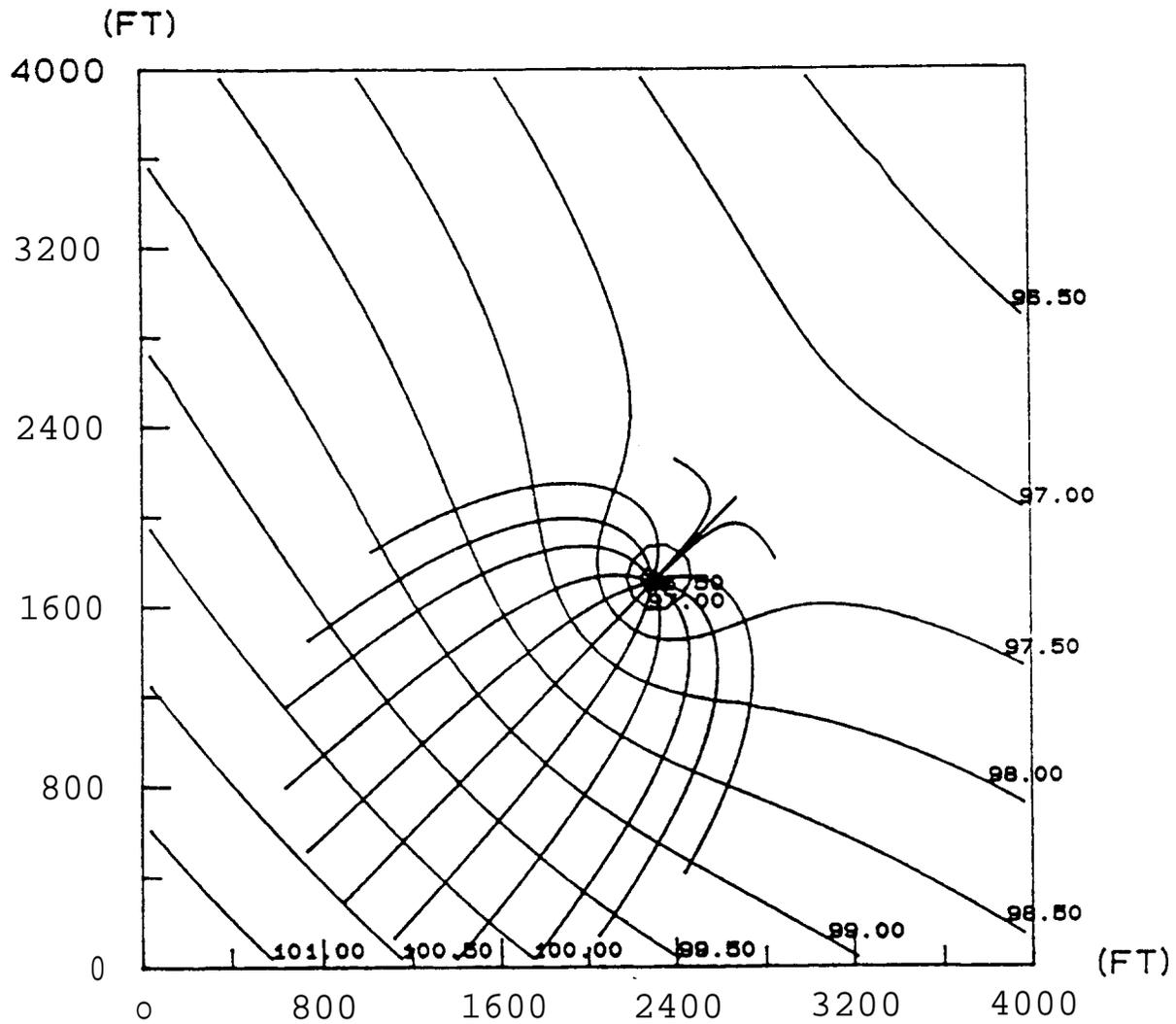
Simulation Options	Aquifer Parameters	Well No. 1
Units = ft and days	T = 14.3	X = 2,300
XMIN = 0.0 XMAX = 4,000	b = 10.0	Y = 1,700
YMIN = 0.0 YMAX = 4,000	i = 0.001	Q = 50.0
Step Length = 25	α = 45°	No. of Pathlines = 10
No. of pumping wells = 1	θ = 0.25	Time = 2×10^5
XREF = 0	No Boundary	
YREF = 2,000	NCOLS = 50	
HREF = 100.0	NROWS = 50	

Figure 2.2   Verification Example 2: Single pumping well in a uniform ambient flow field in a confined aquifer.

8

each of these problems were verified using the WhAEM model (Haitjema and Strack, 1993) soon to be released by EPA. In addition to checking the general shape and location of the contour lines, the minimum and maximum hydraulic head values calculated using both codes (WHPA and WhAEM) were compared.   For the first problem, the minimum and maximum hydraulic head obtained using WHPA are 8.62 and 25.4 ft, respectively, while the equivalent values obtained using WhAEM are 8.05 and 25.54 ft, respectively. For the second problem. the minimum and maximum WHPA code heads are 95.92 and 101.46 ft, respectively, and the equivalent values obtained from WhAEM are 95.87 and 101.53 ft, respectively.   These differences are minor and are probably due to the different griding configurations used by the two models: WHPA calculates hydraulic heads at the center of the grid blocks, while it appears that the WhAEM code calculates heads at the intersections of gridlines. Therefore, if a grid of 50 rows and 50 columns is specified for each model. the two codes will not calculate head values at identical locations.

The first two examples clearly illustrate some general features of the analytical solutions employed. First of all, the ground-water flow pathlines are everywhere perpendicular to the equipotential lines (hydraulic head contours), as is necessary for isotropic conditions. In addition, the influence of the cone of depression caused by the well on the capture zone shape is clearly evident in the vicinity of the well, and the transition of ground-water flow to an ambient magnitude and direction upgradient of the well is obvious.

The third example (Figure 2.3) is the Albuquerque example (Newsom and Wilson, 1988) presented in Chapter 7 of the WHPA Code Users's Guide. For this example, a reference head of 4,910 ft was selected on the stream boundary at the origin; the fact that the reference head was maintained during the simulation is evidenced by the 4,91O ft contour line terminating at the origin. Furthermore, along the right side of the plot, away from the pumping well, it can be verified that the ambient hydraulic gradient (0.0013) and the ambient direction of ground-water flow (-90°, or due south) are very nearly maintained. This example may be reproduced using either the MWCAP or the GPTRAC modules of the WHPA code, or the RESSQC module if an injection image well is input explicitly.
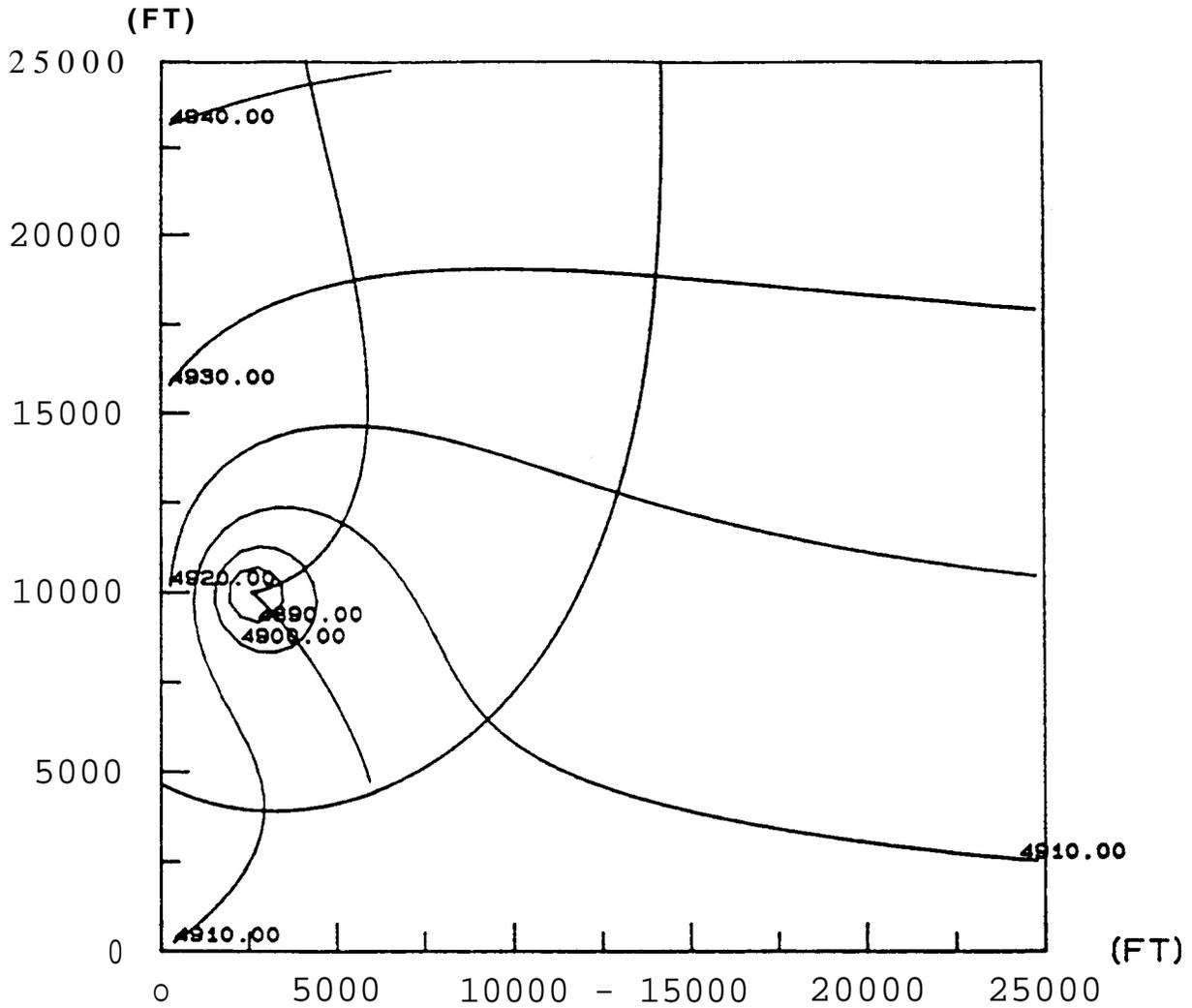
Simulation Options		Well No. 1
Units = ft and days	X = 2,600	b = 200
XMIN = 0.0 XMAX = 25000	Y = 10,000	Stream Boundary
XMIN = 0.0 YMAX = 25000	Q = 712,247	Distance to Boundary = 2,600
Step Length = 200	T = 6,690	Boundary Orientation = 0.0
No. of pumping wells = 1	i = 0.0013	Steady-State Capture Zone
XREF = 0.0	α = -90°	No. of Pathlines = 0
YREF = 0.0	θ = 0.25	
HREF = 4,910		

Figure 2.3   Steady-state capture zone and associated hydraulic head field for pumping well near a stream boundary (Albuquerque, New Mexico, example from Chapter 7 of WHPA User's Guide).

2.4   Model Calibration

Model calibration is the process of comparing model output, such as hydraulic heads and ground-water flow velocities, with values observed in the field. If the difference between the simulated and observed values are "significantly" different, then the values of one or more model input parameters may be adjusted (within reasonable bounds) in an attempt to obtain a better match, or the conceptual model of the site may be reevaluated. If a model calibration is conducted using the WHPA code or similar analytical and semi-analytical solutions, the following suggestions and observations may prove useful:

1)   In general, it is better to match the overall shape of a hydraulic head field and the magnitude of hydraulic gradients; local irregularities in observed head fields will be difficult (and perhaps impossible) to reproduce, and may often have little influence on a capture zone delineation.

2)   Analytical solutions are generally not very accurate in the immediate vicinity of a well and at large distances from the well. These general regions therefore, should not be emphasized during the calibration process. By "immediate vicinity of the well" we mean a distance from the well bore equivalent to 1-2 times the aquifer thickness. Inaccuracies in the vicinity of the well area due to partial penetration effects, well losses, the formation of a seepage face for unconfined conditions, etc., all of which are neglected in the analytical solutions.   By "large distances from the well" we mean distances substantially beyond the reference point provided for a given problem.

3.0 POTENTIAL EQUATIONS

In this chapter, the potential equations used to compute hydraulic heads are presented. Most of the equations are also presented in the appendices of the WHPA Code User's Guide.

3.1   Confined Aquifer

The hydraulic heads are solved for in terms of the potential function, Φ, where

$$\Phi = Kh + C \tag{3.1}$$

where K is the hydraulic conductivity, h is the hydraulic head, and C is an arbitrary constant (scc. for example, Javandel et al, (1984)).   The potential functions for uniform ambient groundwater flow and the drawdown due to multiple pumping and injection wells may be superposed as follows

$$\Phi = -U\left(x\cos\alpha + y\sin\alpha\right) + \sum_{i=1}^{N_p} \frac{Q_i}{4\pi b} \ell n\left[(x-x_i)^2 + (y-y_i)^2\right]$$

$$-\sum_{i=1}^{N_i} \frac{Q_i}{4\pi b} \ell n\left[(x-x_i)^2 + (y-y_i)^2\right] + C \tag{3.2}$$

where U is the Darcy velocity of the ambient uniform flow, α is the angle of ambient flow, b is the aquifer thickness, Q is the discharge or recharge rate for well i located at (x_i, y_i), N_p is the number of pumping wells, N_i is the number of injection wells, and C is a combined constant of integration, Equation 3.2 is solved to obtain hydraulic heads in the RESSQC, MWCAP, and GPTRAC (confined aquifer semi-analytical) modules.   Heads are solved for at the nodal locations (x,y) of a uniform grid.

Note that the incorporation of boundary conditions is handled implicitly by the above equation, since both a stream and a barrier boundary are incorporated via image well theory.

3.2   Semi-Confined (Leaky) Aquifer

The potential solution for a pumping well in a semi-confined aquifer may be written (Bear, 1979)

$$\Phi = \frac{Q}{2\pi b} K_0 (r/\lambda) + C \tag{3.3}$$

where K_0 is the modified Bessel function of the second kind of zero order, r is radial distance from the well defined as

$$r = \left[(x-x_w)^2 + (y-y_w)^2 \right]^{1/2} \tag{3.4}$$

where (x_w, y_w) is the well location, and λ is a leakage factor defined as

$$\lambda^2 = Kbb'/k' \tag{3.5}$$

where k' and b' are the vertical hydraulic conductivity and thickness, respectively , of the aquitard through which leakage occurs.   Equation 3.3 may be combined with the potential function for uniform ambient flow, and multiple pumping and injection wells may also be implemented (Q would be positive for injection wells).

3.3   Unconfined Aquifer with Recharge

To determine the drawdown due to pumping wells in unconfined aquifers. the following definition of the potential function is introduced to mathematically linearize the problem (account for the variation in aquifer saturated thickness in the vicinity of the pumping well):

$$\Phi = \frac{Kh^2}{2} \tag{3.6}$$

where h is the hydraulic head above the base of the aquifer. The potential solution for a fully penetrating pumping well in an areally infinite unconfined aquifer with areal recharge applied over a circular area bounded by $0 < r \le R$. It is assumed that at r = R, the hydraulic head (h),

13

and thus the saturated thickness, is a maximum value of H. For this case,, the analytical solution may be expressed as

$$\Phi = \Phi_0 - \frac{Q}{2\pi} \ell n \, (R/r) + \frac{N}{4} (R^2 - r^2) \quad \text{for } r \leq R \tag{3.7}$$

and

$$\Phi = \Phi_0 \qquad\qquad \text{for } r > R \tag{3.8}$$

Equation 3.7 is linear (in h^2) and thus the effects of multiple wells may be superposed. Note also that there is no constant of integration to evaluate, since the solution is bounded at r = R.

In practice, Equation 3.7 is combined with a uniform ambient flow field in the following manner. Equation 3.7 is rearranged and solved for drawdown. s, due to the well

$$s = H - h \tag{3.9}$$

If drawdown is negative (h > H), a warning message is written and drawdown is set equal to H. If this situation occurs, the simulation results should be closely examined and the input parameter (such as well pumping rate) should be reexamined. It should also be noted that this condition generally occurs at small radial distances from the well, and therefore may sometimes be avoided by artificially increasing the well radius a small amount (perhaps several feet). This approach may not be unreasonable in many cases since the analytical solution does not provide a highly accurate estimate of the hydraulic head in the vicinity of the well bore (i.e. the solution neglects well losses, the presence of a seepage face, etc.).

Once the drawdown (in terms of h, not h^2) is determined, it is subtracted from the ambient head field as defined by the first term in Equation 3.1. This procedure is approximate, since it assumes ambient flow under confined conditions (constant thickness aquifer); while the unconfined flow condition is directly incorporated in the solution in the vicinity of the pumping well(s) only.

14

3.4   Confined Strip-Aquifer

The potential solutions for confined strip aquifers (two parallel barriers, two parallel streams, or a parallel barrier and stream) were derived using conformal transformations of the complex potential; the boundary conditions for this aquifer type are not implemented using simple image well theory. The potential functions for a pumping well in the various types of strip aquifers are as follows:

1)   Strip aquifer with two barrier boundaries:

$$\Phi = \frac{-Q}{2\pi b} \ell n \frac{r'' r_w}{rr'} + C \tag{3.10}$$

where r_w, is the radius of the well bore,

$$r = \left[(u - u_0)^2 + (v - v_0)^2 \right]^{1/2} \tag{3.11}$$

$$r' = \left[(u - u_0)^2 + (v + v_0)^2 \right]^{1/2} \tag{3.12}$$

$$r'' = \left[u^2 + v^2 \right]^{1/2} \tag{3.13}$$

and

$$u = e^{\pi x/a} \cos\left(\frac{\pi y}{a}\right) \tag{3.14}$$

$$v = e^{\pi x/a} \sin\left(\frac{\pi y}{a}\right) \tag{3.15}$$

$$u_0 = e^{\pi x_0/a} \cos(\pi y_0/a) \tag{3.16}$$

$$v_0 = e^{\pi x_0/a} \sin(\pi y_0/a) \tag{3.17}$$

where a is the width of the strip, and the well is located at (x_0, y_0).

15

2)   Strip aquifer with two stream boundaries:

$$\Phi = \frac{Q}{4\pi b} \ell n \left(r^2/(r')^2 \right) + C \tag{3.18}$$

where r and r' are defined previously.

3)   Strip aquifer with a stream boundary (bottom) and a barrier boundary (top):

$$\Phi = \frac{Q}{2\pi b} \ell n \frac{r_1 r_2}{r_3 r_4} + C \tag{3.19}$$

where

$$r_1 = \left[(u - u_0)^2 + (v - v_0)^2 \right]^{1/2} \tag{3.20}$$

$$r_2 = \left[(u + u_0)^2 + (v - v_0)^2 \right]^{1/2} \tag{3.21}$$

$$r_3 = \left[(u + u_0)^2 + (v + v_0)^2 \right]^{1/2} \tag{3.22}$$

$$r_4 = \left[(u - u_0)^2 + (v + v_0)^2 \right]^{1/2} \tag{3.23}$$

and

$$u = e^{\pi x/2a} \cos (\pi y/2a) \tag{3.24}$$

$$v = e^{\pi x/2a} \sin (\pi y/2a) \tag{3.25}$$

$$u_0 = e^{\pi x_0/2a} \cos (\pi y_0/2a) \tag{3.26}$$

$$v_0 = e^{\pi x_0/2a} \sin (\pi y_0/2a) \tag{3.27}$$

The fourth case (barrier on top and stream on bottom) is a special case of solution 3. It should be noted that the above solutions are applicable to a horizontal (with respect to a Cartesian coordinate system) strip aquifer with the origin at (0,0). Vertical strip aquifers that have boundary conditions parallel to the y-axis can be handled by simple geometric transformation of the above solutions.

The potential solution for strip aquifers may be superposed upon a uniform ambient flow field as were the other solutions. As is also the case with the other potential solutions, however, the ambient flow field is not influenced by the presence of boundary conditions.

3.5   Determination of Constants of Integration

For each of the potential solutions (except for drawdown in an unconfined aquifer) there is a combined constant of integration, C, that must be evaluated. Since the constant is added to the entire solution, it simply has the effect of shifting the potential field up or down. The constant is evaluated by solving the potential equations (3.1, for example) at the reference point (x_{ref}, Y_{ref}) input by the user. The difference between the head simulated using the potential equations without the constant, and the head reference (h_{ref}) is the constant, C, which is added to the potential solution for head at each node. This procedure is the same as applied by Strack (1989). Note that for the unconfined aquifer solution, the reference point and head is only used to solve for the ambient uniform flow field.

17

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⊕EPA WHPA

A Modular Semi-Analytical Model for the Delineation of Wellhead Protection Areas

Version 2.0

W H P A

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Disclaimer

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In order to demonstrate use of the WHPA model, and to provide example problems so that users may verify that the code is working correctly, several WHPA delineation examples based upon actual hydrogeological studies in Coming, NY, Albuquerque, NM and Seattle, WA are included in this document. These examples are presented for *instructional purposes only;* due to a variety of simplifying assumptions and inferred data, these case study examples *may not be indicative of actual site conditions.*

Abstract

WHPA is a modular, semi-analytical ground-water flow model designed to assist State and local technical staff with the task of Wellhead Protection Area (WHPA) delineation. The model is PC-based and very user-friendly.

The WHPA model consists of four independent computational modules that may be used to delineate capture zones. Three of the modules contain semi-analytical capture zone solutions; they are applicable to homogeneous aquifers that exhibit two-dimensional, steady ground-water flow in an areal plane. Multiple pumping and injection wells may be present. Barrier or stream boundary conditions which exist over the entire aquifer depth may be simulated. Available aquifer types include confined, leaky-confined and unconfined with areal recharge. One of the three modules is a Monte Carlo module that provides an uncertainty analysis capability. This module allows the effects of uncertain input parameters on the delineated capture zone(s) to be assessed quantitatively.

The fourth module is a general particle tracking module that maybe used as a postprocessor for two-dimensional numerical models of ground-water flow. Because this module uses the hydraulic heads output from a numerical model to delineate capture zones, the hydrogeological scenarios that may be investigated are only limited by the capabilities of the numerical code.

Table of Contents

Appendices

List of Figures

List of Tables

1.0 Introduction

The Amendments to the Safe Drinking Water Act (SDWA), which were passed in June 1986, established the first nationwide program to protect ground-water resources used for public water supplies from all (anthropogenic) potential threats. Unlike previous Federal programs, that have tended to focus on individual contaminant sources, this new effort approaches the assessment and management of pound-water quality fron a more comprehensive perspective. The SDWA seeks to accomplish this goal by the establishment of State Wellhead Protection (WHP) Programs that "protect wellhead areas within their jurisdiction from contaminants which may have any adverse effect on the health of persons." A WHP Program is part of a State's Ground Water Protection Strategy.

One of the major elements of WHP is the determination of zones within which contaminant source assessment and management will be addressed. These zones, called Wellhead Protection Areas (WHPAs), are defined in the SDWA as "the surface and subsurface area surrounding a water well or wellfield, supplying a public water system, through which contaminants are reasonably likely to move toward and reach such water well or wellfield."

The States are given flexibility in determining appropriate operational approaches to WHPA delineation. The U.S. Environmental Protection Agency (EPA) is required by the SDWA to provide technical guidance on the hydrogeologic aspects of this task In June 1987, EPA published the technical background document "Guidelines for Delineation of Wellhead Protection Areas." In this report EPA outlined five criteria that can be used as a technical basis for WHPA delineation:

- Distance
- Drawdown
- Time of travel
- Flow boundaries
- Assimilative capacity

States may select one, or some combination, of the above criteria to form a technical basis for their WHP program. A State's choice of a criteria will likely be based on a combination of technical and nontechnical (e.g., administrative) considerations.

Delineation methods are used to translate the criteria selected by the States to actual, mappable delineation boundaries. EPA, based upon existing ground-water protection programs in the United States and Western Europe, has identified six primary methods for WHPA delineation. The methods are listed below in order of increasing technical sophistication:

- Arbitrary fixed radii
- Calculated fixed radii
- Simplified variable shapes
- Analytical methods
- Hydrogeologic mapping
- Numerical flow/transport models

A detailed explanation of each of these methods may be found in Chapter 4 of the EPA Guidelines document (U.S. EPA, 1987).

The development of a user-friendly computer model to assist State and local technical staff with the delineation of WHPAs is an outgrowth of EPA's Guidelines document. This report documents the capabilities and proper use of the WHPA model, which is a modular semi-analytical and numerical code for the delineation of WellHead Protection Areas. Two of the five delineation criteria, time of travel and flow boundaries, may be addressed using the model. Although one model option is based on numerical model results, the delineation methods used by the model are primarily semi-analytical.

All users are strongly encouraged to read this manual thoroughly prior to applying the WHPA model. Chapter 2 is designed for those of you who refuse to do so -- if you are an experienced ground-water flow modeler it should provide enough information to get you up and running. Chapter 3 is a general overview of the capture zone delineation problem, while chapter 4 is an introduction to one of the most commonly used techniques to delineate capture zones (particle tracking). Chapter 5 is an in-depth overview of the WHPA model. Chapters 6-9 describe in detail the capabilities and limitations of, and provide examples for, the individual capture zone delineation options contained in the WHPA model. Chapter 10 is the last and perhaps most important chapter; it describes some of the errors that may occur if the WHPA model is applied improperly.

2.0 Getting Started

.1 WHPA **Model** Installation

The WHPA model is designed to run on any standard, IBM or compatible XT, AT, or 386 microcomputer (PC) operating under MS DOS version 21 or later. The machine must have a minimum of 640K RAM (Random Access Memory), a hard disk and CGA EGA, VGA or Hercules graphics capability (EGA or VGA is highly recommended). The model will automatically detect and use the math coprocessor if one is present but one is not required

A hard copy of capture zone plots observed on the monitor may be obtained using EPSON, OKIDATA NEC PinWriter and IBM Proprinter dot matrix printers and compatibles, Hewlett-Packard (HP) Laserjet laser printers and compatibles, and Hewlett-Packard and Houston Instruments pen plotters and compatibles. A summary of the available graphics devices supported by WHPA is provided in Table 2.1. If you do not have access to any of the supported hard copy output devices, you may save plot files in standard HPGL format (see section 5.2.3.2) and subsequently use any number of software packages, such as WordPerfect (see Appendix D), PrintAPlot or just about any CAD package, to output the plot on other output devices.

To install the WHPA model on your computer, perform the following steps:

1.   Establish a sub-directory on the hard disk

```
MKDIR WHPA
```

2.   Change directory

```
CD\WHPA
```

3.   Place diskette in drive A

able 2.1

Graphics Devices Supported by WHPA

Device Type	Standard Models Supported
Video	CGA EGA VGA Hercules Graphics Card (HGC)
Dot Matrix Printer	EPSON FX, MX, LQ800, LQ1000, LQ1500, LQ2500 and compatibles OKIDATA and compatibles NEC Pinwriter and compatibles IBM Proprinter and compatibles
Laser Printer	HP LaserJet and compatibles (such as HP DeskJet)
Pen Plotter	Hewlett-Packard and other HPGL-compatibles Houston Instruments and other DM/PL-compatibles

4. Copy files on WHPA diskette to hard disk. Note that steps 3 and 4 must be performed two times.

```
COPY  A:*.*
```

Once step 4 is completed the following files should exist in your WHPA subdirectory.

```
WHPA.EXE        PREGP.EXE
GRAF.EXE        GPTRAC.EXE
PRERQC.EXE      PREMC.EXE
RESSQC.EXE      MONTEC.EXE
PREMW.EXE       SETUP.EXE
MWCAP.EXE       HEDCON.EXE
```

The next step is to execute the setup program by typing

```
                         SETUP
```

The setup program will display a series of menus that prompt for information concerning graphical output. The program first attempts to determine the type of graphics card installed in your computer if the program determines the correct graphics card type, type "Y" to select the default and continue on to select a hard copy output device. If you type "N", a menu will appear that allows selection of the appropriate graphics mode (CGA EGA VGA or Hercules). Once the correct graphics card type is determined, a menu will appear from which any of the hard copy output devices listed in Table 2.1 maybe selected. You must also select the port that the device is connected to (LPT1, LPT2, PRN, COM1 or COM2) and possibly some additional parameters that are device specific (e.g., the number of pens available for a given pen plotter). The communication parameters specfic to your output device, such as baud rate, should be set using the MS DOS "MODE" command. The MODE command will generally be located in your AUTOEXEC.BAT file. Refer to your MS DOS Users Manual for more details.

To execute the WHPA mode, simply type "WHPA".

```
                         WHPA
```

2.2 A Brief Overview of the WHPA Model

The primary objective of the WHPA model is to assist State and local technical staff with the task of WHPA delineation. The WHPA model is an easy-to-use, widely applicable tool for WHPA delineation based on state-of-the-art technology of the ground-water industry. The WHPA model can be divided conceptually into two major sections. The computational modules section contains the Fortran programs that compute the capture zone(s) for a given physical scenario. All of the "number crunching" is performed by these computational modules. The remaining portion of the WHPA model is the user-interface. The interface provides an efficient mechanism for data entry as well as the viewing of model results.

The WHPA model contains four major computational modules: RESSQC, MWCAP, GPTRAC and MONTEC. The capabilities of each of these modules is summarized in Table 2.2. Some users may recognize RESSQCas a modified version of the computer code RESSQ presented by Javandel et al. (1984). The remaining three modules were developed specifically for the EPA Office of Ground-water Protection (OGWP) using state-of-the-technology and some recently published studies available in the literature (e.g., Newsom and Wilson, 1988 and Pollock 1988). The capabilities assumption& limitations, and input requirements for each of the computational modules are discussed in detail m Chapters 6-9. A matrix of the input requirements for each of the computational modules is provided in Table 23. The MONTEC module is not listed in Table 23; it has the same input requirements as MWCAP and semi-analytical GPTRAC with the addition that the uncertain aquifer parameters and their associated probability distributions must be specified. Note that each of the computational modules operate entirely independent of one another.

There are two major assumptions common to <u>all</u> of the computational modules; 1) flow in the aquifer is at steady state, and 2) flow in the aquifer is horizontal (two-dimensional in areal view)The first assumption implies that the aquifer is under equilibrium conditions, and therefore temporal variations in sources and sinks (including pumping) are not considered. The WHPA model is therefore most applicable to continuously used water-supply wells. For RESSQC, MWCAP, and MONTEC the second assumption implies that the aquifer is confined or unconfined if the drawdown-to-initial saturated thickness ratio is small (approximately less than 0.1). This assumption is also applicable for the confined aquifer option in GPTRAC, but this module also has a special unconfined aquifer option that may handle drawdown ratios much larger than 0.1 with minimal error. None of the modules simulate vertiical flow of water within the aquifer explicitly.

The preprocessor is very straightforward to use. The user is prompted, through a series of pop-up windows, for input required by the selected computational module. The following key sequences will be useful when using the preprocessor:

Menu Commands:

<Esc>   H   -   Invoke a series of 1-4 pop-up help screens that define model input parameters and provide guidance on propermodel option selections.

<Esc>   M   -   Return to the main model menu. Any model input parameters that were entered or any changes made to an existing data set <u>will</u> be saved. May also use to Home or End keys.

Table 2.2

Description of WHPA Model Computational Modules

Module Name	Description
RESSQC	Delineates time-related capture zones around pumping wells, or contaminant fronts around injection wells, for multiple pumping and injection wells in homogeneous aquifers of infinite arcal extent with steady and uniform ambient ground-water flow. Well interference effects are accounted for.
MWCAP	Delineates steady-state, time-related or hybrid capture zones for pumping wells in homogeneous aquifers with steady and uniform ambient ground-water flow. The aquifer may be infinite in areal extent or the effects of nearby stream or barrier boundaries can be assessed. If multiple wells are examined the effects of well interference are ignored.
GPTRAC	Semi-analytical Option: Delineates time-related capture zones for pumping wells in homogeneous aquifers with steady and uniform ambient ground-water flow. The aquifer may be of infinite areal extent or it may be bounded by one or two (parallel) stream and/or barrier boundaries. The aquifer may be confined, leaky confined or unconfined with areal recharge. Effects of well interference are accounted for.
	Numerical Option: Delineates time-related capture zones about pumping wells for steady ground-water flow fields. Since this option performs particle tracking using a head field obtained from a numerical (finite difference or finite element) ground-water flow code, many types of boundary conditions as well as aquifer heterogeneities and anisotropies maybe accounted for.
MONTEC	Performs uncertainty analysis for time-related capture zones for a single pumping well in homogeneous aquifers of infinite areal extent. The aquifer may be confined or leaky confined.

Table **2.3**

Required Input for WHPA Model Computational Modules

Required Input	RESSQC	MWCAP	GPTRAC	
			Semi-analytical	Numerical
Units used	■	■	■	■
Aquifer type*			■	
Study area limits	■	■	■	■
Maximum step length	■	■	■	
No. of pumping wells	■	■	■	■
No. of recharge wells	■		■	■
Well locations	■	■	■	■
Pumping/Injection rates	■	■	■	■
Aquifer transmissivity	■	■	■	■
Aquifer porosity	■	■	■	■
Aquifer thickness	■	■	■	■
Angle of ambient flow	■	■	■	
Ambient hydraulic gradient	■	■	■	
Areal recharge rate			■	
Confining layer hydraulic conductivity			■	
Confining layer thickness			■	
Boundary condition type		■	■	
Perpendicular distance from well to boundary		■		
Orientation of boundary		■	■	
Capture zone type		■		
No. of pathlines used to delineate capture zones	■	■	■	■
Simulation time	■		■	■
Capture zone time	■	■	■	■
Rectangular grid parameters				■
No. of forward/reverse pathlines	■		■	■
Starting coordinates for foward/reverse pathlines	■		■	■
Nodal head values				■
No. of heterogeneous aquifer zones				■
Heterogeneous aquifer properties				■

• Confined, unconfined or leaky confined.

```
Menu Commands (cont'd):

<Esc> N          -    Move to the next input screen. May also use the Page
                      Up key.

<Esc> P          -    Move to the previous input screen. May also use the
                      Page Down key.

<Esc> S          -    Obtain a summary of the input parameters.

<Esc> Q          -    Quit editing/input session and return to main model
                      menu. Entered model parameters or changes made to
                      an existing file will not be saved.

F1               -    Exit to DOS. To return to the WHPA model, type
                      EXIT at the DOS prompt.

Input Field Commands:

<Del>            -    Clear the entire input field and reposition the cursor to
                      the beginning of the field.

<Backspace>      -    Standard destructive backspace.

<Enter>          -    Accept the current value in an input field, and position
                      the cursor at the start of the next input field. If an
                      input field is left blank, a value of zero is assigned to
                      the corresponding model parameter. One beep will
                      sound if inappropriate input is entered.
```

2.3 A Brief Example

The best way to introduce the WHPA model is to go through a step-by-step example. This section is designed to do just that so sit down at your computer and type "WHPA". The first screen that will appear is the disclaimer:

```
              ** DISCLAIMER **

Neither the U.S. EPAs Office of Ground-Water Protection, HydroGeoLogic,
Inc., nor any person acting on behalf of either of these entities:

   a)    makes any warranty, express or implied, with respect to this
         software; or

   b)    assumes any liabilities with respect to the use or misuse of
         this software, or the interpretation or misinterpretation of
         any results obtained from this software, or for damages
         resulting from the use of this software.
```

The disclaimer screen may be erased by pressing any key on the keyboard. The next screen is the main menu for the WHPA code.

```
╔══════════════════════════════════╗
║  M A I N   M E N U    F O R    T H E  ║
║                                      ║
║      W H P A    C O D E             ║
╚══════════════════════════════════╝
```

```
┌────────────────────────────────────────────────┐
│                                                  │
│   RESSQC    Modified version of the RESSQ code   │
│   MWCAP     Capture zones for single or multiple │
│             (non-interfering) production wells   │
│   GPTRAC    General particle tracking            │
│   MONTEC    Monte Carlo analysis                 │
│   QUIT      Halt execution of WHPA program       │
│                                                  │
└────────────────────────────────────────────────┘
```

[↑↓] move cursor, <Enter> to select option

This screen allow the user to select one of five available options. Select the MWCAP option by moving the cursor down one line using the down arrow key and depressing "Enter." The next screen is the main menu for the MWCAP option.

```
╔══════════-- MWCAP OPTION --══════════╗
║                                       ║
║        (N)ew Problem                  ║
║                                       ║
║        (C)ontinue Current Problem     ║
║                                       ║
║        (S)ave Current Problem         ║
║                                       ║
║        (L)oad Previous Problem        ║
║                                       ║
║        (R)un Model                    ║
║                                       ║
║        (P)lot Results                 ║
║                                       ║
║        (D)irectory                    ║
║                                       ║
║        (H)elp                         ║
║                                       ║
║        (E)xit                         ║
║                                       ║
╚═══════════════════════════════════════╝
```

Press "N" to input the parameters for a new problem. Next a series of input screens will appear that prompt you for required model input. Type in the numeric values shorn on each screen.

```
╔══════════════════ MWCAP ══════════════════╗
║      Run Title: BRIEF WHPA MODEL EXAMPLE      ║
║                                               ║
║      Units to use for Current Problem:  0     ║
║             0 - meters and days               ║
║             1 - feet and days                 ║
║                                               ║
║           Number of Wells for which           ║
║           Capture-Zones are desired:  1       ║
║                                               ║
║               Minimum X-Coordinate:           ║
║               Maximum X-Coordinate:  3000     ║
║               Minimum Y-Coordinate:           ║
║               Maximum Y-Coordinate:  3000     ║
║                                               ║
║          Maximum Spatial Step Length:  50     ║
║                                               ║
║   ┌─────────────────────────────────────┐    ║
║   │  Change Any Values On This Screen (Y/N)?  │    ║
║   └─────────────────────────────────────┘    ║
╚═══════════════════════════════════════════════╝
```
<Enter> - select value   <Esc> - options menu   <F1> - DOS shell

At the bottom of each input screen the user may change values entered on the screen by typing 'Y. If the input values are all correct type "N" to continue to the next screen.

```
╔═══════════════════════════════════════════════╗
║       AQUIFER PROPERTIES AND LOCATION FOR WELL # 1   ║
║                                               ║
║                    X Coordinate (L):  500     ║
║                    Y Coordinate (L):  1500    ║
║          Well Discharge Rate (L**3/T):  4000  ║
║               Transmissivity (L**2/T):  1000  ║
║   Hydraulic Gradient (dimensionless):  0.00150║
║       Angle of Ambient Flow (degrees):  180   ║
║      Aquifer Porosity (dimensionless):  0.25  ║
║                 Aquifer Thickness (L):  50     ║
║                                               ║
║   ┌─────────────────────────────────────┐    ║
║   │ (H)ELP  (M)AIN  (N)EXT  (P)REVIOUS  (S)UMMARY  (Q)UIT │  ║
║   └─────────────────────────────────────┘    ║
╚═══════════════════════════════════════════════╝
```
<Enter> - select value   <Esc> - options menu   <F1> - DOS shell

The options menu that is displayed at the bottom of the above input screen is obtained by pressing the Escape key at any time. This menu allows you to obtain HELP information, save the values that have been entered and return to the MAIN MWCAP menu go to the NEXT input screen go to the PREVIOUS input screen obtain a SUMMARY of information already entered or QUIT the current application (entered input data not saved). Press "H" for help, and the following menus will appear:

```
═══════════════════════ MWCAP HELP ═══════════════════════

Well Location:
  The location of each well is specified by a Cartesian coord-
  inate pair (x,y). Well locations must reside within the study
  area defined on the previous MWCAP input screen, or an error
  will occur.

Well Discharge:
  The pumping value for each well must be in ft**3/day or
  m**3/day. Because the flow field is assumed to be at steady
  state, only one discharge value per well is required. MWCAP
  assumes that all wells are pumping wells. The sign of the
  pumping value does not matter, it is set in the code.

Transmissivity:
  The transmissivity (T) of an aquifer is a measure of the ease
  with which water can travel through the porous media. T is
  often computed from the equation T=Kb, where K=hydraulic
  conductivity and b=aquifer thickness. The units of T are
  ft**2/day or m**2/day.
```

```
═══════════════════════ MWCAP HELP ═══════════════════════

Gradient:
  The hydraulic gradient (ft/ft or m/m - dimensionless) is most
  commonly measured from a map of piezometric surface or water
  table elevations. The average ambient gradient should be in-
  put to the model, and therefore gradients prior to pumping, or
  gradients not affected by the cone of depression should be used.

Direction of Ground-Water Flow:
  Ground water flows from areas of high hydraulic head towards
  areas of low hydraulic head; for homogeneous, isotropic
  aquifers the direction of ground-water flow is perpendicular to
  the hydraulic head contours. At a given site, the direction of
  ground-water flow may be variable; in this case the average,
  most dominant direction should be used. The direction of flow
  may be 0-360 degrees, with 0=due east, 90=due north, etc.

              Press any key to continue  <ESC=abort>
```

```
┌──────────────── MWCAP HELP ────────────────┐
│                                             │
│ Porosity:                                   │
│   Porosity (dimensionless) is defined as the volume of the
│   voids within the aquifer divided by the total volume of the
│   aquifer. It must always be less than one by definition, and
│   values of 0.15-0.30 are characteristic of most aquifers.
│                                             │
│ Thickness:                                  │
│   The aquifer thickness has units of ft or m.  If the aquifer
│   has a variable thickness, an average value for the aquifer
│   (generally in the vicinity of the pumping well) should be
│   used.                                     │
│                                             │
│                                             │
│                                             │
│                                             │
│                                             │
│            Press any key to continue        │
└─────────────────────────────────────────────┘
```

At any point while these help screens are displayed pressing the Escape key will return you to the appropriate model input screen, while pressing any other key will advance you to the next help screen. Once you have entered the required values for the present input screen, you will move through two more input screens in sequence

```
┌─────────────────────────────────────────────┐
│                                             │
│        BOUNDARY CONDITION INPUT FOR WELL # 1 │
│                                             │
│                                             │
│            Boundary Type:  0                │
│                                             │
│        0 - no boundary                      │
│        1 - stream boundary                  │
│        2 - barrier boundary                 │
│                                             │
│                                             │
│      ┌──────────────────────────────────┐   │
│      │ Change Any Values On This Screen (Y/N)? │
│      └──────────────────────────────────┘   │
└─────────────────────────────────────────────┘
    <Enter>- select value <Esc> - options menu <F1> = DOS shell
```

```
  CAPTURE-ZONE TYPE OPTION FOR WELL # 1


       Capture-Zone Type Option:   2

       0 - steady-state
       1 - hybrid
       2 - time-related


                    Travel Time:   3650

       Number of Pathlines Desired: 20
                (default - 20)
       Plot Capture Zone Boundary ?  1
                (0-No, 1-Yes)
  ┌─────────────────────────────────────────┐
  │ Change Any Values On This Screen (Y/N)? │
  └─────────────────────────────────────────┘
```

<Enter>- select value <Esc> - options menu <F1> DOS shell

The above input screen is the last one for MWCAP. After entering the appropriate values and typing "N", the main MWCAP menu will reappear.

```
═══════════ MWCAP OPTION ═══════════

        (N)ew Problem

        (C)ontinue Current Problem

        (S)ave Current Problem

        (L)oad Previous Problem

        (R)un Model

        (P)lot Results

        (D)irectory

        (H)elp

        (E)xit
```

At this point type "R" in order to execute the MWCAP module. The message will appear

```
**   MWCAP Running   **
```

When the MWCAP run is completed, the main MWCAP menu will appear again. At this point, type "T" to plot the results of the MWCAP run. Hit "Enter" to plot the current graph, and the following figure will appear
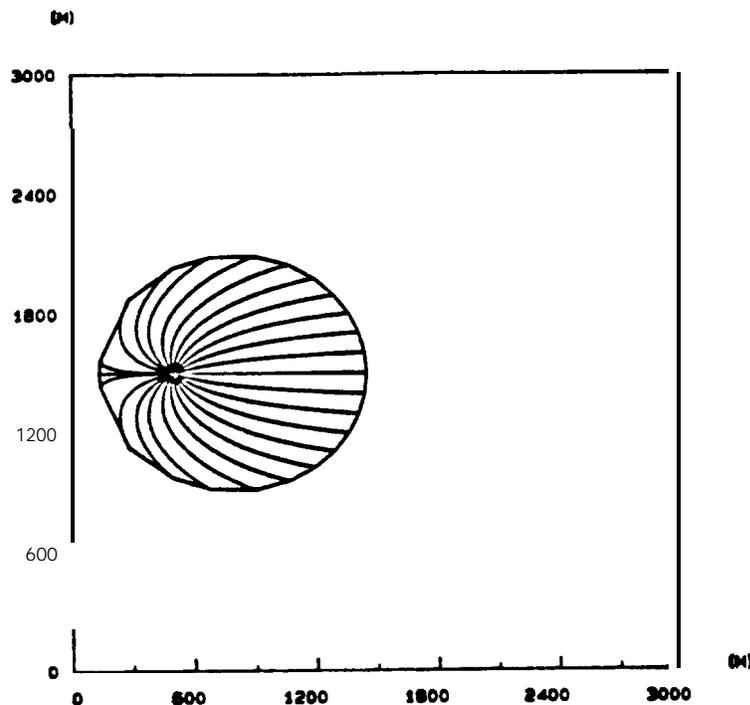

```
(S)ave Plot   (H)ard Copy (O)verlay (R)etrieve Plot (M)ap Scale (E)xit
```

At this point the plotting module (GRAF) options may be used to save the plot file in ASCII, HPGL or ARC/INFO format, to obtain a hard copy if you have access to one of the output devices listed in Table 2.1, to overlay the results of up to fifteen different WHPA model runs (this can not be done at this point because only one plot file has been created thus far), to retrieve a previously created plot file, to scale the plot arbitrarily or to correspond to some map scale, or you may exit the plotting module.

To exit the brief WHPA model example, type "E" to exit from the plotting module, type another "E" to exit from the main MWCAP menu, and finally move the cursor to the "Exit" option on the main WHPA model menu. Users are strongly encouraged to read the remainder of the user's guide prior to applying the WHPA model for capture zone delineation purposes.

3.0 Problem Description

3.1 Introduction

A capture zone is defined as the zone surrounding a pumping well that will supply ground-water recharge to the well. The zone of contribution (ZOC) of a well is identical to the capture zone of a well as defined in OGWP'S "Guidelines for Delineation of Wellhead Protection Areas" (U.S. EPA 1987). For two-dimenensional areal ground-water flow problems, the capture zone corresponds to the area of contribution surrounding the well.

A capture zone for a single well in a homogeneous, isotropic aquifer with an ambient uniform flow is shown in Figure 3.1. Note that the extent of the capture zone in the downgradient direction is defined by the location of a stagnation point. Water particles between the well and the stagnation point travel towards the well in a direction opposite to the regional hydraulic gradient. Water particles downgradient of the stagnation point travel in the direction of regional flow, even though they may be located within the cone of depression of the pumping well. The stagnation point itself is defined mathematically as a point of zero ground-water flow velocity.

3.2 Capture Zone Types

The WHPA model may be used to delineate three types of capture zones; steady-state, time-related, and hybrid. Steady-state and hybrid capture zones can only be obtained using the MWCAP option, while the remaining options as well as MWCAP maybe used to obtain time-related capture zones. This section describes the three types of capture zones.

3.2.1 Steady-State Capture Zones

A steady-state capture zone is the surface or subsurface area surrounding a pumping well that will supply wound-water recharge to the well over an infinite period of time. The typical outline of a steady-state capture zone for a single pumping well is depicted in Figure 3.2. The open-ended shape of the capture zone is due to the fact that given enough time, any particle of water upstream of the well, within the capture zone

Figure 3.1

Terminology for Basic Capture Zone Analysis

<u>Cross section</u>

Ground-water
divide

Pumping Well

Stagnation
point

Ambient
Flow

<u>Plan View</u>

Streamline

Stagnation
point
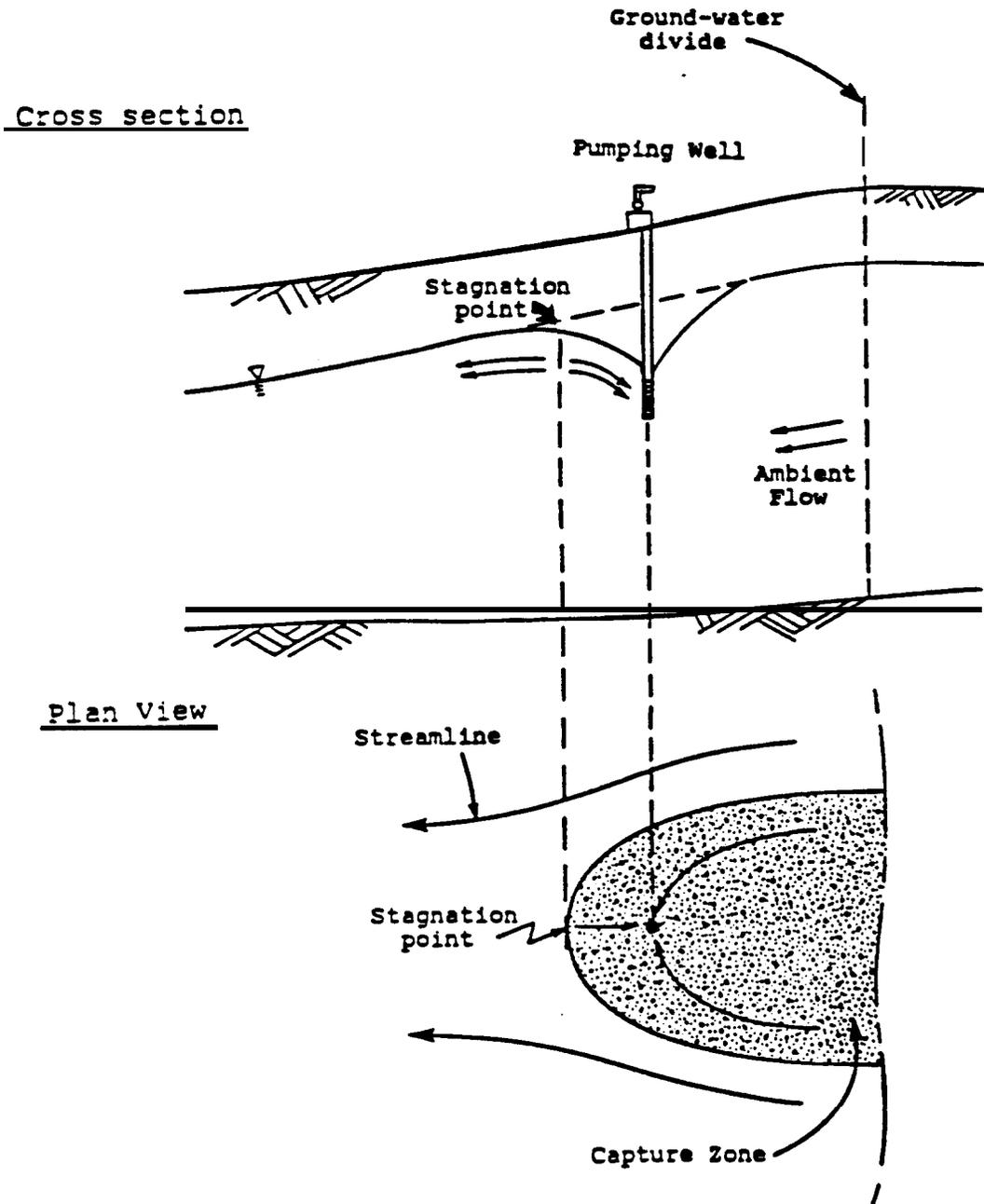
Capture Zone

Figure 3.2

Generic Steady-State, Time-Related, and Hybrid Capture Zone Shapes

Capture Zone Types

Steady-State

Time-Related   AMBIENT FLOW

Hybrid
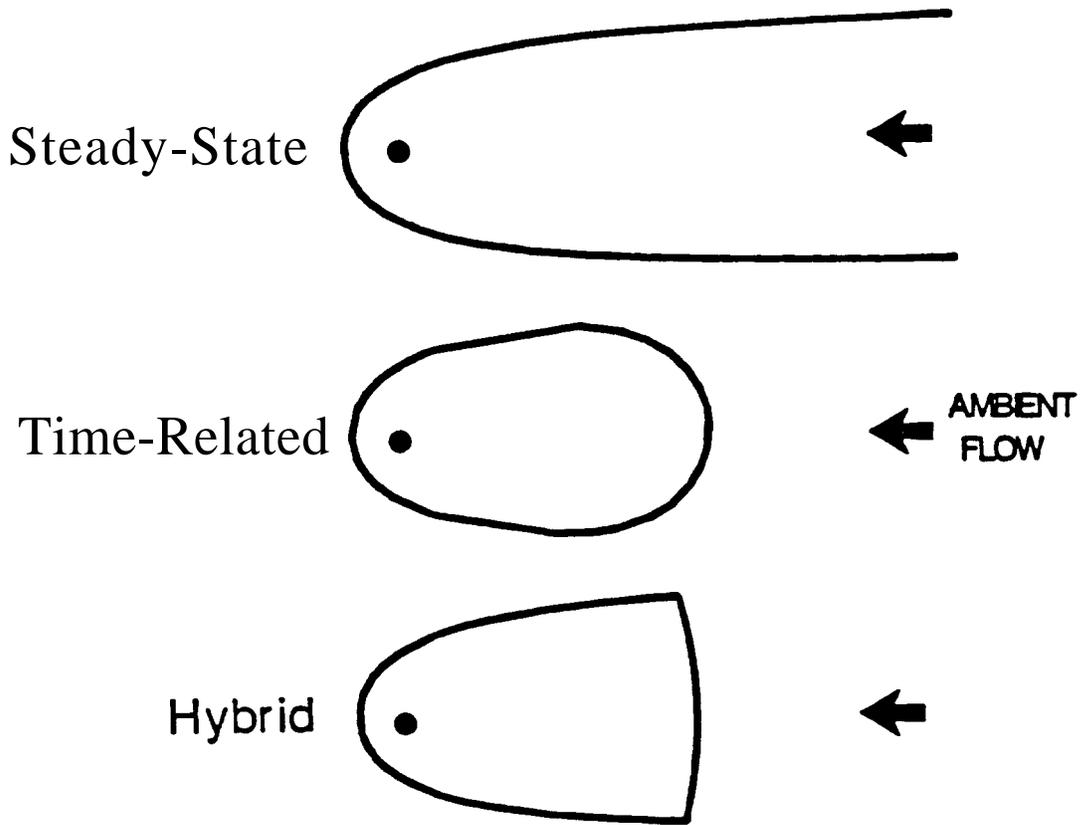
boundaries, will eventually travel to the well. In practice, the upstream end of the capture zone would be "capped" in some manner due to physical and/or managerial restrictions. For example, a steady-state capture zone may terminate at a ground-water flow divide.

3.2.2 Time-Related Capture Zones

A time-related capture zone is the surface or subsurface area surrounding a pumping well that will supply ground-water recharge to the well within some specified period of time. When calculating time-related capture zones, OGWP generally recommends that time periods of 10-25 years be considered

A typical outline of a time-related capture zone for a single pumping well is depicted in Figure 3.2. A time-related capture zone is always represented by some closed shape. In general, time-related capture zones are less conservative (enclose smaller areas) than steady-state or hybrid capture zones. As the specified time increases, however, differences between the three capture zone types in the proximity of the pumping well become negligible.

Note that time-related capture zones may be calculated when the ground-water flow field is at steady-state. A steady flow field implies that the direction and magnitude of the ground-water flow velocity at any point within the aquifer is constant for all time; this concept should not be confused with the fact that it takes some finite period of time for a water particle within a capture zone to travel to a pumping well located within a steady-state flow field.

3.2.3 Hybrid Capture Zones

As the name implies, a hybrid capture zone is a combination between a steady-state and a time-related capture zone. A typical outline of a hybrid capture zone is shown in Figure 3.2. The hybrid capture zone is identical to the steady-state capture zone in all respects except that it is "capped" on the upstream end (Figure 3.2). A particle of water released from the mid-point of the capping segment will reach the pumping well within some specified time. Therefore, the cap on the hybrid capture zone approximates a segment of a time-related capture zone. The hybrid capture zone can be viewed as an implementable alternative to the steady-state capture zone.

4.0 Solution Techniques

The WHPA model delineates capture zones about pumping wells using the particle tracking technique. The term "particle" is used only for conceptual purposes. One may view a particle as an individual water molecule or an individual molecule of a conservative tracer that moves through the aquifer coincident with the bulk movement of ground-water flow; dispersion and diffusion do not affect the particle location.

To obtain steady-state or hybrid capture zones, particles are released from the stagnation point(s) of the system. Time-related capture zones arc obtained by tracing the pathlines formed by a series of particles placed around the well bore of the pumping well. The code uses both forward and reverse particle tracking depending upon the option(s) selected. Forward tracking involves the tracking of panicles in the direction of ground-water flow, while reverse tracking involves the tracking of particles in the direction opposite to ground-water flow. The following two sections provide an introduction to the delineation of capture zones using the particle tracking technique. For a more detailed explanation, refer to Appendix A-3.

Although the term pathline is used throughout this document it should be noted for completeness sake that pathlines correspond to streamlines for the case of steady ground-water flow. The term streamline, rather than pathline, is used often in the relevant literature.

4.1 Particle Tracking

The particle tracking method requires knowledge of the ground-water flow velocity at any point within the aquifer. The flow velocities are expressed in terms of Darcy's Law, which may be written as:

$$Q = KiA \tag{4-1}$$

where Q is the volumetric flow rate, K is the hydraulic conductivity of the porous medium, i is the hydraulic gradient (change in hydraulic head over some specified horizontal distance) and A is the cross-sectional area of flow. The specific discharge (or Darcy velocity) is defined **as:**

$$q = Q/A = Ki \tag{4-2}$$

The average pore-water velocity for an individual fluid particle moving through the porous medium may be written as

$$v = q/\theta \tag{4-3}$$

where v is the seepage velocity and θ is the effective porosity of the medium. Equation (4-3) may be generalized to describe the x and y components of seepage velocity for two-dimensional, horizontal flow;

$$v_x = q_x/\theta \qquad v_y = q_y/\theta \tag{4-4}$$

Several methods are available to obtain the seepage velocity components, v_x and v_Y for a given flow field. For the RESSQC, MWCAP, MONTEC and semi-analytical GPTRAC options of the WHPA model, the required velocities are obtained analytically. That is, there are exact mathematical solutions for seepage velocity programmed into the Fortran code. Using these solutions, the code solves for v_x and v_y at any specified location (x_i, y_i) within the aquifer.

The numerical option of the GPTRAC module uses a slightly different method to calculate velocities. This option requires that hydraulic head values at the nodes of a rectangular grid be supplied to the code. The grid may be a finite element or a finite difference grid. In the latter case, the nodes may be located at the grid-block centers (block-centered grid) or at the intersection of the grid lines (mesh-centered grid). Velocities at any location are then calculated using a simple analytical solution within each grid block (see Appendix C.3). The computed velocities are dependent upon the nodal hydraulic head values, and the grid block hydraulic conductivity and effective porosity values.

Once velocities can be determined, pathlines (the route that an individual particle of water follows through an aquifer) may be delineated using particle tracking. Particle tracking delineates pathlines by calculating the distance $d\ell$, that is traversed in a given time dt. The distance a particle travels during a given period of time is defined by

$$d\ell = (dx^2 + dy^2)^{\frac{1}{2}} \tag{4-5}$$

where

$$dx = v_x dt = q_x dt / \theta \tag{4-6a}$$

$$dy = v_y dt = q_v dt / \theta \tag{4-6b}$$

where dx and dy are the projections of $d\ell$ on the x and y axis, respectively. In practice, equations 4-5 and 4-6 are solved using some form of numerical integration; i.e. the differential dt is approximated by a finite time step Δt, and the differential $d\ell$ is approximated by a finite spacial increment $\Delta\ell$. Therefore, the path of a water particle may be traced using

$$x_{i+1} = x_i + \Delta x = x_i + v_x \Delta t \tag{4-7a}$$

$$y_{i+1} = y_i + \Delta y = y_i + v_y \Delta t \tag{4-7b}$$

where (x_i, y_i) is the location of the water particle at time t, and (x_{i+1}, y_{i+1}) is the position of the particle at time $t + \Delta t$.

The terms forward and reverse particle tracking are used frequently throughout this document. Forward tracking refers to the procedure of tracking water panicles in the direction of ground-water flow, while reverse tracking refers to the procedure of tracking water particles in the direction opposite to that of ground-water flow. Since ground water flows towards a pumping well, reverse tracking is used when particles are released about the circumference of a well bore. If particles arc released upgradient of a pumping well, forward tracking is used to determine whether or not the particle will be captured by the well. Forward tracking is based upon equations (4-7a) and (4-7b), and reverse tracking is based upon these equations with the sign of the velocity terms v_x and v_y reversed (multiplied by negative one).

Forward tracking can be used to determine whether or not a pumping well will be contaminated by a particular contaminant source. For example, panicles released at the edge of a waste disposal facility may be forward-tracked for a specified time to determine if they will enter a pumping well. If a production well has been contaminated, reverse tracking may be used to determine potential sources of contamination. To do this, particles would be released at the contaminated well and reverse-tracked through time to identify potential sources of the contaminated water.

4.2 Pathline and Capture Zone Delineation

Using the particle tracking method, pathlines within a region can be delineated for any specified travel distance or time. The general procedure is illustrated in Appendix B (Figure B.5).

Time-related capture zones are delineated by placing a series of water particles (generally about 20-50) at sequential locations along the perimeter of a small circle representing the well boundary. Individual pathlines for each of these particles are then traced using reverse tracking. Pathlines arc terminated when the assigned travel time value is reached or when a plotting boundary is encountered (Figure 4.la). The capture zone consists of the entire region enclosed by the delineated pathlines.

To delineate the boundaries of steady-state and hybrid capture zones, it is convenient to release particles from the stagnation point(s). Pathlines that are forward tracked will terminate at the pumping well, while pathlines that are reverse tracked will end at a study area boundary (Figure 4.lb). The pathlines that emanate from the stagnation point(s) form the steady-state capture zone boundary.

Note that in the case of Figure 4.lb where the capture zone intercepts the stream boundary, the stream itself forms a segment of the capture zone boundary, and the two pathlines extending from the stagnation points to the well partition the well recharge attributable to the stream and the ambient aquifer flow respectively. The portion of the capture zone attributable to the stream is refereed to as the "stream capture zone".

The perimeter of a well bore and stagnation points are convenient locations to release particles for capture zone delineation purposes; however, it is often desirable to release particles from other locations within the study area (see previous section on reverse and forward particle tracking). The RESSQC and GPTRAC options of the WHPA model allow the user to specify arbitrary starting particle locations. The particles may be either forward or reverse tracked.

Figure 4.1

**Pathline Tracking to Delineate Time-Related (a)
and Steady-State (b) Capture Zones**

(a)

(b)
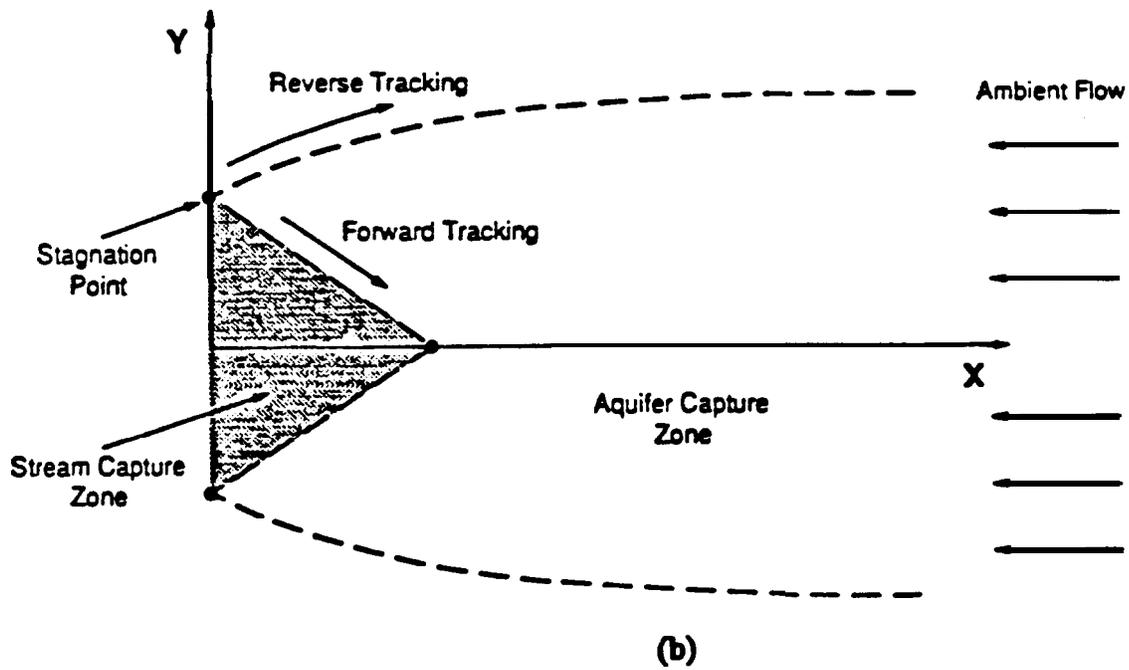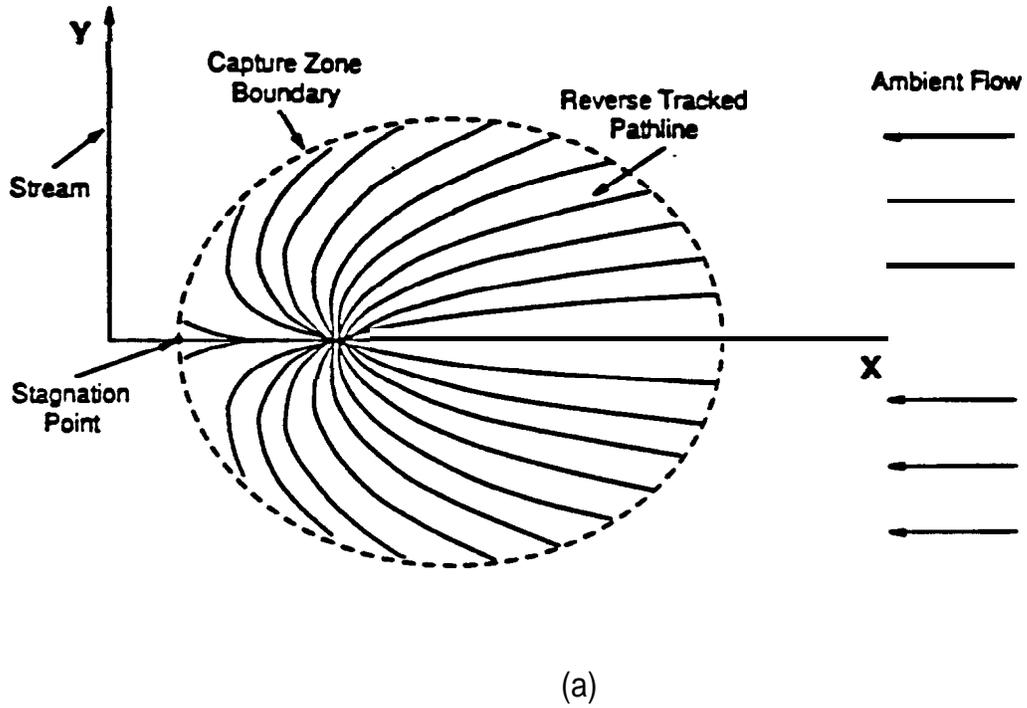
5.0 Overview of the WHPA Model

5.1 Objectives

The primary objective of the WHPA model is to assist State and local technical staff with the task of WHPA delineation. The WHPA model is an easy-to-use, widely applicable tool for WHPA delineation based on state-of-the-art technology of the ground-water industry. The model is designed for widespread usc among technology staff who may have only a basic understanding of ground-water flow processes and computer model applications on the IBM PC

5.2 Structure and Organization of the WHPA Model

The WHPA model can be divided conceptually into two major sections. The computational modules section contains the Fortran programs that compute the capture zone(s) for a given physical scenario. All of the "number crunching" is performed by these commutational modules. The remaining portion of the WHPA model is the user-interface. The interface provides an efficient mechanism for data entry as WHPA as the viewing of model results. The composition of, and the relationship between these two portions of the model is discussed in the next two sections.

5.2.1 Computational Modules

The WHPA model contains four major computational modules: RESSQC, MWCAP, GPTRAC, and MONTEC. The capabilities of each of these modules is summarized in Table 5.1. Some users may recognize RESSQC as a modified version of the computer code RESSQ presented by Javandel et al. (1984). The remaining three modules were developed specifically for OGWP using state-of-the-art technology and some recently published studies available in the literature (e.g., Newsom and Wilson, 1988). The capabilities, assumptions, limitations, and input requirements for each of the computational modules are discussed in detail in Chapters 6-9. A matrix chart of the input requirements for each of the computational modules **is** provided in Table 5.2. The MONTEC module is not listed in Table 5.2; it has similar input requirements as MWCAP and semi-analytical GPTRAC with the addition that the uncertain aquifer parameters and their associated probability distributions must be specified. Note that each of the computational modules operate entirely independent of one another.

Table 5.1

Description of WHPA Model Computational Modules

Module Name	Description
RESSQC	Delineates time-related capture zones around pumping wells, or contaminant fronts around injection wells, for multiple pumping and injection wells in homogeneous aquifers of infinite areal extent with steady and uniform ambient ground-water flow. Well interference effects are accounted for.
MWCAP	Delineates steady-state, time-related or hybrid capture zones for pumping wells in homogeneous aquifers with steady and uniform ambient ground-water flow. The aquifer may be infinite in areal extent or the effects of nearby stream or barrier boundaries can be assessed. If multiple wells are examined the effects of well interference are ignored.
GPTRAC	Semi-analytical Option: Delineates time-related capture zones for pumping wells in homogeneous aquifers with steady and uniform ambient ground-water flow. The aquifer may be of infinite areal extent or it may be bounded by one or two (parallel) stream and/or barrier boundaries. The aquifer may be confined, leaky confined or unconfined with areal recharge. Effects of well interference are accounted for.
	Numerical Option: Delineates time-related capture zones about pumping wells for steady ground-water flow fields. Since this option performs particle tracking using a head field obtained from a numerical (finite difference or finite element) ground-water flow code, many types of boundary conditions as well as aquifer heterogeneities and anisotropies maybe accounted for.
MONTEC	Performs uncertainty analysis for time-related capture zones for a single pumping well in homogeneous aquifers of infinite areal extent. The aquifer may be confined or leaky confined.

Table 5.2

Required Input for WHPA Model Computational Modules

Required Input	RESSQC	MWCAP	GPTRAC	
			Semi-analytical	Numerical
Units used	■	■	■	■
Aquifer type*			■	
Study area limits	■	■	■	■
Maximum step length	■	■.	■	
No. of pumping wells	■	■	■	■
No. of recharge wells	■		■	■
Well locations	■	■	■	■
Pumping/injection rates	■	■	■	■
Aquifer transmissivity	■	■	■	■
Aquifer porosity	■	■	■	■
Aquifer thickness	■	■	■	■
Angle of ambient flow	■	■	■	
Ambient hydraulic gradient	■	■	■	
Areal recharge rate			■	
Confining layer hydraulic conductivity			■	
Confining layer thickness			■	
Boundary condition type		■	■	
Perpendicular distance from well to boundary		■		
Orientation of boundary		■	■	
Capture zone type		■		
No. of pathlines used to delineate capture zones	■	■	■	■
Simulation time	■		■	■
Capture zone time	■	■	■	■
Rectangular grid parameters				■
No. of forward/reverse pathlines	■		■	■
Starting coordinates for forward/reverse pathlines	■		■	■
Nodal head values				■
No. of heterogeneous aquifer zones				■
Heterogeneous aquifer properties				■.

● Confined, unconfined or leaky confined.

There are two major assumptions common to __all__ of the computational modules; 1) flow in the aquifer is at steady-state, and 2) flow in the aquifer is horizontal (two-dimensional in areal view). The fit assumption implies that the aquifer is under equilibrium conditions, and therefore temporal variations in sources and sinks (including pumping) are not considered. The WHPA model is therefore most applicable to continuously used water-supply wells. For RESSQC and MWCAP, the second assumption implies that the aquifer is confined or unconfined if the drawdown-to-initial saturated thickness ratio is small (approximately less than 0.1). This assumption is also applicable for the confined aquifer option in GPTRAC but this module also has a special unconfined aquifer option that may handle drawdown ratios much larger than 0.1 with minimal error. None of the modules simulate vertical flow of water within the aquifer explicitly.

5.2.2 **Preprocessor**

The desired computational module (RESSQC, MWCAP, GPTRAC or MONTEC) is selected from the main WHPA model menu that appears immediately after the disclaimer screen when the code is run. Each of the modules have preprocessors that provide for the convenient interactive input of parameters. Parameter values are entered through a series of input screens that appear on the monitor. Each input screen has one or more associated help screens that define the input parameters and guide the user in the selection of appropriate modeling options. The user is prompted only for those parameter values that are required for a given application.

5.2.2.1 Computational Modules Main Menu

The "main menu" for each of the computational modules will appear after the desired module is selected from the main WHPA model menu. The available options are as follows:

```
(N)ew  Problem
(C)ontinue Current Problem
(S)ave Current Problem
(L)oad Previous Problem
(R)un Model
(P)lot Results
(Directory
(H)elp
(E)xit
```

The desired option is invoked by depressing the letter key marked by parenthesis.

The "New Problem" option initiates a new run of the computational module. In this case, all of the problem input parameters will need to be entered at the appropriate input screen.

The "Continue Current Problem" option maybe used when a problem has been run and the user wishes to rerun the code using the same, or similar, simulation options and/or input parameters. When this option is chosen, the input parameters (e.g. , well location) and simulation options (e.g., capture zone type) will be echoed to the screen as each input window appears. The user may then selectively change any input value, and input parameters for the entire problem need not be reentered.

The "Save Current Problem" option is useful for saving the input associated with a particular capture zone delineation scenario. The input is saved in a user-specified file.

Users should not confuse this option with the "Save Plot" option available in the GRAF module. The "Save Plot" option saves the actual capture zone plot file output by a computational module; the "Save Current Problem" option saves only the input parameters required to calculate the capture zone(s).

The "Load Previous Problem" option is used to retrieve applications that were saved previously using the "Save Current Problem" option.

Note that the "Save Current Problem" and "Load Previous Problem" options support the use of full DOS pathnames. Therefore, files maybe saved to, or retrieved from, drives and directories other than the current drive and the current directory.

The "Run Model" option initiates execution of the selected computational module (e.g. GPTRAC). The computed pathlines and capture zones are automatically written to the WHPA.PLT "file for subsequent plotting using the "Plot Results" option. Another, more extensive output file that contains an echo of the input parameters as well as the model output is written for each run (section 5.2.3.4).

Once an application has been run, the "Plot Results" option will produce a plot of the calculated capture zone(s) on the screen. When this option is selected, the file WHPA.PLT is plotted by default, or other plot files may be retrieved or overlayed.

The "Directory" option may be used to display a listing of the files that reside in any directory. When this option is selectecd the user is prompted for a pathname for which a directory is to be displayed. The default (Enter key) is to display the contents of the current directory. The directory option also supports use of the DOS wildcard character (*) in file names.

The "Help" option will display a brief description of the other options, and the "Exit" option returns the user from the selected computational module to the main menu of the WHPA code.

5.2.2.2 Input Screens

If the "New Problem", "Continue Current Problem" or "Load Previous Problem" are selected from the main menu of the executable module, the user is prompted for the required model parameters through a series of input screens. A typical input screen is shown m Figure 5.1a; this particular screen was selected from the MWCAP module preprocessor. For the application show the user has already input the location of pumping well number one, and the next value that must be entered is the well discharge rate. At this point the user simply types in the discharge value. Only numerals and decimal points will be accepted - letters or other symbols will not appear on the screen. The arrow keys may be used to move to the left or right of the current cursor position; they may not be used to move the cursor up or down. The input field width is 10 spaces for real values and 1-5 spaces for integer values. If the cursor is moved past the end of this invisible "box", it will appear at the first space again. Real and integer values are distinguished automatically by the program, and therefore a decimal point does not need to be typed if a value is real. If a mistake is made typing in the value, the Backspace or the Delete key maybe used. The Delete key clears the entire input field and positions the cursor at the beginning of the field. Finally, the Enter key will enter the typed value into the program and position the cursor at the beginning of the next input field. If an input field is left blank a zero value will be assigned to the corresponding parameter if a non-zero default is not specified.

Certain input values are not admitted if they are inappropriate for the current parameter. For example, WHPA will not accept negative values for transmissivity or aquifer thickness, and porosity values must be between zero and one.

Figure 5.1

Typical WHPA Model Input Screen (a) and
Typical Input Screen With The Options Menu Invoked (b)

AQUIFER PROPERTIES AND LOCATION FOR WELL # **1**

X Coordinate (m): 500
Y Coordinate (m): 1500
Well Discharge Rate (rn**3/d): —
Transmissivity (m**2/d):
Hydraulic Gradient (dimensionless):
Angle **of** Ambient Flow (degrees):
Aquifer **Porosity** (dimensionless):
Aquifer Thickness (m):

<Enter>- select value <Esc> options menu <F1> - DOS shell
(a)

AQUIFER PROPERTIES AND LOCATION FOR WELL # 1

X Coordinate (m): 500
Y Coordinate (m): 1500
Well Discharge Rate **(m**3/d): —**
Transmissivity (m**2/d):
Hydraulic Gradient (dimensionless):
Angle of Ambient Flow (degrees):
Aquifer Porosity (dimensionless):
Aquifer Thickness (m):

| (H)ELP | (M)AIN | (N)EXT | (P)REVIOUS | (S)UMMARY | **(Q)UIT** |

<**Enter**>-- select value <Esc> **options** menu <F1> - DOS shell
b)

If the "Load Previous Problem" or the "Continue Current Problem" is selected, the values of each input parameter and model option that exist in the current data set will appear automatically on the screen. These values may be changed either by typing a new value, in which case the previous value is erased or by using the arrow keys to selectively change one or more digits in an input field. In any case, the value that exists on the screen when the Enter key is depressed will be the value that is read by the code.

Another useful option available by typing the F1 key is the ability to exit to DOS. When this option is invoke& the WHPA model resides in memory, and you may return to the model at any time by typing "EXIT' (this procedure is the same as that used by Lotus 123 and other commercial software packages). Exiting to DOS maybe useful if you want to view certain files or directories at the DOS level, but you do not wish to exit the WHPA model to do so. If this option is invoked, remember to return to the WHPA model at some point and exit the code in a normal fashion.

Once all of the required parameters on a given screen have been entered the prompt "Change Any Values on This Screen (Y/N)?" will appear. If a T' is typed the cursor will be repositioned at the beginning of the first input field so that one or more parameter values can be changed. The Enter key can be used to move down the screen to each parameter input field. If a "N" is typed the next input screen will appear.

5.2.23 Options Menu

The options menu can be accessed from any input screen by depressing the Escape key. Figure 5.lb shows the same input screen as in Figure 5.la after the Escape key has been depressed. The options available are as follows:

Help		Invoke a series of 1-4 pop-up help screens to assist the user in selecting appropriate parameter values and modeling options.
Main	·	Exit the current application and return to the main menu of the current computational module. Changes (if any) to the current data set will be saved. May also use the Home or End keys.
Next		Move to the next input screen. May also use the Page Down key.
Previous	-	Move to the previous input screen. May also use the Page Up key.
Summary	-	Obtain a summary of the input values associated with the current application and each well.
Quit	·	Stop execution of the current computational module. Changes (if any) to the current data set will] not be saved.

The desired function is selected by typing the first letter of the corresponding word (e.g., type 'H' to access the help screens). Depressing the Escape key again will clear the options menu. Note that you can perform some of the functions on the options menu by using the Home, End, Page Up or Page Down keys directly.

5.2.2.4 Input Files

Each time one of the WHPA code modules is used to run a problem, the parameter values input via the preprocessor are saved in a file in the current directory. The default file names are as follows: .

Executable Module	Input File Name
RESSQC	RESSQC.SAV
MWCAP	MWCAP.SAV
GPTRAC	GPTRAC.SAV
MONTEC	MONTEC.SAV

These files are used by some of the main menu options. For example, if the user has run an application using MWCAP, and then depresses "S" for "Save Current Problem", the file MWCAP.SAV would be copied to the user-specified file name. If the user wishes at a later time to rerun the problem, the file could be retrieved using the "Load Previous Problem" option and the file that the input parameters were stored in would be copied to MWCAP.SAV.

5.2.3 Postprocessor

The postprocessor of the WHPA code is a plotting routine named GRAF. When any of the executable modules has been successfully run, the GRAF module may be invoked to plot the capture zone results on the monitor. The capture zones for multiple wells will be plotted in different colors if a color monitor is used, or in different shades of amber (or the default display color) if a monochrome monitor is used. If, in addition to capture zone analysis, forward- and/or reverse-tracked pathlines are specified, all of the forward-tracked pathlines and/or all of the reverse- tracked pathlines will be plotted in the same color. A hard copy of the plot can be obtained from any of the printer or plotter output devices listed in Table 2.1.

5.2.3.1 GRAF Module Options

The plot of an example application of MWCAP is shown in Figure 5.2 as it would appear on a monitor with EGA resolution (colors not reproduced). Once the capture zones are plotted the user may select one of the six listed options to continue execution of the code. The function of each option is documented in Table 5.3. The options are invoked by typing the first letter of the description (e.g., type "S" to save the current plot file).

The default plot file generated by WHPA is WHPAPLT. This file is copied to a user-specified file name if the "Save Plot" option is invoked. The file can be replotted using the new file name and the "Retrieve Plot" option. The "Overlay" option retrieves up to 15 plot files consecutively, and plots them one on top of the other. When the overlay option is used, the plotting information for the overlay plot is saved in the file WHPA.BLD. Therefore, the "Save Plot" option may be used subsequent to the "overlay" option to save a series of related plots that have been overlayed. The overlay feature is particularly useful for sensitivity analysis, where the effect of varying input parameter values (e.g., transmissivity) on the size and shape of a capture zone is investigated

The output from all four computational modules is stored in a compatible format and therefore plots produced using different modules may be overlayed. However, prior to overlaying two plots, GRAF checks if the length units (ft or m) for each plot are compatible. If they are not an error message is displayed and the user must choose another GRAF option. If two plot files contain different values for the minimum and maximum x and y coordinates, the smallest values will be used for the minimum coordinates and the largest values will be used for the maximum coordinates when the plots are overlayed. This procedure ensures that a portion of a plot is not erased inadvertently.

The "Map Scale" option allows arbitrary scaling of the plot or automatic scaling of the plot to one of five standard USGS topographic map scales. The map scales available are listed in Table 5.3. This option enables the user to transfer capture zone results directly from WHPA model hard copy output to project base maps. Note that the physical area available for plotting varies with the selected output device, and therefore capture zones that are large relative to the selected map scale may be truncated in the x and/or y plotting directions. Most of the available output devices (standard EPSON, OKIDATA, NEC and IBM dot matrix printers and HP LaserJet laser printers) are limited by a maximum plot size of 10x 8 inches. The wide carriage version of the dot matrix printers have a maximum plot size of 13.6 x 10 inches. The available plot size for the Hewlett-Packard and Houston Instruments pen plotters varies widely with the model type.

Figure 5.2

Typical WHPA Model Plot Displayed on CRT Monitor Using the GRAF Module
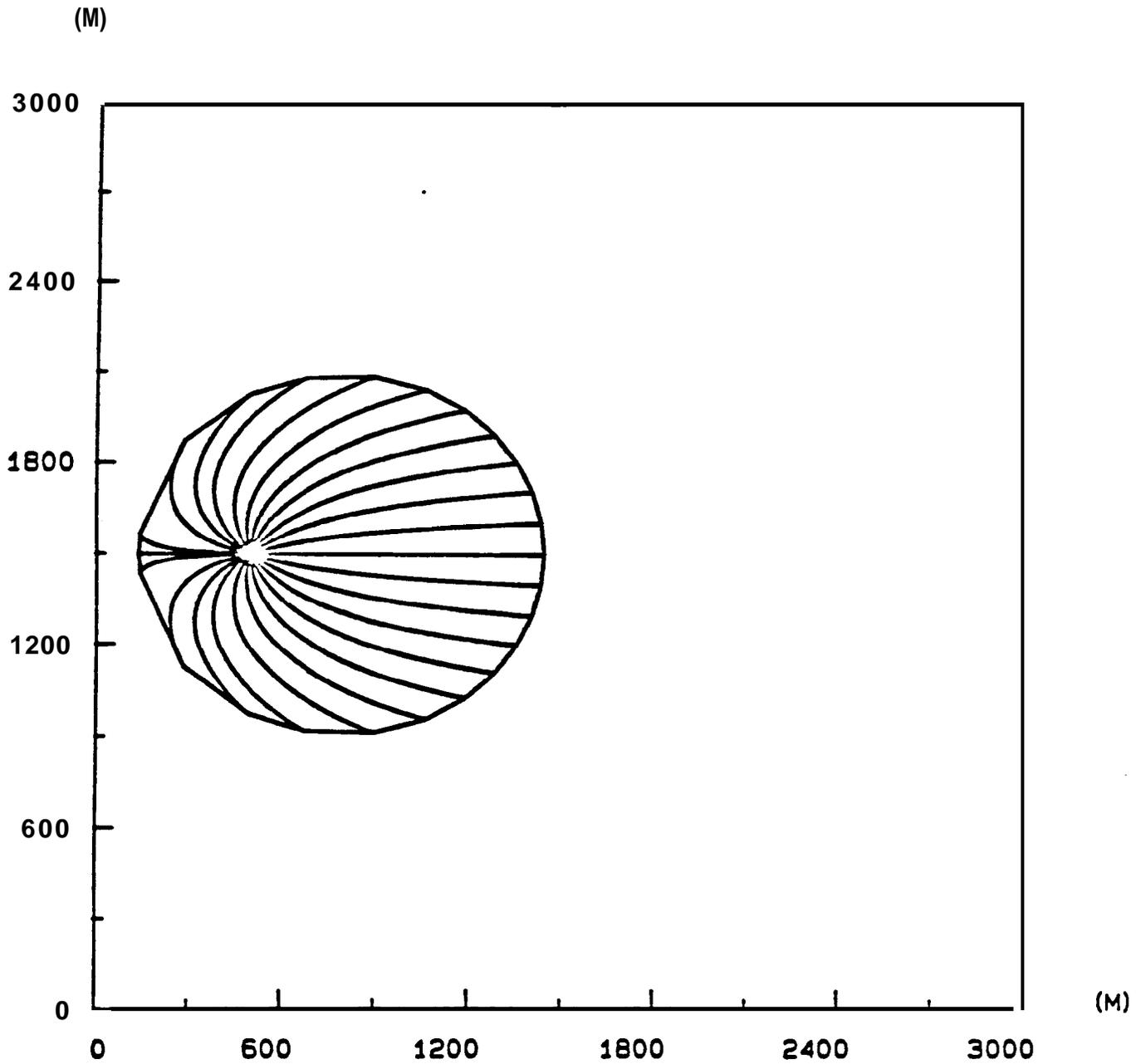
(S)ave Plot   (H)ard Copy   (O)verlay   (R)etrieve Plot   (M)ap Scale   (E)xit

Table 5.3

GRAF Module Options

Option	Function
Save Plot	Saves the current plot file (WHPA.PLT) to a user-specified file name. File may be saved in ASCII, HPGL, or ARC/INFO format.
Hard Copy	Generates a hard copy of the capture zone plot on any of the output devices listed in Table 2.1.
Overlay	Plots up to 15 plot files, one on top of the other. The user is prompted for the names of the files to plot. Plot will not be generated if the units specified for each plot file are not compatible.
Map Scale	Allows the user to scale the plot (up or down) to any arbitrary ratio or to one of 5 standard USGS topographic map scales (7.5 minutes, 7.5 × 15 minutes, 15 minutes, 30 × 60 minutes, 1 × 2 degree).
Retrieve Plot	Plots a single, user-specified plot file.
Exit	Exit the GRAF module and return to the main menu of the current computational module.

The "Hard Copy option allows the user to obtain a capture zone plot on EPSON, OKIDATA, NEC Pinwriter or IBM Proprinter (or compatible) dot matrix printers; HP LaserJet or compatible laser printers; and Hewlett-Packard and Houston Instruments pen plotters (or compatibles). The output device and the appropriate port specification (LPTl, LPT2, COM1 or COM2) are selected using the SETUP program (see section 21). The dot matrix and laser printers are monochrome output devices and only one color is used for plotting. Most pen plotters have six or more pens available. If a monochrome plotting mode was selected in the setup routine, only pen 1 of the plotter will be used to plot the WHPA model results. If the color plot option was selected the axis and borders of the plot will be plotted using pen 1, but the capture zones and pathlines will be plotted using the remaining pens in sequential order (i.e., pen 2 for the first capture zone, pen 3 for the next one, etc.).

It should be noted that when the GRAF module is first invoked the six options described above appear in menu form prior to the actual plot of the capture zone(s). To proceed with the plot at this point simply depress the Enter key. However, you may also invoke any of the options listed prior to plotting the graph. For example, you may use the "overlay" option to enter two or more file names, and then the overlayed plot will appear when the capture zone(s) are plotted. This procedure is useful because the GRAF module options may be invoked prior to viewing the plot.

The GRAF module is designed in such a way that scale distortions will not occur when capture zones are plotted: 1 ft or m along the x-axis will always equal 1 ft or m along the y-axis. For example, if the x-axis represents a distance of 6,000 ft when plotted, and they-axis represents a distance of 4,000 ft, the length of the plotted y-axis will be equal to two thirds the length of the plotted x-axis. The scaling is precise when model results are plotted on an output device, but only approximate when results are plotted on the monitor.

5.2.3.2   HPGL File Option

The "Save Plot" option allows the user to save plot files in Hewlett-Packard Graphics Language (HPGL) format. HPGL is a commonly used standard in the computer graphics industry, and consequently many word processing, desktop publishing, computer aided design (CAD) and specialized computer graphics packages have the capability to import and process HPGL files. Most of these software packages also have the capability to output graphics images (capture zone plots) on numerous types of laser and dot-matrix printers. Step-by-step instructions for incorporating a HPGL file into WordPerfect are presented in Appendix D. This option was included to aid users that do not have access to any of the

output devices listed in Table 2.1, or who may wish to incorporate capture zone plots directly into reports or documents.

Users are cautioned that the original plot scale may not be maintained by all software packages. If secondary software is used to import and subsequenty output WHPA model HPGL files, the size of the resulting plot should be carefully checked.

5.2.3.3   ARC/INFO File Option

A geographic information system (GIS) can be a valuable tool in a WHP program. GIS technology is commonly used to integrate and analyze numerous types of spatial data. A particularly common use of a GIS is to develop maps or "coverage". A coverage may consist of the spatial representation of a single attribute such as land use, or of multiple attributes, such as land use, aquifer type, and municipal well locations. Schooley (1989) used a GIS in a pilot project to eliminate wells from the WHP program that were not immediately susccptiile to contamination; to prioritize the remaining wells for WHPA delineation; and to target problem sites for more intensive monitoring, enforcement and remediation efforts.

The "Save Plot" option provides a facility for saving WHPA model results in an ASCII file that may be used as input to the ARC/INFO proprietary GIS developed by the Environmental Systems Research Institute (ESRI). The ARC/INFO file option is designed to construct files compatible with the ARC GENERATE LINES command. Note that once an ARC/INFO input file is obtained using WHPA additional processing may be required to convert the WHPA model Cartesian coordinates to the appropriate coordinate system (perhaps latitude and longitude or state plane) used for the GIS application. Such processing should be performed by a GIS specialist.

Although the WHPA model supports output specifically for the ARC/INFO software, it is a relatively simple matter to process the standard WHPA model plot files for input into other GIS packages.

5.2.3.4   General Output Files

Each time an executable module of the WHPA code is run a default ASCII output file is generated. The output file names are as follows:

Executable Module	Output File Name
RESSQC	RESSQC.OUT
MWCAP	MWCAP.OUT
GPTRAC	GPTRAC.OUT
MONTEC	MONTEC.OUT

Each output file contains an echo of the problem-specific input parameters, and the output (capture zone and pathline coordinates) calculated by the code. Refer to Chapter 9 for a description of additional fies created when MONTEC is used.

5.3 Selection of Appropriate Modeling Options

Selection of the appropriate modeling options depends on the problem at hand. Tables 5.1 and 5.2 can be used as guides in determining the appropriate computational module to use. For example, if a user wishes to delineate capture zones for multiple, closely spaced pumping wells in a well field, the RESSQC or GPTRAC semi-analytical modules should be used because the effects of well interference are accounted for. If a user wishes to delineate steady-state or hybrid capture zones, the MWCAP module must be used. If recharge wells exist and their effect on the flow field is deemed important the RESSQC or GPTRAC semi-analytical modules should be used. If observed hydraulic head values in the field or output heads from a two-dimensional numerical model are available, the GPTRAC numerical option may be used.

To better understand the capabilities and limitations of each computational module, as well as simplifying assumptions that may or may not be appropriate, users are strongly encouraged to work through the practical examples presented for each module at the end of Chapters 6-9.

6.0 RESSQC Module

6.1 Introduction

The RESSQC module is a slightly modified version of the RESSQ code presented by Javandel et al., 1984. The "C" was added to the program name because the code was specifically modified for "C"apture zone delineation purposes. RESSQ was originally designed to delineate contaminant fronts about injection wells, and this capability is retained in RESSQC.

6.2 Capabilities

RESSQC can be used to delineate time-related capture zones for a system of one or more pumping/injection wells that fully penetrate a homogeneous aquifer. The presence of a stream or barrier boundary can be simulated using image well theory, but the image wells need to be supplied explicitly to the code. If a stream or barrier boundary exists, the user may save time and avoid mistakes by using the MWCAP or semi-analytical GPTRAC option. The effects of well interference are accounted for through superposition of solutions. A maximum of 50 pumping wells and 20 injection wells may be used in RESSQC.

The number of pathlines reverse tracked from each pumping well may be defined interactively by the user.   In addition, particles can be released at any point within the system to be subsequently forward or reverse tracked (depending upon whether contaminant . fronts or capture zones are delineated).

63 Assumptions and Limitations

Capture zones and contaminant fronts delineated using RESSQC are valid for fully penetrating pumping and injection wells screened in aquifers that are essentially homogeneous. Ground-water flow must be three-dimensional in the x-y plane, and therefore the aquifer may be confined or unconfined if the drawdown-to-initial saturated thickness ratio is small (less than approximately 0.1). Steady ground-water flow is assumed.

If a stream or a barrier boundary is implemented using image well theory, the boundary is assumed to be a straight line and fully penetrate the aquifer. The latter assumption is often violated in cases where stream boundaries exist. The effect of a partially penetrating stream may be an important one and each application should be examined on a site-by-site basis. In general, the greater the depth and breadth of the stream in relation to the aquifer thickness, the more valid the fully penetrating stream assumption. Also, stream boundary partial penetration effects decrease as the distance from the stream to the well increases. The stream and the aquifer are assumed to be in perfect hydraulic connection; the effects of a "clogging layer" between the streambed and the aquifer are not considered.

If, in actuality, the stream is partially penetrating and/or there is a clogging layer of fine grained material that lines the streambed, the capture zone obtained using RESSQC will be smaller than the "true" capture zone. The amount of error incurred will be dependent upon the degree to which the above assumptions are violated.

6.4 Input Requirements

The input requirements for the RESSQC option are outlined in Table 6.1. The well-specific parameters must be input for each well specified in the study area.

6.5 Example Applications

Two examples are presented that illustrate use of the RESSQC module. The first example is a hypothetical one taken from Javandel et al. (1984). The second example is a site application in the vicinity of Corning, New York.

6.5.1 Hypothetical Example

Because the RESSQC module is an amended version of the RESSQ Code (Javandel et al. 1984), the example problems presented in Javandel et al. were run using RESSQC to ensure that the changes made to the code did not alter its original capability. The original RESSQ code has been verified, field validated and used extensively by numerous users (van der Heijde and Beljin, 1988).

The second example problem presented by Javandel et al. is depicted in Figure 6.1. In this example there is one injection well and one pumping well with equal rates of injection and pumping. Uniform ambient flow within the aquifer occurs at an angle of 45°

Table 6.1

RESSQC Input Requirements For Delineation of Capture Zones
(Input Differs Slightly For Delineation of Contaminant Fronts)

Program Variable	Description
For each problem —	
IUNIT:	Default units of input parameters (feet and days or meters and days)
NWP:	Number of pumping wells within the study area
NWI:	Number of recharge (injection) wells within the study area
XMIN:	Minimum x-coordinate of study area (ft or m)
XMAX:	Maximum x-coordinate of study area (ft or m)
YMIN:	Minimum y-coordinate of study area (ft or m)
YMAX:	Maximum y-coordinate of study area (ft or m)
TRANSM:	Transmissivity of the aquifer (ft^2/d or m^2/d)
GRADNT:	Regional hydraulic gradient (ft/ft or m/m)
ALPHA:	Angle of ambient ground-water flow (0-$360°$)
POR:	Aquifer porosity (dimensionless)
HEIGHT:	Aquifer saturated thickness (ft or m)
DL:	Largest allowable step length, dℓ (ft or m) see section 4.1
TMAX:	Maximum amount of time for calculating the trace of a pathline (days)
NCAPZ:	Number of time-related capture zones to be calculated for each pumping well (maximum = 7)
NRPATH:	Number of reverse-tracked pathlines started at arbitrary locations within the study area
For each capture zone (I=1, NCAPZ) —	
DATE(I):	Time value for capture zone (days)

Table 6.1 (cont'd)

RESSQC Input Requirements For Delineation of Capture Zones
(Input Differs Slightly For Delineation of Contaminant Fronts)

Program Variable	Description
For each pumping well (I=1, NWP) --	
XW(1,I):	x-coordinate of well (ft or m)
XW(2,I):	y-coordinate of well (ft or m)
QPWELL(I):	Well discharge rate[a/] (ft^3/d or m^3/d)
RADW(I):	Well radius (ft or m) - default = 0.3 ft or 0.1 m
ITRW(I):	Ratio of number of pathlines to the number plotted (=1 to plot all pathlines, =2 to plot every other pathline, etc.)
NPATH(I):	Number of pathlines to be computed to delineate time-related capture zone (default = 20)
For each injection well (I=NWP + 1, NWP + NWI) --	
XW(1,I):	x-coordinate of well (ft or m)
XW(2,I):	y-coordinate of well (ft or m)
QPWELL(I):	Well recharge rate[a/] (ft^3/d or m^3/d)
RADW(I):	Well radius (ft or m) - default = 0.3 ft or 0.1 m
For each forward tracked pathline (I=1, NRPATH) --	
RSTART(I,1):	x starting coordinate (ft or m)
RSTART(I,2):	y starting coordinate (ft or m)

[a/] The sign (+,-) of the discharge or recharge rate need not be specified.

Figure 6.1

Contaminant Fronts Delineated Using RESSQC for Hypothetical Example

(M)

Simulation Options	Aquifer Properties	Injection Well	Pumping Well
Units = m and days	T = 100	X = -300	X = 300
Step Length = 10	b = 10	Y = 300	Y = -300
Simulation time = 73,000	θ = 0.25	Q = 1,200	Q = 1,200
No. Fronts = 3	i = 0.00343	r = 1.0	r = 1.0
@ 183, 730 and 1,460 days	α = 45	No. Pathlines = 40	
		Plotting Interval = 4	

with respect to the x-axis. Note that the values of transmissivity (T) and hydraulic gradient (i) agree with the 0.14 m/d pore water velocity specified by Javandel et al.

Because the original RESSQ code was designed to track the location of contaminated water emanating from injection wells, option 2 of RESSQC (delineate contaminant fronts about injection wells) was used to obtain Figure 6.1. In addition, 40 pathlines (plotted at intervals of four) were specified. A comparison of Figure 6.1 with Figure 19 in Javandel et al. (1984) shows a perfect correspondence. The three concentric rings about the injection well in Figure 6.1 represent the area] extent of the injected water front for the time periods of 0.5, 2 and 4 years.

To test the capture zone delineation capability of the RESSQC code, the problem specified above was rerun with the only change being that simulation option 1 was used (delineate capture zones about pumping wells). The results of this run are shown in Figure 6.2. As expected, Figure 6.2 is a rotated image of Figure 6.1. In Figure 6.3 the concentric rings about the pumping well represent the 0.5-, 2- and 4-year capture zones for the pumping well. Note that when delineating contaminant fronts the forward tracking method is used (particles are tracked in the fiction of ground-water flow), while when delineating capture zones the reverse tracking method is used (particles are tracked in the direction opposite to that of ground-water flow).

6.5.2 Corning Example

For the next example, RESSQC was used to delineate the capture zones for three wells withdrawing water from the surficial aquifer in the vicinity of Corning, New York. The data for this example was taken from Ballaron (1988).

Figure 6.3 is a general site map of the study region. The valley sediments in the vicinity of Coming consist of stratified glacial drift deposits that are primarily interbedded silty to clean sands and gravels. Relatively thin deposits of lacustrine clay, silt and fine sand exist over much of the valley and separate a surficial, unconfined aquifer from a confined to semi-confined aquifer at depth. Two cross sections through the study area are presented in Figure 6.4.

For the current example three wells screened in the surficial aquifer are considered. Recharge from the Chemung River, local recharge from precipitation, and leakage between the surficial and lower aquifer units were neglected. Hence, the capture zones computed

Figure 6.2

Capture Zones Delineated Using RESSQC for Hypothetic] Example

(M)

Simulation Options	Aquifer Properties	Injection Well	Pumping Well
Units = m and days	T = 100	X = -300	X = 300
Step Length = 10	b = 10	Y = 300	Y = -300
Simulation time = 73,000	θ = 0.25	Q = 1,200	Q = 1,200
No. Fronts = 3	i = 0.00343	r = 1.0	r = 1.0
@ 183, 730 and 1,460 days	α = 45	No. Pathlines = 40	
		Plotting Interval = 4	

Figure 6.3

General Site Map of Chemung River Valley in the Vicinity of Corning, New York
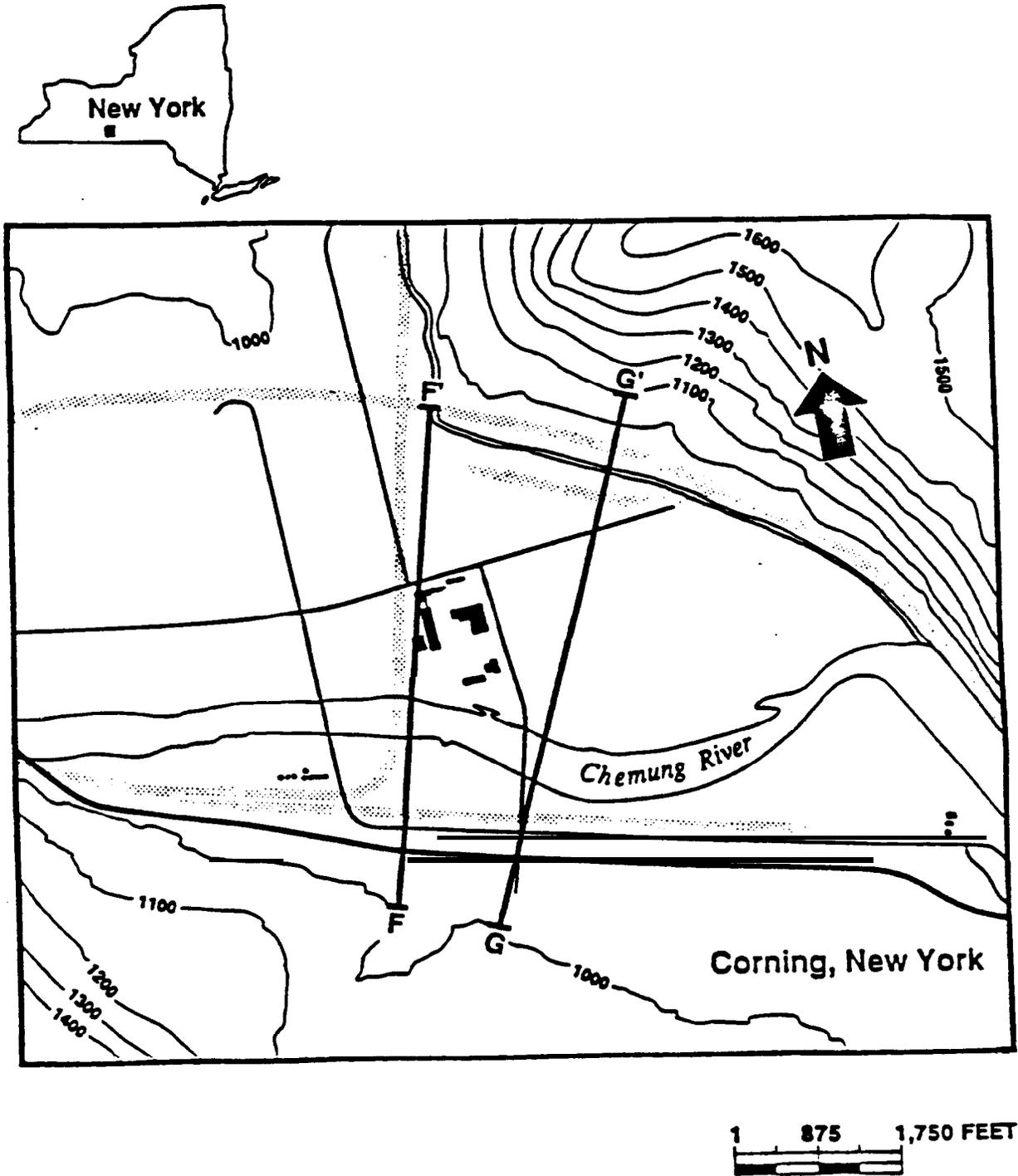
Figure 6.4

Cross Sections F-F and G-G' in the Vicinity of Corning
Reproduced from Ballaron (1988)
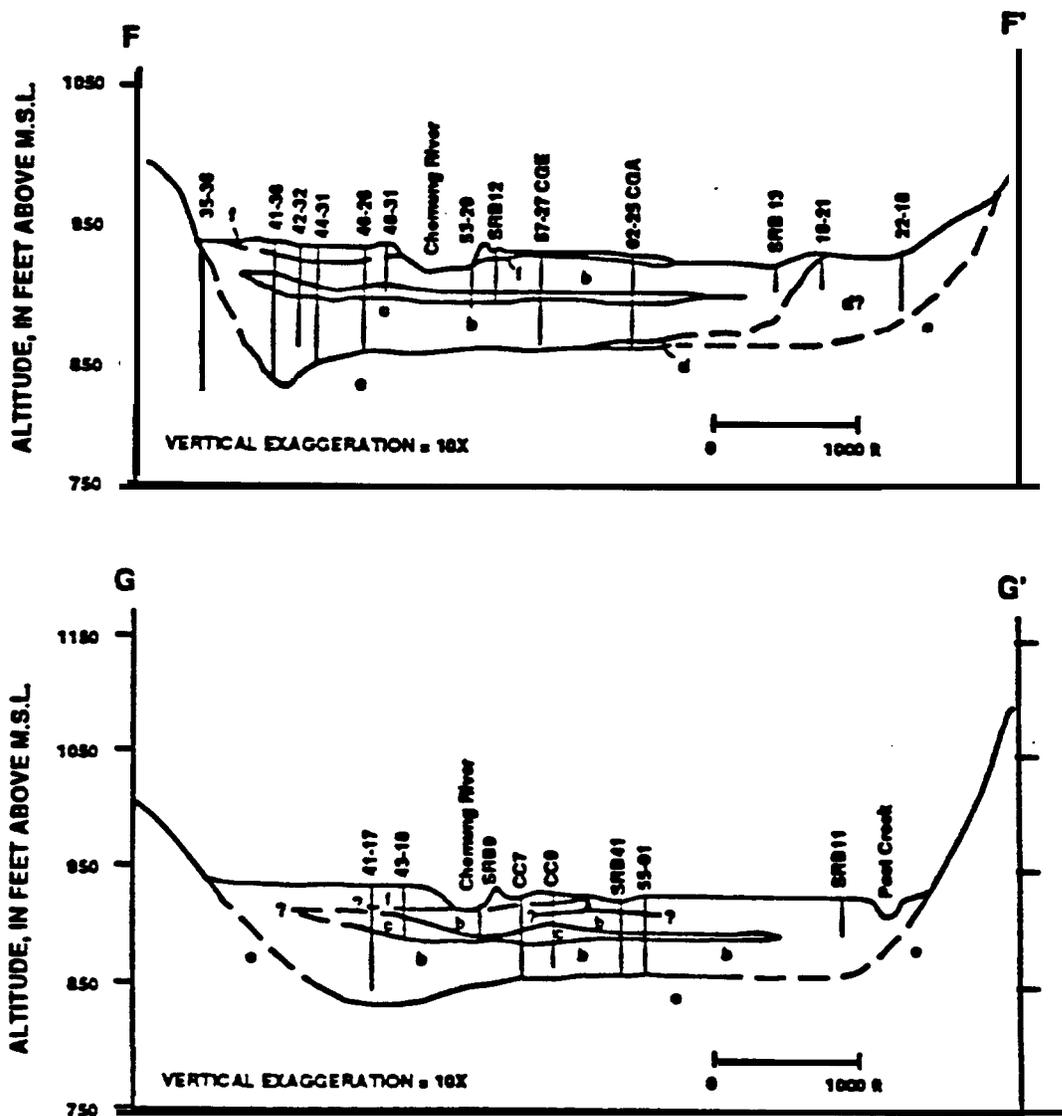
EXPLANATION

a FLOOD - PLAIN SILT AND SAND	d TILL
b OUTWASH AND ICE - CONTACT SAND AND GRAVEL	e BEDROCK
c LACUSTRINE SILT AND SAND	f FILL
40-20 WELL OR TEST BORING AND IDENTIFICATION NUMBER	

using RESSQC are conservative estimates (they are largcr in areal extent than they would be if all sources of recharge to the well were incorporated into the analysis).

The locations of the three pumping wells are superimposed on a pre-pumping steady-state head map (refer to Section 83.4.2 for details on how the head map was obtained) in Figure 6.5. From this map the hydraulic gradient (=0.0019) and the direction of ambient ground-water flow (-45⁰) was obtained. Additional required information such as reasonable pumping rates for the wells, an average hydraulic conductivity of 150 ft/d an average saturated thickness of 25 ft were taken from Ballaron (1988).

The five-year capture zones for the three pumping wells delineated using RESSQC as well as the input data used are illustrated in Figure 6.6. Note that in this example interference effects between the three wells are significant; the two wells farthest upgradient (about in the middle of the study area) intercept a major portion of the ambient aquifer flow that would otherwise supply recharge to the third well. The capture zone of the third well, therefore, assumes a complex contorted shape because it must draw water from regions of the aquifer that are not enclosed by the capture zones of the first two wells.

The three pumping wells examined in this exercise were assumed to be screened over the entire saturated thickness of the surficial aquifer. Because the aquifer is unconfined, its saturated thickness decreases as water is withdrawn by pumping wells due to dewatering of the effective pore space.   The assumptions inherent in the RESSQC, MWCAP, and MONTEC modules are only valid for this type of system if the ratio of the drawdown at (or near) the pumping well(s) is small compared to the initial saturated thickness of the aquifer. In general this ratio should not exceed 20%, or 10% if one desires to be conservcative. As a GPTRAC example in Chapter 8, the Coming case study was modeled using a numerical ground-water flow code. The results of this simulation indicate a maximum drawdown to initial saturated thickness ratio of approximately 15-20%. This ratio is small enough that errors incurred due to using the confined aquifer ground-water flow equations are acceptable for demonstration purposes.

Finally, the Corning example was rerun using the input parameters from Figure 6.6, only for this run one capture zone for 1,825 days (5 years) was specified. The results are shown in Figure 6.7.   The crescent shapes are the 5-year capture zones that RESSQC delineates for each well.

. Figure 6.5

Predevelopment Water Table Map for Corning Region (Obtained From Numerical Simulation) and Locations of Three Surficial Aquifer Pumping Wells
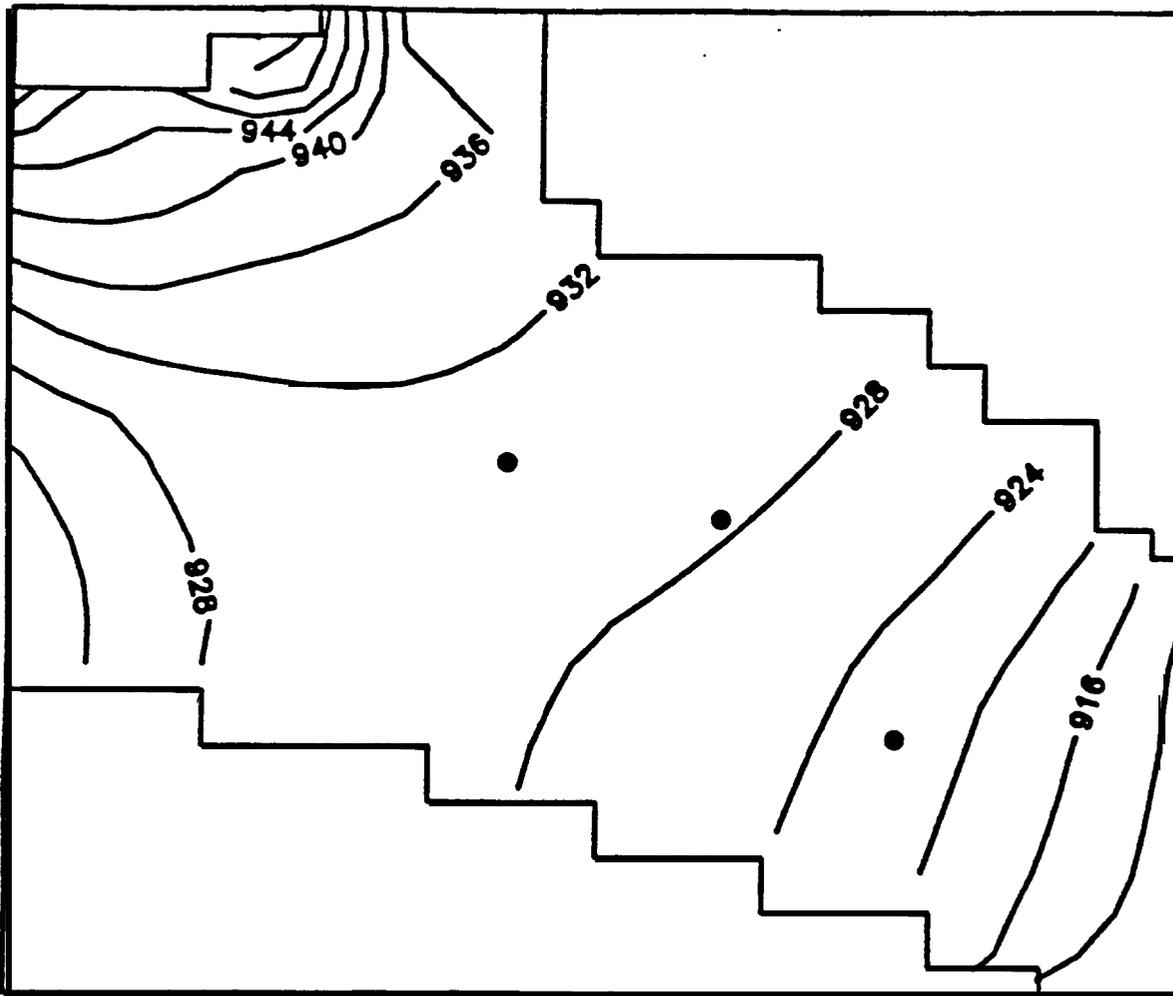
Figure 6.6

**Five-Year Capture Zones Delineated Using RESSQC and
Corresponding Input Parameters for Corning Example**

(FT)
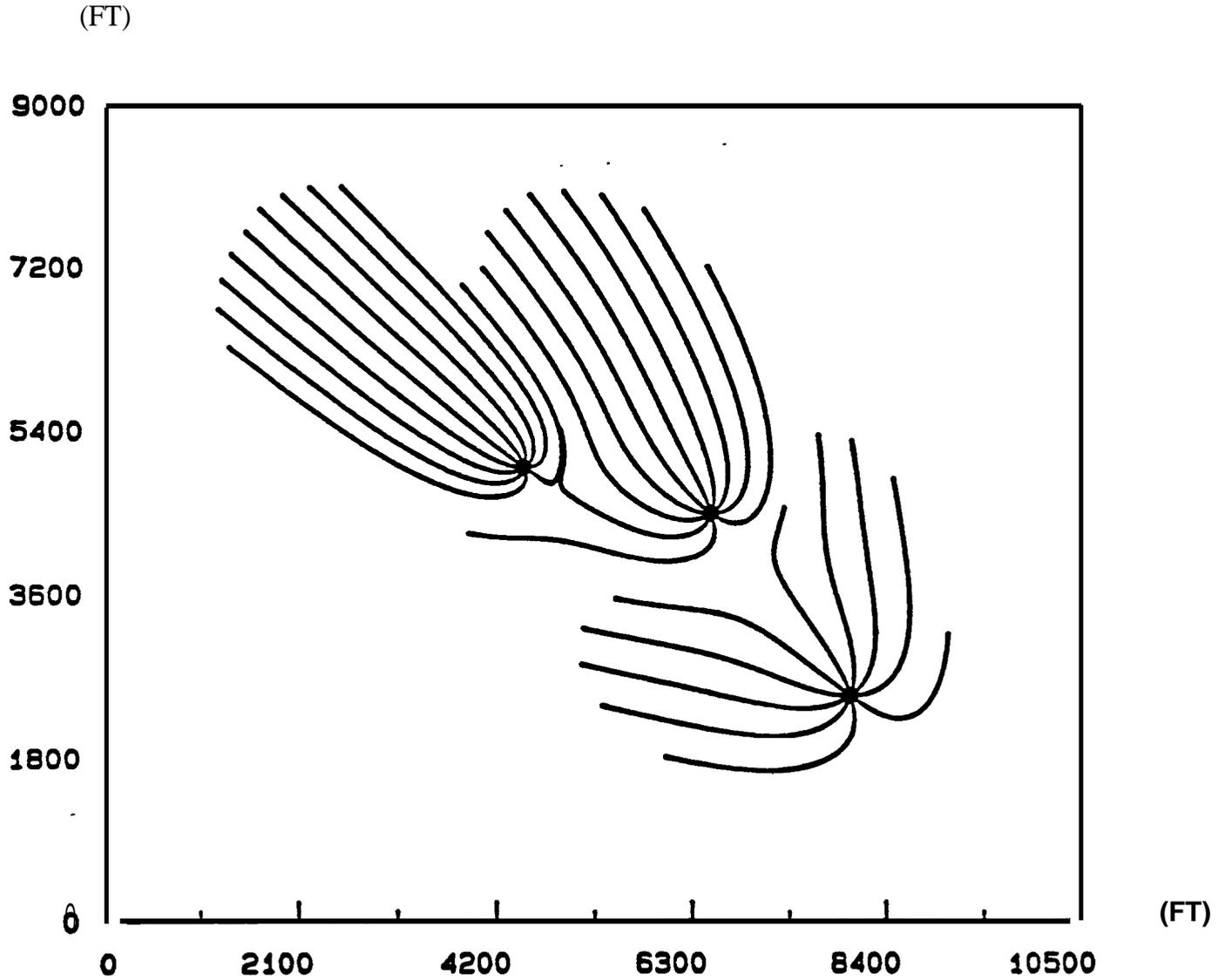
Simulation Options	Aquifer Properties	Well #1	Well#2	Well #3
Units = ft and days	T = 3,750	X = 8,000	6,500	4,500
Step Length = 25	b = 25	Y = 2,500	4,500	5,000
Simulation time = 1,825	θ = 0.22	Q = 30,000	30,000	25,000
No. Capture Zone times = 0	i = 0.0019	No. Pathlines = 10	10	10
	α = -45°	Plotting Interval = 1	1	1

Figure 6.7

**Five-Year Capture Zones for Corning Example Delineated Using
RESSQC With One Capture ZoneTime Specified**

(FT)

(FT)
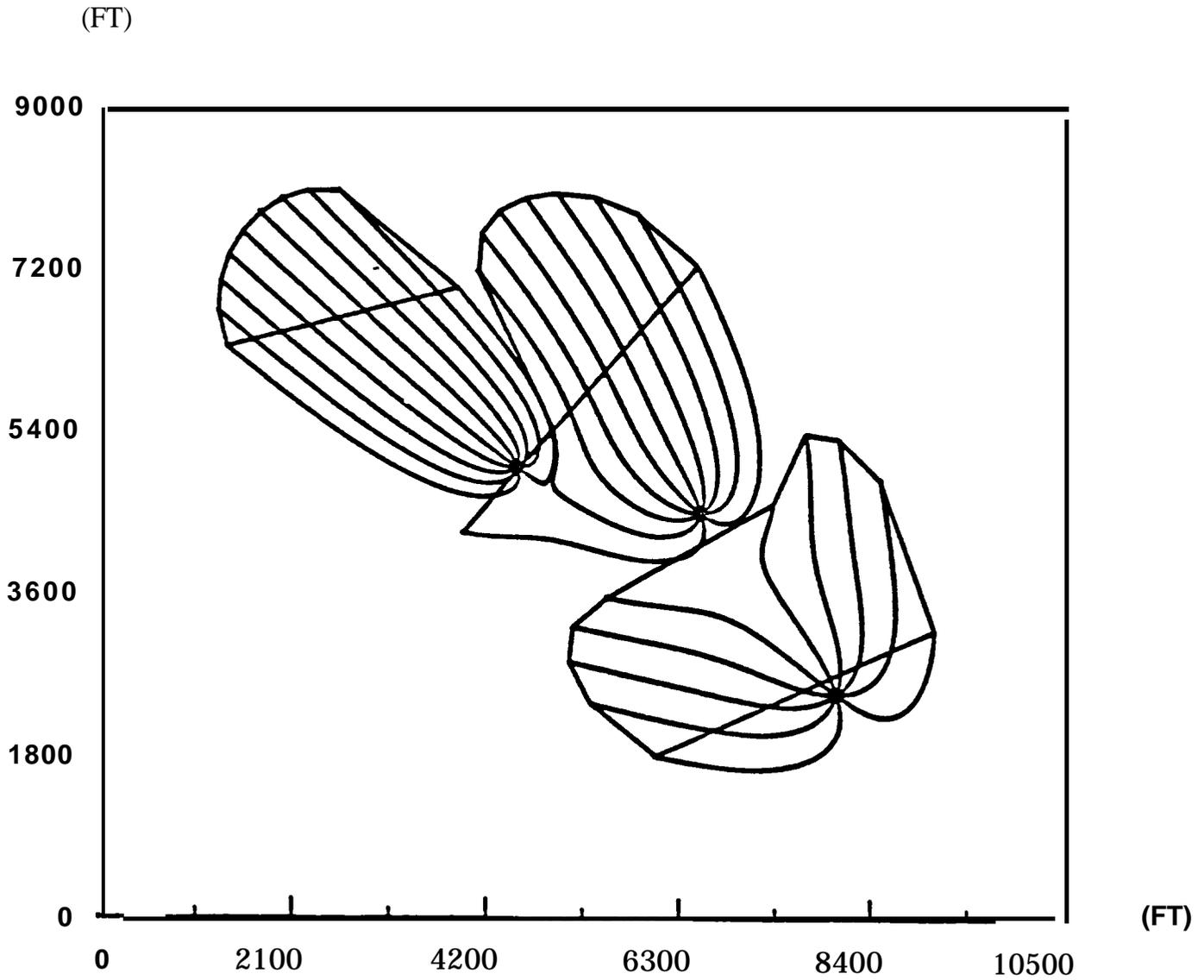
These odd shapes often occur when capture zones are delineated using RESSQC for long periods of time - they obviously do not enclose the entire capture zone of the well. They occur because, in order to delineate time-related capture zones, the code traces a series of reverse pathlines from each well for a specified period of time. When a capture zone time is reached, the corresponding point on each pathline is saved. These points are then connected in sequential order (i.e. the point on pathline 1 is connected to the corresponding point on pathline 2 then the point on pathline 2 is connected to pathline 3, etc.) When the last pathline is reached, its capture zone point is connected to the capture zone point on pathline 1; this final connection causes the line to be drawn that cuts across the pathlines and truncates the capture zone. The simplest way to avoid this shortcoming is to set the simulation time equal to the capture zone time desired and then specify zero capture zone time values as was done for the first Corning run This method produces clear plots and there is no ambiguity as to what area is enclosed by the capture zone(s).

7.0 Multiple Well Capture Zone Module (MWCAP)

7.1 Capabilities

MWCAP is designed to provide efficient delineation of steady-state, time-related and hybrid capture zones for one or more pumping wells in homogeneous aquifers. Each well specified may be operating in an aquifer without a lateral boundary (an areally infinite aquifer), or in an aquifer with a stream or a barrier boundary (semi-infinite aquifer). If a stream or barrier boundary is present the angle of ambient flow in relation to the boundary, as well as the orientation of the boundary itself may be completely arbitrary. MWCAP requires that stream or barrier boundaries be represented by straight lines in plan view.

Although multiple wells within a study area maybe specified MWCAP assumes that the wells operate independently of one another. Therefore, physical processes such as increased drawdown due to well interference effects are ignored.

MWCAP is very efficient due to the small number of pathlines required to delineate steady-state or hybrid capture zones. If a stream boundary is present and the capture zone intersects the stream, the zone of induced recharge from the stream to the well will be delineated automatically. MWCAP can also be used to delineate time-related capture zones.

7.2 Assumptions and Limitations

Capture zones delineated using MWCAP are valid for fully penetrating pumping wells screened in aquifers that are essentially homogeneous. Ground-water flow must be two-dimensional in the areal x-y plane, and therefore the aquifer maybe confined or unconfined if the drawdown-to-initial saturated thickness ratio is small (less than about 0.1). A steady-state ground-water flow field is assumed.

If a stream or a barrier boundary is present, the boundary is assumed to be linear and fully penetrating. The latter assumption is often violated in cases where stream boundaries exist. The effect of a partially penetrating stream may be an important one and each application should be examined on a site-by-site basis. In general, the greater the depth and

breadth of the stream in relation to the aquifer thickness, the more valid the fully penetrating stream assumption. Also, stream boundary partial penetration effects decrease as the distance from the stream to the well increases. The stream and the aquifer are assumed to be in perfect hydraulic connection: the effects of a "clogging layer" between the streambed and the aquifer are not considered.

If, in actuality, the stream is partially penetrating and/or there is a clogging layer of fine grained material that lines the streambed the capture zones obtained using MWCAP will be smaller than the "true" capture zones. The amount of error incurred will be dependent upon the degree to which the above assumptions are violated.

Capture zones for multiple pumping wells within a study area maybe delineated with one run of MWCAP, but each well is assumed to operate independently of every other well. Therefore, each well may have a potentially unique set of input parameters. The effects of well interference (increased drawdown due to overlapping cones of depression) are neglected.

7.3 Input Requirements

The input requirements for MWCAP are outlined in Table 7.1. Note that the well-specific parameters must be input for each well specified in the study area.

7.4 Example Applications

In this section four examples of capture zones delineated using MWCAP are presented. The first example compares steady-state and time-related capture zones; the second example illustrates the effects of boundary conditions (stream or barrier) on capture zone morphology; and the third and fourth examples demonstrate the application of MWCAP to actual field sites near Albuquerque, New Mexico and Seattle, Washington, respectively.

7.4.1 Time-Related and Steady-State Capture Zone Comparison

Figure 7.1 shows the steady-state, 10-year and 25-year capture zones delineated using MWCAP for a hypothetical set of input parameters. The time-related capture zones are enclosed entirely by the steady-state capture zone. However, as the specified time

Table 7.1

Input Requirements for MWCAP Module

Program Variable	Description
For each problem --	
IUNIT:	Default units of input parameters (feet and days or meters and days)
NWELL:	Number of pumping wells for which capture zones are to be delineated
XMIN:	Minimum x-coordinate of study area (ft or m)
XMAX:	Maximum x-coordinate of study area (ft or m).
YMIN:	Minimum y-coordinate of study area (ft or m)
YMAX:	Maximum y-coordinate of study area (ft or m)
DLMAX:	Largest allowable step length, $d\ell$ (see section 4.1)
For each well (I=1, NWELL) --	
XWELL(I):	x-coordinate of well (ft or m)
YWELL(I):	y-coordinate of well (ft or m)
QWELL(I):	Well discharge rate[a] (ft^3/day or m^3/d)
TRAN(I):	Transmissivity of the aquifer (ft^2/d or m^2/d)
GRAD(I):	Regional hydraulic gradient (ft/ft or m/m)
ANGLE(I):	Angle of ambient ground-water flow (0-360°)
POR(I):	Aquifer porosity (dimensionless)
THICK(I):	Aquifer saturated thickness (ft or m)
IBOUND(I):	Associated boundary type (no boundary, stream boundary, or barrier boundary)
DSW(I):	Perpendicular distance from stream or barrier boundary to the well (ft or m)
THETA(I):	Orientation of stream or barrier boundary (0-360°)
ICZTYP(I):	Capture zone type option (steady-state, time-related, or hybrid) .
TMCZ(I):	Time value associated with capture zone (days); time-related and hybrid capture zones only
NSTLIN(I):	Number of pathlines to be computed for the well in addition to pathlines delineated automatically by the code
ICZPLT(I):	Flag indicating if capture zone boundary is to be plotted

[a] The sign (+,-) of the discharge rate does not need to be specified.

Figure 7.1

**Steady-State, and 10- and 25-Year Time-Related Capture Zones Delineated
Using MWCAP. For The Time-Related Capture Zones the Number of Pathlines is 50.**
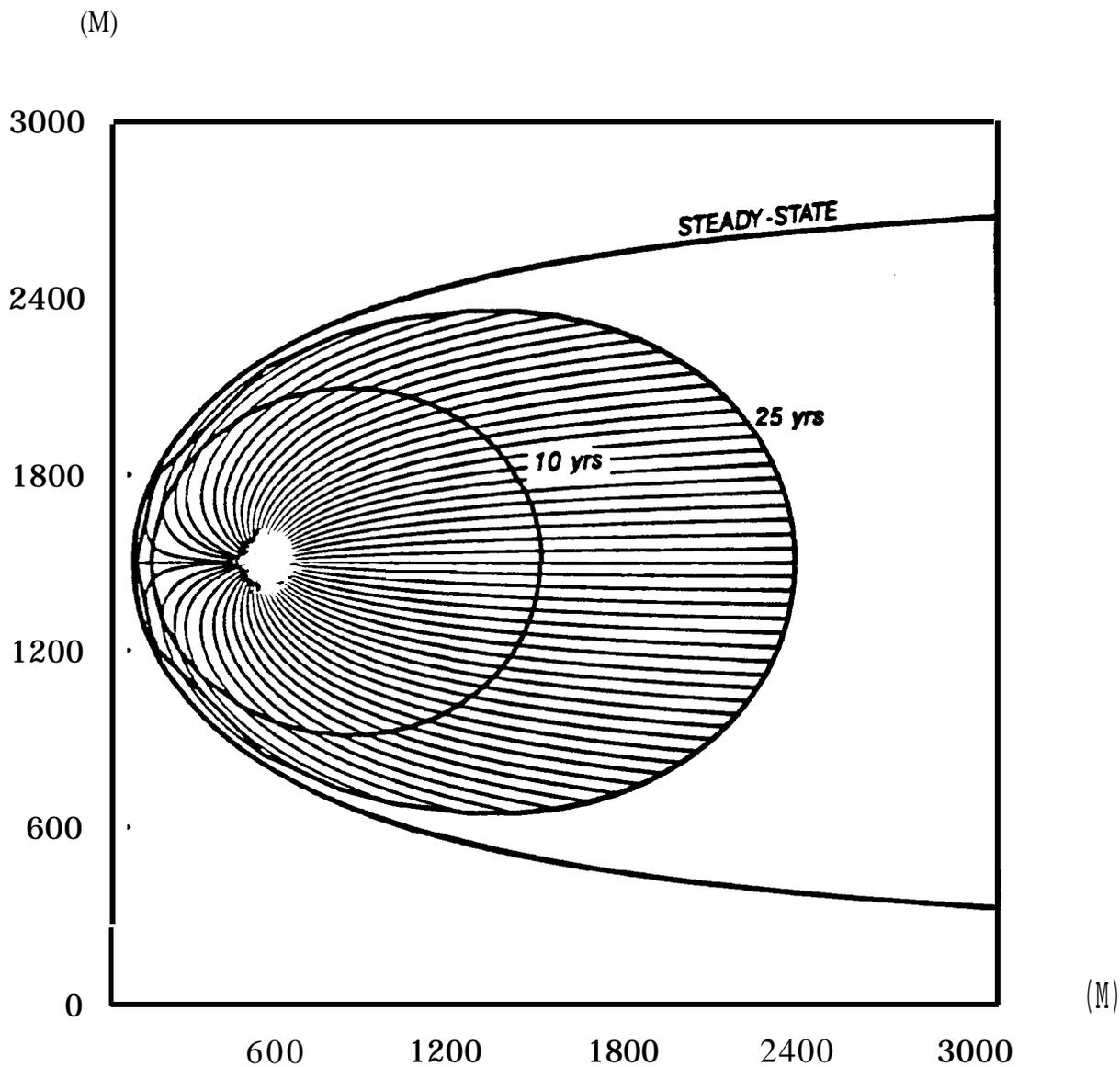
Simulation Options		Well No. 1	
Units = m and days	X = 500	θ = 0.25	
Step Length = 50	Y = 1,500	b = 50	
XMIN = 0.0 XMAX = 3000	Q = 4,000	No boundary	
YMIN = 0.0 YMAX = 3000	T = 1,000	Steady-State Capture Zone	
No. Pumping Wells = 1	i = 0.0015	No. of Pathlines = 0	
	α = 180°		

increases, the time-related capture zones "expand" toward the steady state solution. This makes intuitive sense because the steady state condition can be viewed as the case where time is infinitely large. Figure 7.1 also indicates that the time-related capture zones most closely resemble the steady-state solution in the region close to the well. The user may find it beneficial to check the steady-state capture zone depicted in Figure 7.1 using the analytical solution presented in Todd (1980) and Javandel and Tsang (1986).

Figure 7.1 was constructed by making three separate runs of MWCAP and using the 'Save Plot" and "Overlay" options of the postprocessor to save the plotting information for each run and then to subsequently overlay the three plots. Once the input for the first run (the steady-state example) was typed in the subsequent two scenarios were run very quickly using the "Continue Current Problem" option in the main MWCAP menu.

7.4.2 Boundary Effects Example

The second hypothetical example is designed to illustrate the effects that aquifer boundary conditions may have on capture zone morphology. The input parameters for this example are summarized in Table 7.2.

Figure 7.2 illustrates the MWCAP output for this example. The first capture zone (Figure 7.2a) was obtained for a pumping well that was not influenced by an aquifer boundary condition.   Figures 7.2b and 7.2c portray the effects of a stream and a barrier boundary respectively on the shape and areal extent of the same capture zone. Each respective boundary condition was oriented north to south (parallel to the y-axis) and was located 100 m due west of the pumping well (Table 7.2).

Because the stream boundary acts as a source of water to the well, the capture zone in Figure 7.2b is smaller than that in either Figure 7.2a or c. Since the stream boundary is considered to be fully penetrating, the capture zone expands in width along the stream, but it does not extend beyond the stream. When a capture zone intersects a stream boundary, the pumping well induces flow from the stream to the well.

Figure 7.2c shows the effect of a barrier boundary near the well. Because the barrier boundary limits the portion of the aquifer from which the well can withdraw water, the capture zone "fans out" to capture a greater proportion of ambient flow upstream of the well. The areas enclosed by the capture zones in Figures 7.2a and 7.2c are equal because the only source of water to the well in each of these cases is the ambient ground-water

Table 7.2

MWCAP Input Parameters for Second Hypothetical Example

Simulation Options

Units = m and days

```
XMIN=0        YMIN=0
XMAX = 4,500 .  YMAX = 4,500
```

Step Length = 50
No. of Pumping Wells = 3

Input Parameter	Well No. 1	Well No. 2	Well No. 3
X Coordinate	1,000	1,000	1,000
Y Coordinate	3,500	2,300	1,000
Discharge (Q)	4,000	4,000	4,000
Transmissivity (T)	1,000	1,000	1,000
Hydraulic Gradient (i)	0.0015	0.0015	0.0015
Angle of Ambient Flow (α)	180°	180°	180°
Porosity (θ)	0.25	0.25	0.25
Aquifer Thickness (b)	50	50	50
Boundary Type	None	Stream	Barrier*
Distance from Well to Boundary	N/A	100	100
Boundary Angle	N/A	0.0	0.0
Capture Zone Type	Time-Related	Time-Related	Time-Related
Travel Time Value	3,650	3,650	3,650
No. of Pathlines	20	20	20
Capture Zone Plotting Option	Yes	Yes	Yes

*   In practice, the direction of ambient ground-water flow will generally not be directly toward a barrier boundary.

Figure 702

**Ten-Year Capture Zone For the Cases of No Boundary (a),
A Stream Boundary (b) and A Barrier Boundary (c)**

(M)
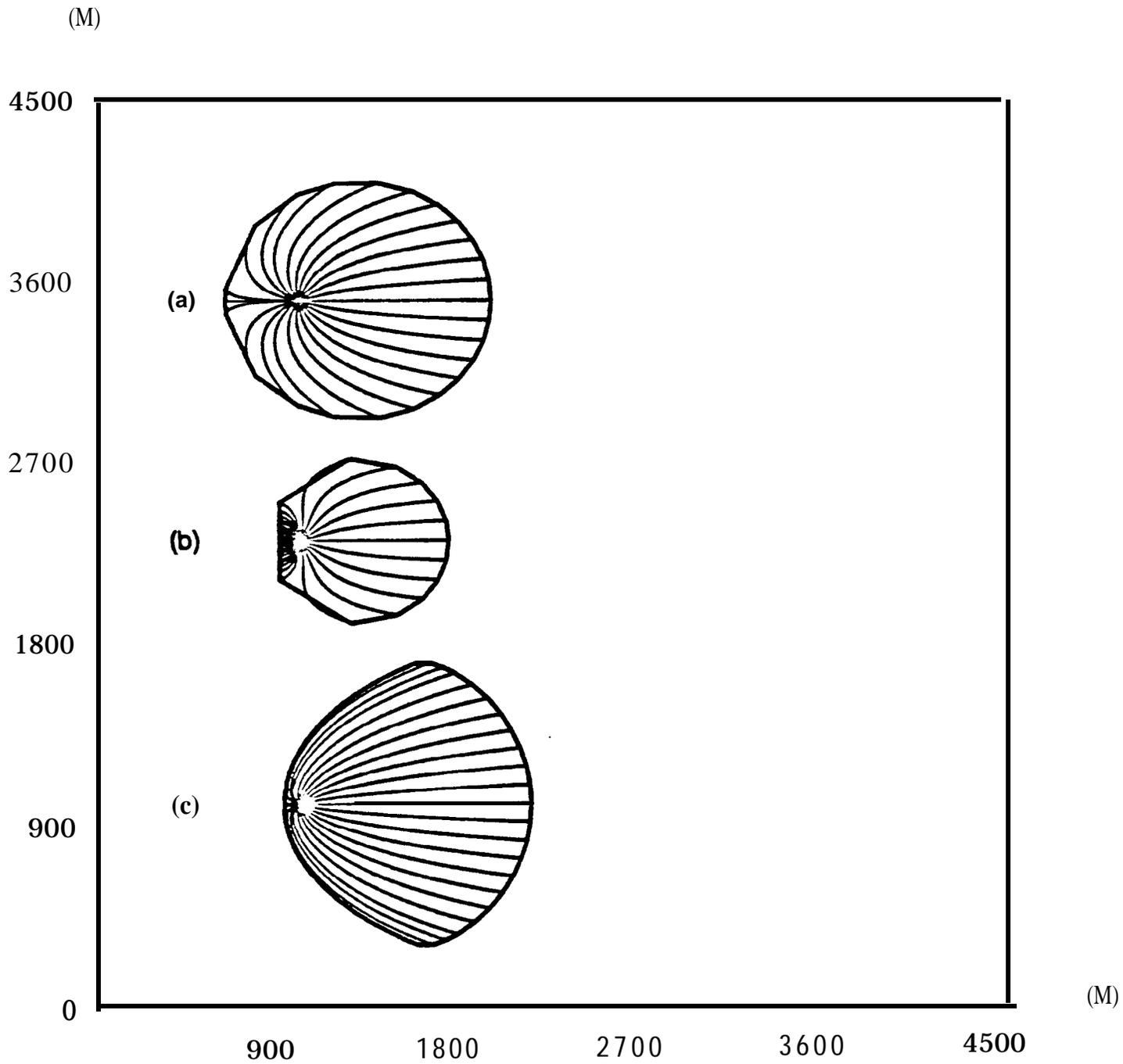
flow within **the** aquifer. The area enclosed by the capture zone that intercepts the stream is smaller than the other two because the stream boundary, in addition to the ambient ground-water flow, acts as a source of water to the well.

7.4.3 Albuquerque Example

The third MWCAP example involves application of the code to an actual municipal well field in New Mexico. The background information for this example was taken primarily from Newsom and Wilson (1988). Figure 7.3 presents the general hydrogeological scenario; there are three closely spaced municipal supply wells located approximately half a mile due east of the Rio Grande in the South Valley of Albuquerque, New Mexico.

The Albuquerque Basin lies within the Basin and Range physiographic province of the United States. The basin fill (often refereed to as "bolson fill") is primarily alluvial in nature and consists of layered gravels, sands, silts and clays; it forms a very prolific aquifer. In the vicinity of Albuquerque water-bearing sediments may have thicknesses on the order of several thousands of feet. Leakage from the Rio Grande and mountain front recharge from the Sandia Mountains to the east are the primary sources of recharge to the aquifer. The climate is semi-and and therefore the assumption of negligible area] recharge due to rainfall is a good one.

The direction of ground-water flow is from north to south ($\alpha = 270°$ or $\alpha = -90°$) in the ambient flow field west of the river which is unaffected by pumping. The sinuosity of the Rio Grande was neglected and the river was approximated as a straight line boundary. Because the three pumping wells are in close proximity to one another, and since MWCAP does not account for well interference effects, the pumping from the three wells was represented by an imaginary model well (marked M on Figure 7.3). The model well has a discharge equal to the average sum of the discharges of the three municipal wells.

The steady-state capture zone delineated using MWCAP is presented in Figure 7.4. Note that the y-axis in the figure corresponds to the stream (Rio Grande) boundary, and therefore a portion of the y-axis forms part of the capture zone boundary. The pathlines that extend from the well to the stagnation point and from the well to the northern boundary of the study area partition the recharge to the well; ground water to the left (west) of these pathlines originates at the Rio Grande, while ground water to the right (east) of these pathlines originates from ambient aquifer flow. All of the pathlines in Figure 7.4 were generated automatically by MWCAP (i.e. the number of pathlines desired was set to zero). If a non-zero number of pathlines had been specified, the additional pathlines would have been started at the well bore and reverse tracked until they reached a study area boundary.

Figure 7.3

General Groundwater Flow System for Albuquerque MWCAP Example
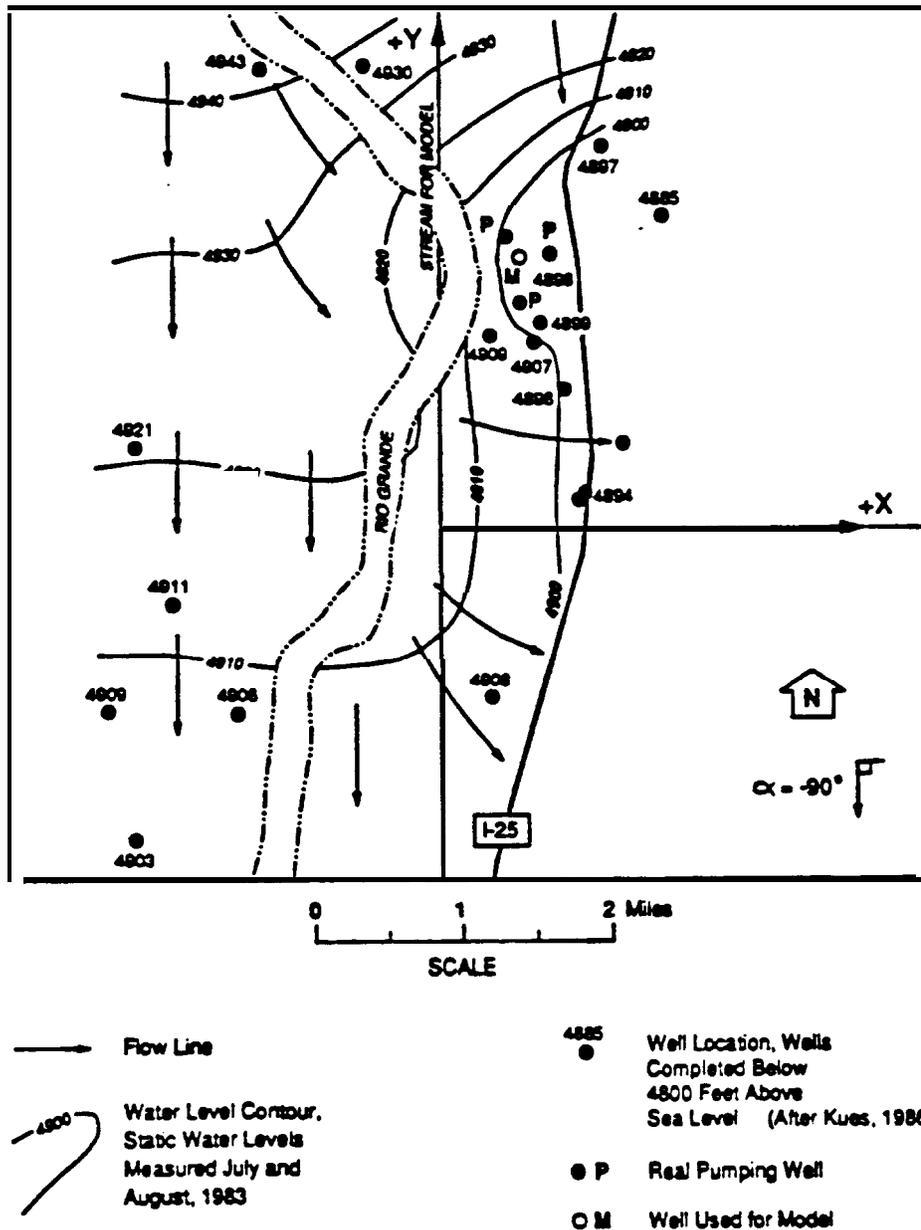
From Newsom and Wilson, 1988. P's represent actual municipal wells, and M represents the imaginary model well. The x and y coordinate axis used by MWCAP are superimposed upon the general flow field.

Figure 7.4

**Steady-State Capture Zone for Albuquerque Municipal
Well Field Delineated Using MWCAP**
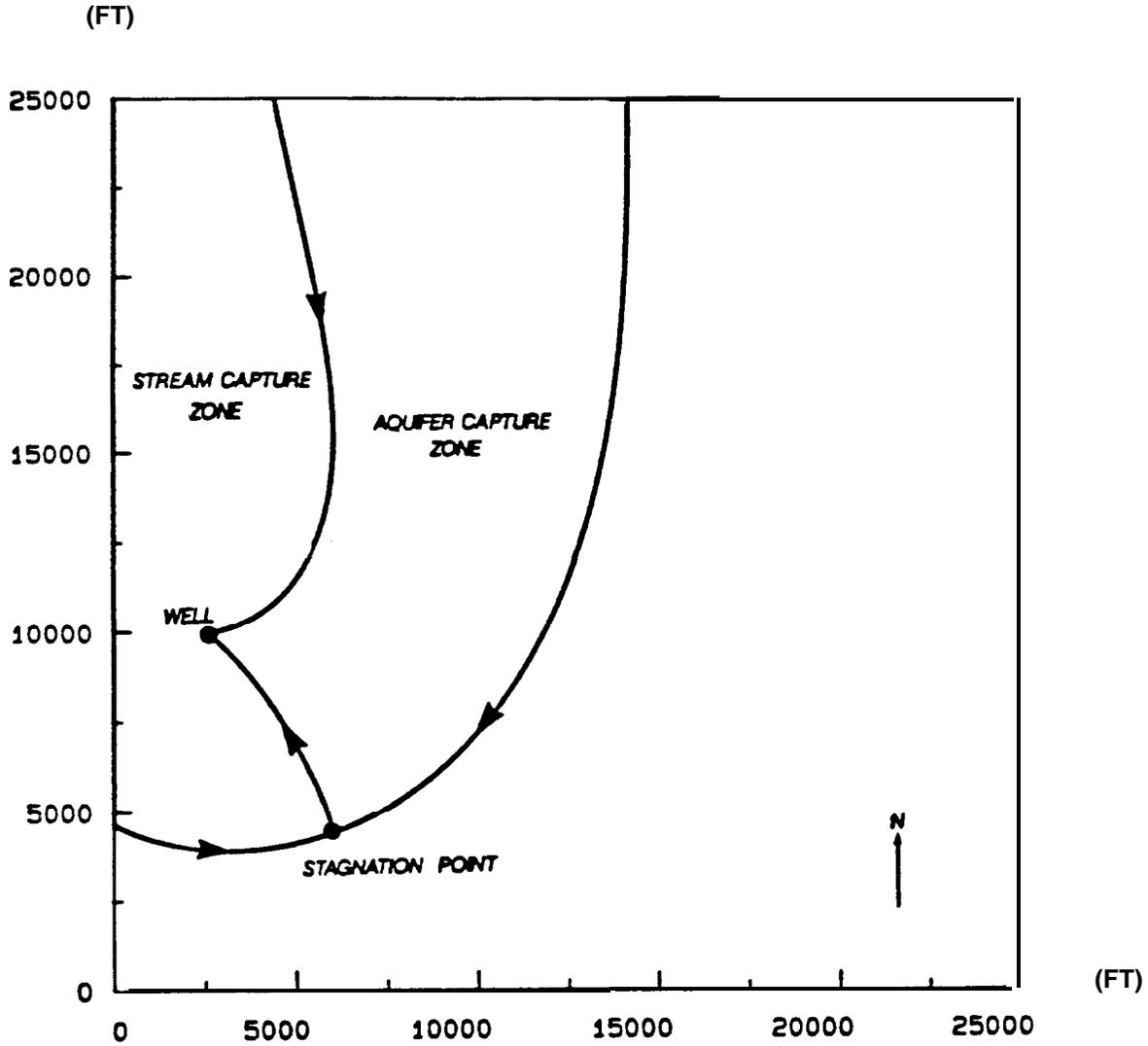
(FT)

Simulation Options		Well No. 1	
Units = ft and days	X =	2,600	b = 200
XMIN = 0.0 XMAX = 25000	Y =	10,000	Stream Boundary
YMIN = 0.0 YMAX = 25000	Q =	712,247	Distance to Boundary = 2,600
Step Length = 50	T =	6,690	Boundary Orientation = 0.0
No. Pumping Wells = 1	i =	0.0013	Steady-State Capture Zone
	α =	-90°	No. of Pathlines = 0
	θ =	0.25	

The actual capture zone for the three Albuquerque wells probably differs somewhat from that computed by MWCAP because the Rio Grande only partially penetrates the aquifer (see Section 10.3 and Newsom and Wilson 1988). The depth of water m the Rio Grande is probably no more than 5 to 10 ft at any given time, while the wells are pumping from depths of up to 200 ft below land surface. Therefore, the capture zone in Figure 7.4 is not conservative because the recharge to the walls from the river is overestimated. A conservative approach to this problem would be to ignore the presence of the stream boundary.

Because the three wells are closely spaced relative to the size (especially the width) of the capture zone, the simulation approach of lumping the discharge of the three wells to one equivalent model well causes no significant errors. This point is illustrated in Section 8.2.4 where the Albuquerque example was run again using the semi-analytical GPTRAC module.

7.4.4 Seattle Example

The final MWCAP example concerns the Highline well field in Seattle, Washington. The background information for this example was taken from Seattle Water Department (1986). A general location map is presented in Figure 7.5, and a local site map, along with the locations of two pumping wells (Riverton Heights and Boulevard Park) is presented in Figure 7.6.

The Highline area is underlain by three hydraulically interconnected aquifers (shallow, intermediate, and deep) that occur within a thick sequence of unconsolidated glacial and interglacial deposits. The aquifers are composed of cobbly sand and gravel deposits, while the interbedded low-permeability aquitards that separate the major aquifer units are composed of silt and clay. A hydrostratigraphic cross section through the Highline area is presented in Figure 7.7.

The shallow aquifer is unconfined and ranges between 50 and 100 ft in saturated thickness. This aquifer is not used as a major source of ground-water supply, but it does supply significant recharge to the aquifers at depth.

Figure 7.5

General Location Map for Seattle's Highline Well Field Example

——— Supply Lines

N
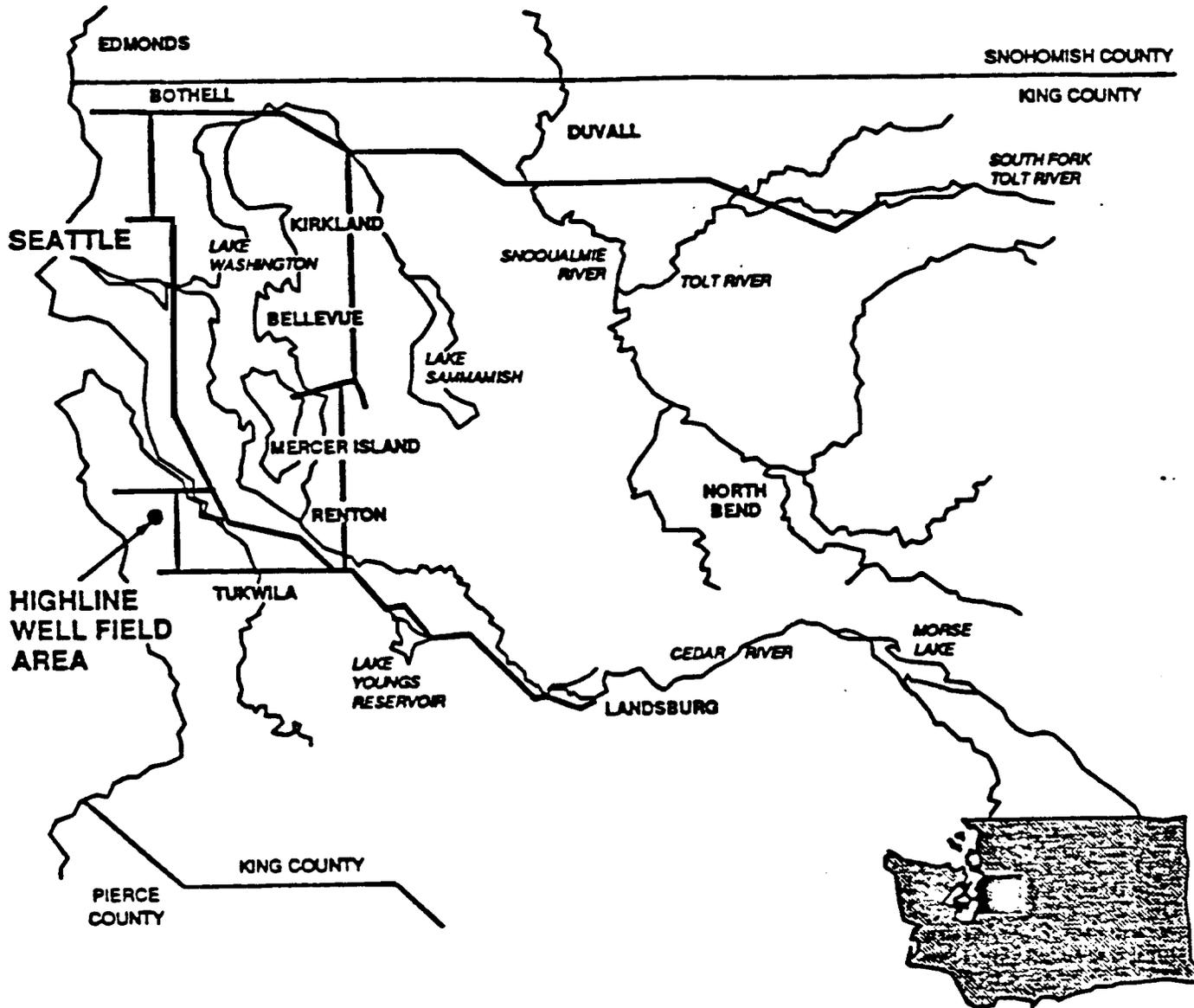
Figure 7.6

**Local Site Map With Intermediate Aquifer Well Locations
for Highline Well Field Example**
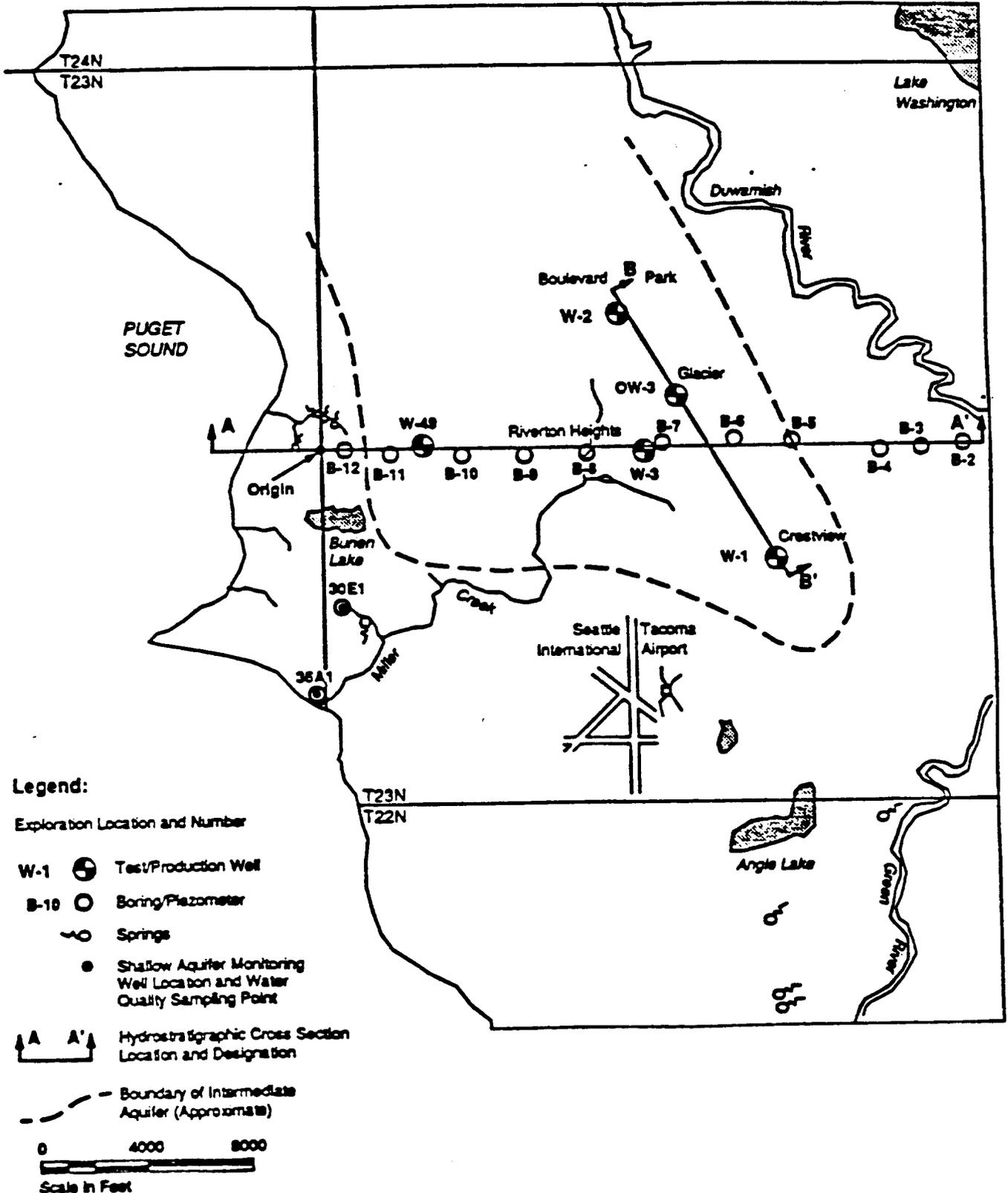
Figure 7.7

Hydrostratigraphic Cross Section B-B' Through Highline Well Field Area
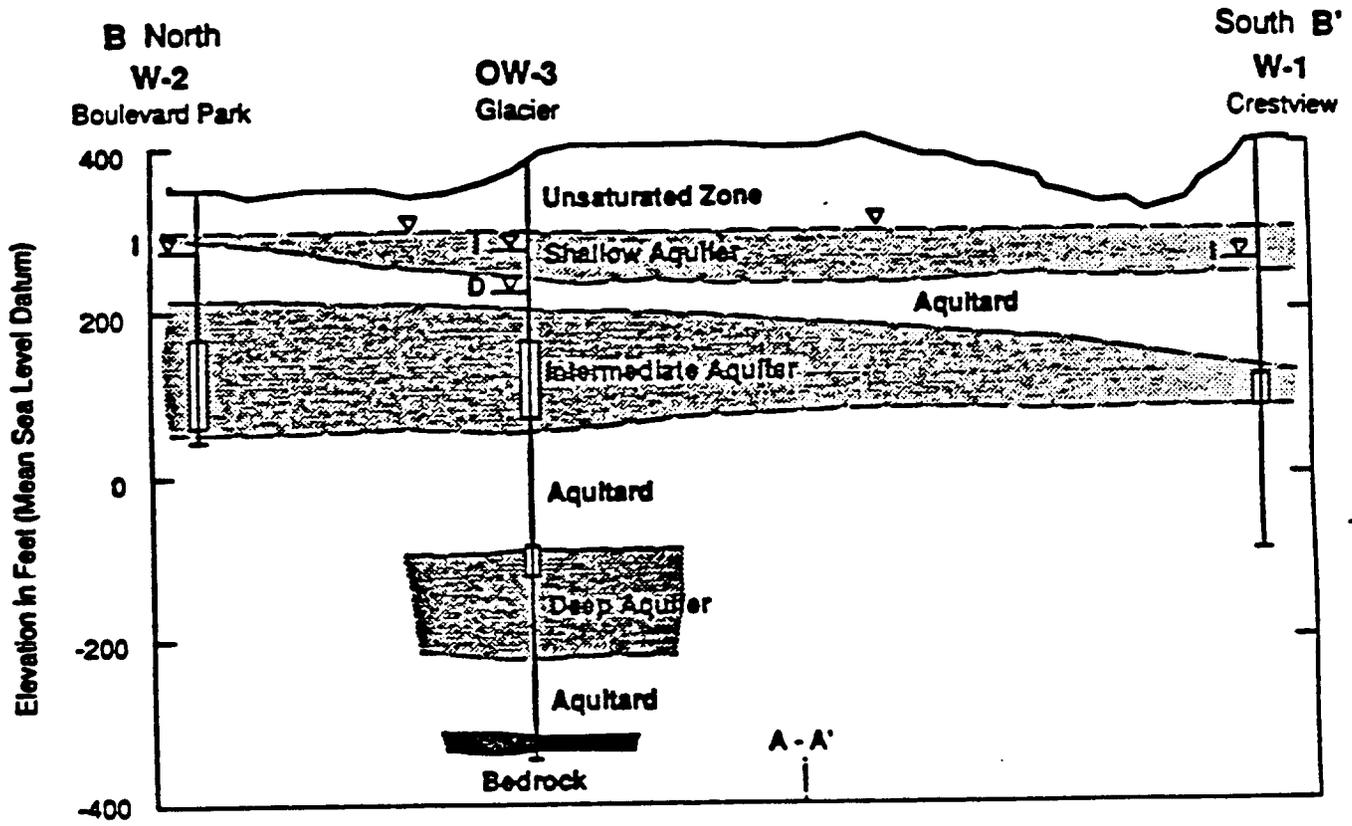
Legend:

W-3   Well Number

[well symbol]   Well Location

    Screened Section

Piezometric Surface

— —∇   Shallow Aquifer

I ∇   Intermediate Aquifer

D ∇   Deep Aquifer

Vertical Exaggeration x 10
Horizontal Scale in Feet
0   2000   4000

0   200   400
Vertical Scale in Feet

March 1986
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The intermediate aquifer is the target of most municipal ground-water development and is the aquifer of interest for this example. It is confined with static water levels typically reaching 100 ft above the top of the aquifer. Most of the confinement is provided by the upper and lower clay units (see cross section) that bound the aquifer above, below, and along the east and west margins of the uplands. This aquifer is generally about 100 ft thick.

The deep aquifer is also confined and averages about 100 ft in thickness. It consists of coarse cobbly sands and gravel deposits with localized silt and clay interbeds. This aquifer is targeted for more limited ground-water devclopment.

Figure 7.8 is a contour map of piezometric head for the intermediate aquifer. This map indicates that the aquifer is recharged within the central upland area by the overlying shallow aquifer, and that the general direction of ground-water flow is from the recharge area toward regional discharge boundaries such as the Green River and Puget Sound.

Because the two production wells are relatively far apart (over 1 mile), an initial assumption of negligible well interference effects was made and the tie-year hybrid capture zone for each well was delineated using MWCAP. The input for this example is provided in Table 7.3. Proposed pumping rates and average transmissivity values in the vicinity of each well were taken from Seattle Water Department (1986). The direction and magnitude of the ambient hydraulic gradient was taken from Figure 7.8. Each well fully penetrates the intermediate aquifer.

The MWCAP results were scaled using the GRAF "Map Scale" option so they could be directly overlaid onto the base map to form Figure 7.9. Note in Figure 7.9 that the capture zones extend across the regional ground-water flow divide in the intermediate aquifer. This was permitted because drawdown due to the production wells will most likely reach the divide and alter its configuration. Ground-water flow divides may sometimes be treated as barrier boundaries if pumping wells are sufficiently distant so as not to affect the ground-water flow field in the vicinity of the divide.

The capture zones computed by MWCAP are conservative estimates since two major sources of recharge to the well, leakage through the overlying aquitard due to pumping and decreased leakage through the lower aquitard due to pumping, were neglected. Also, a uniform ambient ground-water flow in the aquifer from southwest to northeast was assumed to exist over the entire study area. Obviously, once the capture zone boundary

Figure 7.8

Contour Map of Piezometric Head for Highline Well Field Intermediate Aquifer
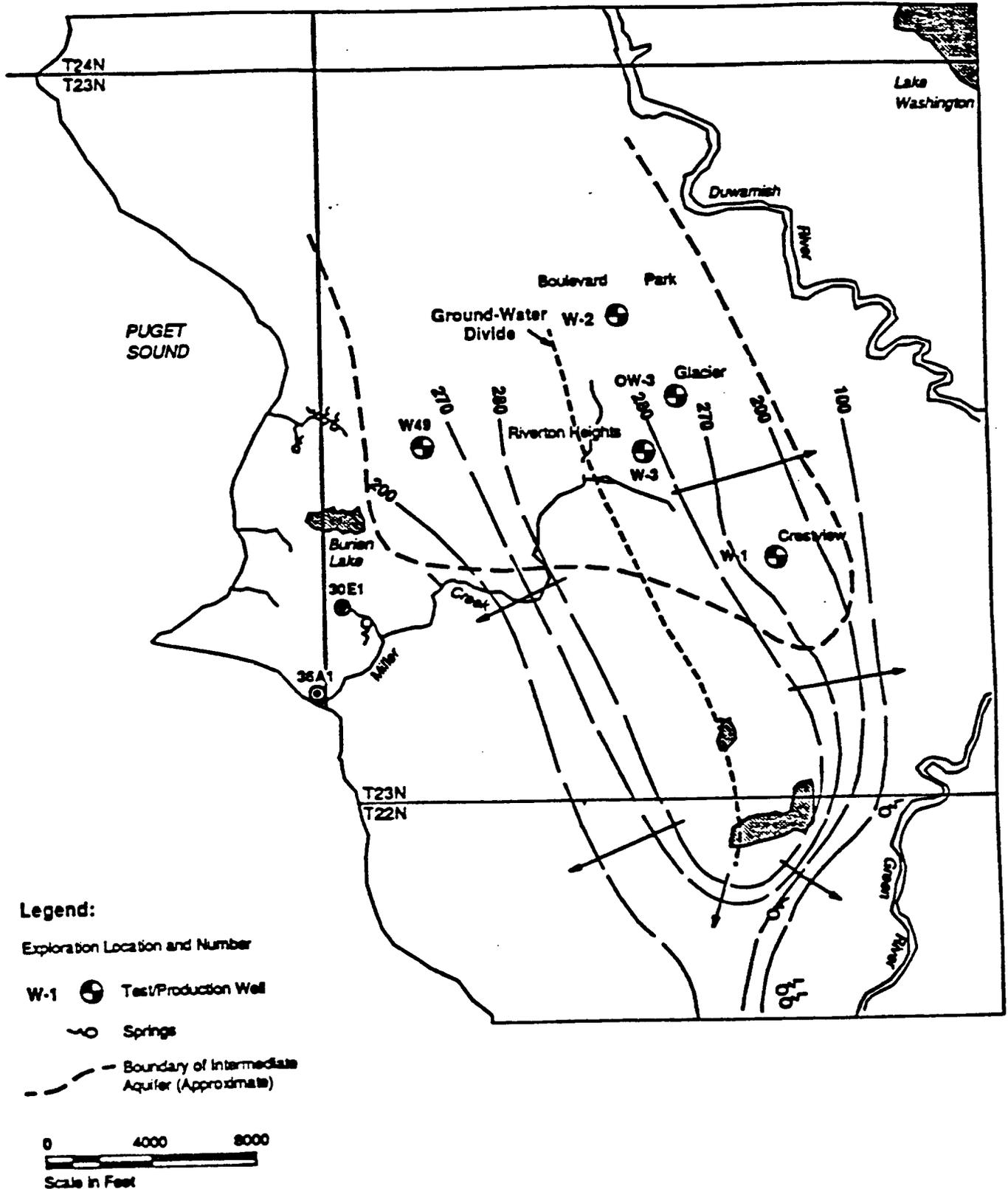
Table 7.3

MWCAP Input Parameters used for Highline Well Field Example

Simulation Options

Units = feet and days

XMIN=0   YMIN = -15,000
XMAX = 15,000   YMAX = 10,OOO

Step Length = 100
No. of Pumping Wells = 2

Input Parameter	Well No. 1[1]	Well No. 2[2]
X Coordinate	12,428	11,556
Y Coordinate	-222	5,170
Discharge	596,748	346,499
Transmissivity	44,573	20,888
Hydraulic Gradient	0.00385	0.00385
Angle of Ambient Flow	45°	45°
Porosity	0.25	0.25
Aquifer Thickness	100	100
Boundary Type	None	None
Capture Zone Type	Hybrid	Hybrid
Travel Time Value	1,825	1,825
No. of Pathlines	0	0

[1] Riverton Heights
[2] Boulevard Park

Figure 7.9

**Five-Year Hybrid Capture Zones Delineated Using MWCAP
For Riverton Heights and Boulevard Park Wells**

Legend:

Exploration Location and Number

W-1 ⊕ Test/Production Well

B-10 ○ Boring/Piezometer

∿○ Springs

● Shallow Aquifer Monitoring
    Well Location and Water
    Quality Sampling Point

▲A   A'▲ Hydrostratigraphic Cross Section
          Location and Designation

∼ ─ Boundary of Intermediate
      Aquifer (Approximate)

0   4000   8000

Scale in Feet
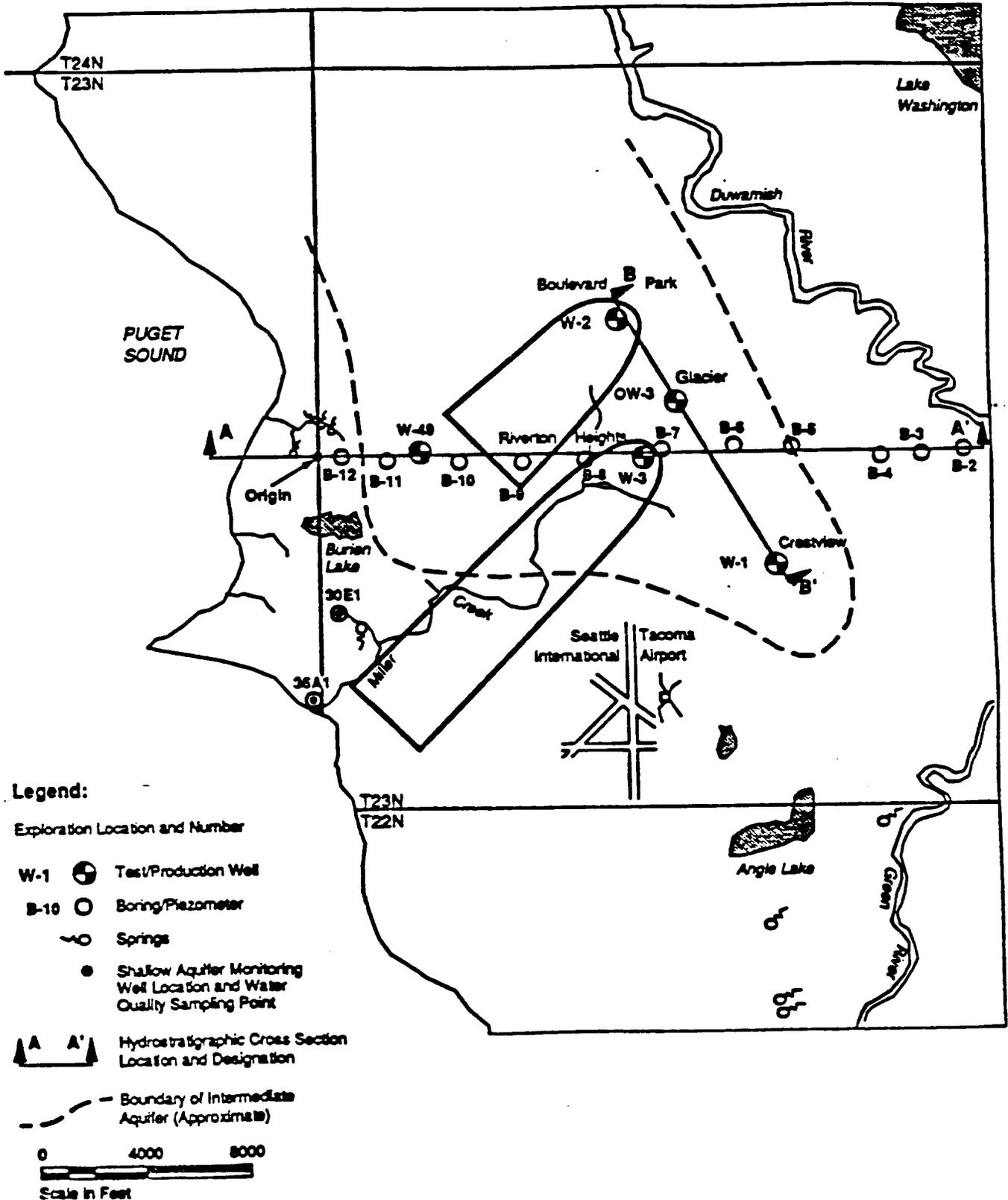
was extended across the ground-water flow divide this assumption became invalid. A numerical ground-water flow model would have to be used to quantitatively assess the effects of the reversal in ambient ground-water flow direction on the capture zones.

The Theis equation maybe used to quickly assess some of the simplifying assumptions made for this example. Jacob's "large time" approximation to the Theis equation may be written:

$$ s = \frac{2.3Q}{4\pi T} \log \frac{2.25Tt}{r^2 S} \tag{7.1} $$

where s is drawdown from an initial static water level at radial distance r from a well pumping at rate Q, t is time since the start of pumping, and T and S are the aquifer transmissivity and storativity respectively. The large time approximation is applicable because only flow conditions that are approaching steady-state are of concern.

The radial distance from each well to the ground-water divide, and the radial distance from each well to the mid-point between the wells were computed from Figure 7.8. Using equation (7.1) the drawdown at each of these locations at various times was calculated; the results of this analysis are presented in Figure 7.10.

Figure 7.10 indicates that significant drawdown maybe observed at each of the selected radial distance values. This analysis would suggest that the assumption of negligible well interference was violated. It would also suggest that drawdown due to pumping will affect the ground-water flow divide and therefore the divide should not be treated as a barrier boundary. However, the simple Theis analysis presented above neglects two important sources of recharge to the wells: ambient aquifer flow, and leakage from the confining beds. To address these physical processes in an appropriate manner, a more sophisticated solution for drawdown (analytical or numerical) would have to be used and perhaps some field observations would be collected.

Figure 7.10

Evaluation of Well Interference Effects and Drawdown At Ground-Water Divide Due to Each Well Using Theis Solution

Jacob's Approximation to Theis Solution:

$$s = \frac{2.3Q}{4\pi T} \log \frac{2.25Tt}{r^2 S} \tag{7.1}$$

Well No. 1- Riverton Heights	Well No. 2- Boulevard Park
$Q = 596{,}748 \text{ ft}^3/\text{day}$	$Q = 346{,}499 \text{ ft}^3/\text{day}$
$T = 44{,}573 \text{ ft}^2/\text{day}$	$T = 20{,}888 \text{ ft}^2/\text{day}$
$S = 4.92 \times 10^{-4}$	$S = 1.04 \times 10^{-3}$

1. Drawdown due to each well at mid-point of line segment connecting the wells (r= 2,916 ft):

Well No. 1			Well No. 2		
r(ft)	t(days)	S(ft)	r(ft)	t(days)	S(ft)
2,916	180	8.91	2,916	180	9.05
2,916	365	9.66	2,916	265	9.98
2,916	1,825	11.37	2,916	1,825	12.1

2. Drawdown due to each well at ground-water divide directly upgradient from well location.

Well No. 1			Well No. 2		
r(ft)	t(days)	S(ft)	r(ft)	t(days)	S(ft)
2,600	180	9.15	4,600	180	7.85
2,600	365	9.90	4,600	265	8.78
2,600	1,825	11.6	4,600	1,825	10.9

8.0 General Particle Tracking Module (GPTRAC)

8.1 Introduction

The GPTRAC module consists of two major components. The first component, referred to as the 'semi-analytical option", provides the option for pathline and time-related capture zone delineation for simple cases using analytical velocity computation techniques similar to those of RESSQC and MWCAP. This option assumes a homogeneous aquifer but is able to accommodate a wider range of aquifer and boundary conditions than the RESSQC and MWCAP modeling options.

The second component referred to as the 'numerical option", provides pathline and time-related capture zone delineation for general cases using numerical velocity computation techniques that require input of hydraulic head values at nodal points of a rectangular grid This option is designed to be used as a postprocessor for numerical ground-water flow models. Additionally, it can be used as a processor for interpolated head values derived from a piezometric map (field data). Once the hydraulic bead values corresponding to the nodal points of a rectangular grid are read into the GPTRAC code, time-related capture zone analysis and general panicle tracking can be performed.

8.2 Semi-Analytical Option

8.2.1 Capabilities

The semi-analytical option of GPTRAC is capable of delineating time-related capture zones for a system of pumping and injection wells that fully penetrate a homogeneous aquifer. A steady flow field is assumed and the aquifer may be confined, unconfined or semi-confined (leaky). For each aquifer type, a stream or barrier boundary can be specified along any edge of the study area. The effects of well interference are accounted for through superposition of solutions resulting from individual wells. If the aquifer is confined, "strip" aquifers (aquifers with two parallel boundaries) may be simulated. A maximum of 50 pumping wells may be used in GPTRAC. For cases involving confined and semi-confined aquifers, injection wells may also be used. The maximum number of injection wells allowed by the code is 20.

The number of pathlines reverse tracked from each pumping well may be defined interactively by the user. In addition, particles can be released at any point within the system to be subsequently forward or reverse tracked.

8.2.2 Assumptions and Limitations

Capture zones delineated using the semi-analytical option of GPTRAC are valid for fully penetrating wells screened in aquifers that are essentially homogeneous. Ground-water flow in the aquifers must be two-dimensional in an areal x-y plane (the Dupuit assumptions are used for unconfined flow cases). A steady-state ground-water flow field is assumed. In the case of a lea& aquifer system, aquitard leakage is assumed to be vertical.

If a stream or a barrier boundary is present, the boundary is assumed to be linear and fully penetrating. The latter assumption is often violated in cases where stream boundaries exist. The effect of a partially penetrating stream may be an important one and each application should be examined on a site-by-site basis. In general, the greater the depth and breadth of the stream in relation to the aquifer thickness, the more valid the fully penetrating stream assumption. Also, stream boundary partial penetration effects decrease as the distance from the stream to the well increases. The stream and the aquifer are assumed to be in perfect hydraulic connection; the effects of a "clogging layer" between the streambed and the aquifer are not considered.

If, in actuality, the stream is partially penetrating and/or there is a clogging layer of the grained material that lines the streambed, the capture zone obtained using GPTRAC will be smaller than the "true" capture zone. The amount of error incurred will be dependent upon the degree to which the above assumptions are violated.

8.23 Input Requirements

The input requirements for the GPTRAC semi-analytical option are outlined in Table 8.1. The well-specific parameters must be entered for each well in the study, area. If a stream or barrier boundary is present, it is assumed to correspond to one edge (top, bottom or either side) of the study area. If the strip aquifer option is selected, the two boundary conditions must correspond to two opposite, parallel sides of the study area (top and bottom, or left and right).

Table 8.1

Input Requirements for GPTRAC Semi-Analytical Option

Program Variable	Description
For each problem --	
IAQFR:	Aquifer type (confined, semi-confined, unconfined)
IUNIT:	Default units of input parameters (feet and days or meters and days)
NPWELL:	Number of pumping wells within the study area
NRWELL:	Number of recharge (injection) wells within the study area
XMIN:	Minimum x-coordinate of study area (ft or m)
XMAX:	Maximum x-coordinate of study area (ft or m)
YMIN:	Minimum y-coordinate of study area (ft or m)
YMAX:	Maximum y-coordinate of study area (ft or m)
DLMAX:	Largest allowable step length, $d\ell$ (see section 4.1)
TRANSM:	Transmissivity of the aquifer (ft^2/d or m^2/d)
GRADNT:	Regional hydraulic gradient (ft/ft or m/m)
ALPHA:	Angle of ambient ground-water flow (0-360°)
POROS:	Aquifer porosity (dimensionless)
B:	Aquifer saturated thickness (ft or m)
KPRIM:	Confining bed hydraulic conductivity[a] (ft/d or m/d)
BPRIM:	Confining bed thickness[a] (ft or m)
CAPN:	Areal recharge rate[b] (ft/d or m/d)
CAPH:	Aquifer saturated thickness prior to pumping [b] (ft or m)
RMAX:	Maximum radius of influence of pumping well[b] (ft or m)
IBOUND:	Boundary condition type (no boundary, stream or barrier boundary on one side of study area, or strip aquifer)
NFPATH:	Number of forward-tracked pathlines
NRPATH:	Number of reverse-tracked pathlines
TMSIM:	Time period for which GPTRAC will be executed[c] (days)
TMCAPZ:	Time value for time-related capture zones[c] (days)

Table 8.1 (continued)

Input Requirements for GPTRAC Semi-Analytical Option

Program Variable	Description
For each pumping well (I=1, NPWELL) –	
XPWELL(I):	x-coordinate of well (ft or m)
YPWELL(I):	y-coordinate of well (ft or m)
QPWELL(I):	Well discharge rate[d/] (ft^3/d or m^3/d)
NSTLIN(I):	Number of pathlines to be computed to delineate time-related capture zone (default = 20)
For each injection well (I=1, NRWELL) –	
XRWELL(I):	x-coordinate of well (ft or m)
YRWELL(I):	y-coordinate of well (ft or m)
QRWELL(I):	Well recharge rate[d/] (ft^3/d or m^3/d)
For each forward-tracked pathline (I=1, NFPATH) –	
FSTART(I,1):	x starting coordinate (ft or m)
FSTART(I,2):	y starting coordinate (ft or m)
For each reverse-tracked pathline (I=1, NRPATH) –	
RSTART(I,1):	x starting coordinate (ft or m)
RSTART(I,2):	y starting coordinate (ft or m)

[a/] Only required for semi-confined (leaky) aquifers.

[b/] Only required for unconfined aquifers.

[c/] A simulation time (TMSIM) different from the capture zone time (TMCAPZ) may be useful when arbitrary forward- or reverse-tracked pathlines are desired. These pathlines will represent the distance that a particle traveled for a time period equal to TMSIM.

[d/] The sign (+,-) of the well discharge or recharge rate does not need to be specified.

8.2.4 Example Applications

To demonstrate some of the capabilities of the GPTRAC semi-analytical module, the New Mexico and Seattle case studies solved previously using MWCAP were re-examined using GPTRAC. The confined aquifer type was used for each of these examples. Additional examples are presented in Section 8.4.

8.2.4.1 Albuquerque Example

The ground-water system at the Albuquerque site was described in Chapter 7. Figure 7.3 portrays the hydrogeological setting of the Albuquerque municipal wells, and the aquifer input parameters were discussed in section 7.43. However, because GPTRAC accounts for the effects of well interference, the three pumping wells were not lumped to one equivalent (imaginary) model well but rather were treated individually. The total discharge of 712,247 ft^3/d was divided equally between the three wells so that each well had a pumping rate of 237,416 ft^3/d. The same coordinate system depicted in Figure 7.3 was used so that the results of both modules could be overlayed. A stream boundary was specified along the left side of the study area.

The 25-year capture zones for the three wells computed using GPTRAC are shown in Figure 8.1. Each well draws water from the Rio Grande, but the capture zones of the top and bottom wells force the middle well to obtain much of its discharge from captured ambient flow. If these results are indicative of actual site conditions, one would expect water quality analysis from the northernmost and southernmost wells to reflect river water characteristics, while water quality for the middle well should reflect a combination of river water and the ambient aquifer flow.

As expected, one can see by overlaying Figures 8.1 and 7.4 that the 25-year capture zones lie within the steady-state capture zone delineated using MWCAP. Therefore, if the objective of the capture zone delineation exercise was to designate a WHPA for the entire well field, and the source of water for each individual well was not of concern, the approach used in section 7.4.3 of analyzing one "equivalent" model well would be valid.

The same limitations addressed in section 7.4.3 apply to this analysis. Although the Rio Grande probably contributes a significant portion of recharge to the pumping wells, the amount **is** certainly overestimated by GPTRAC due to the folly penetrating stream assumption. It is highly likely that the actual capture zones of the three wells extend to the west underneath the river.

Figure 8.1

**Twenty-Five-Year Capture Zones for The Albuquerque
Municipal Wells Located Near the Rio Grande**
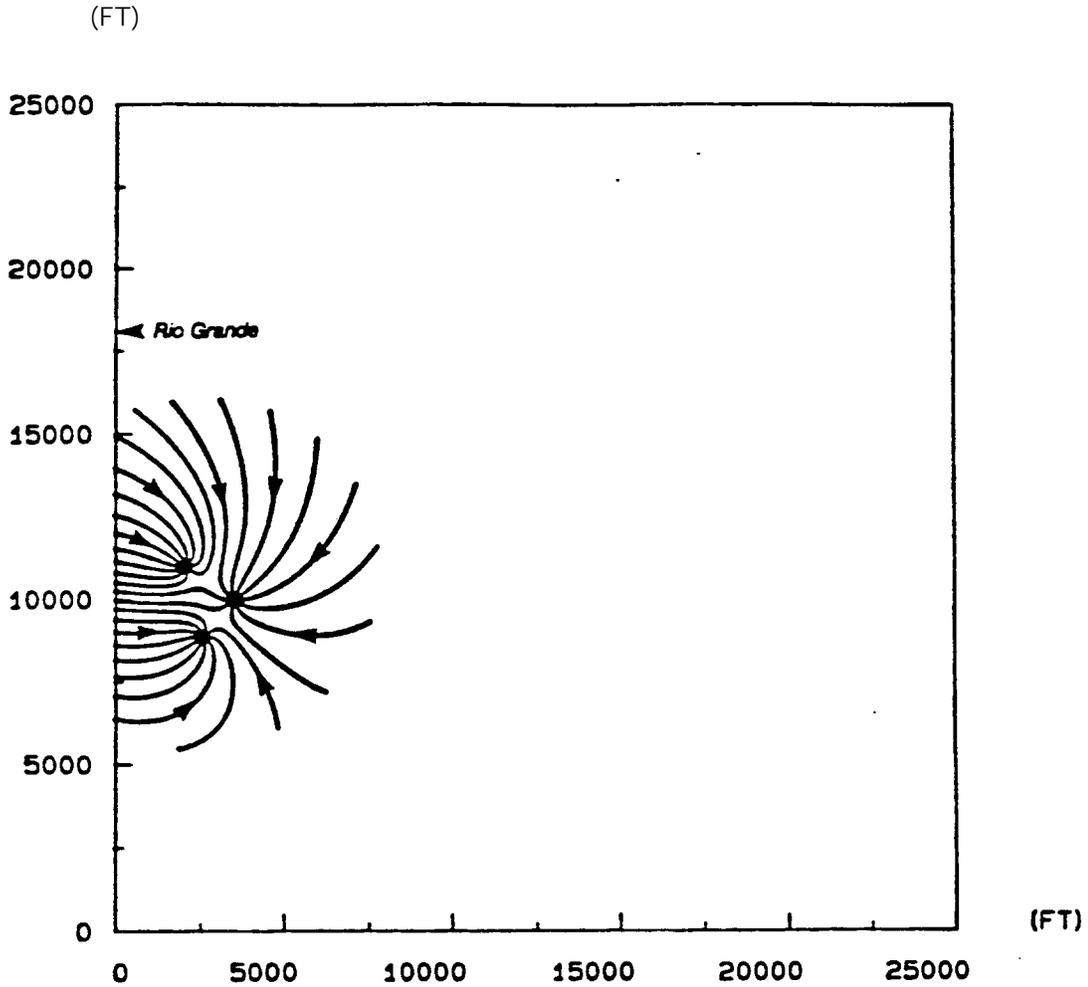
Simulation Options	Aquifer Properties	Well #1	Well #2	Well #3
Units = ft and days	T = 6,690	X = 2,000	3,500	2,100
Aquifer Type = confined	b = 200	Y = 8,900	10,000	11,000
Step Length = 200	ø = 0.25	Q = 237,416	237,416	237,416
No. Pumping Wells = 3	i = 0.0013	No. Pathlines = 10	10	10
Simulation Time = 9,125	a = -90°			
Capture Zone Time = 9,125				
Stream Boundary on Left Side of Domain				

8.2.4.2 **Seattle Example**

The Seattle Highline Well Field examplewas also re-examined using GPTRAC When this example was presented in section 7.4 as an MWCAP problem it was noted that a simple Theis analysis indicated that well interference effects between the two pumping wells were probably not negligible (i.e. the cones of depression for each well overlapped one another). Because the semi-analytical GPTRAC module (unlike MWCAP) accounts for well interference effects, the Seattle example was reanalyzed and differences in the capture zones were compared.

Background information for the Highline well field is presented in section 7.4.4. Recall that although the aquifer thickness remains fairly constant, transmissivity values reported in the vicinity of the two wells are markedly different. Because the semi-analytical GPTRAC module assumes a homogeneous aquifer, the average transmissivities for the Riverton Heights area (T = 44,573 ft2/d) and the Boulevard Park area (T = 20,888 ft2/d) were averaged to obtain an overall transmissivity of 32,730 ft2/d. Although this average value of transmisstivity is sufficient for this example, several additional approaches would be worthy of consideration if the actual WHPAs were to be designated. For example, a sensitivity analysis would be in order where, in two separate model runs, the overall aquifer transmissivity is set equal to the transmissivity values measured in the vicinity of each well.

The capture zone results obtained using MWCAP and GPTRAC are superimposed in Figure 8.2. A transmissivity of 32,730 ft^2/d, 10 pathlines for each well the confined aquifer type, and the additional parameters presented in Table 7.3 were used to obtain the GPTRAC capture zones.　The plot was not scaled to overlay on the base map for this example so that the results of each module could be more easily compared.

The effects of well interference are evident in Figure 8.2 in that the GPTRAC capture zones are not perfectly aligned with the angle of ambient ground-water flow (450), and there also exists a slight curvature in the capture zone outlines (particularly the top well).

The time-related capture zones and the hybrid capture zones do not have compatible lengths despite the fact that they both represent time periods of five years. This is because different transmissivity values were used for each well in MWCAP, but a single

Figure 8.2

Five-Year Hybrid Capture Zones (MWCAP) and Five-Year Time-Related
Capture Zones (GPTRAC) Computed for Highline Well Field

(FT)
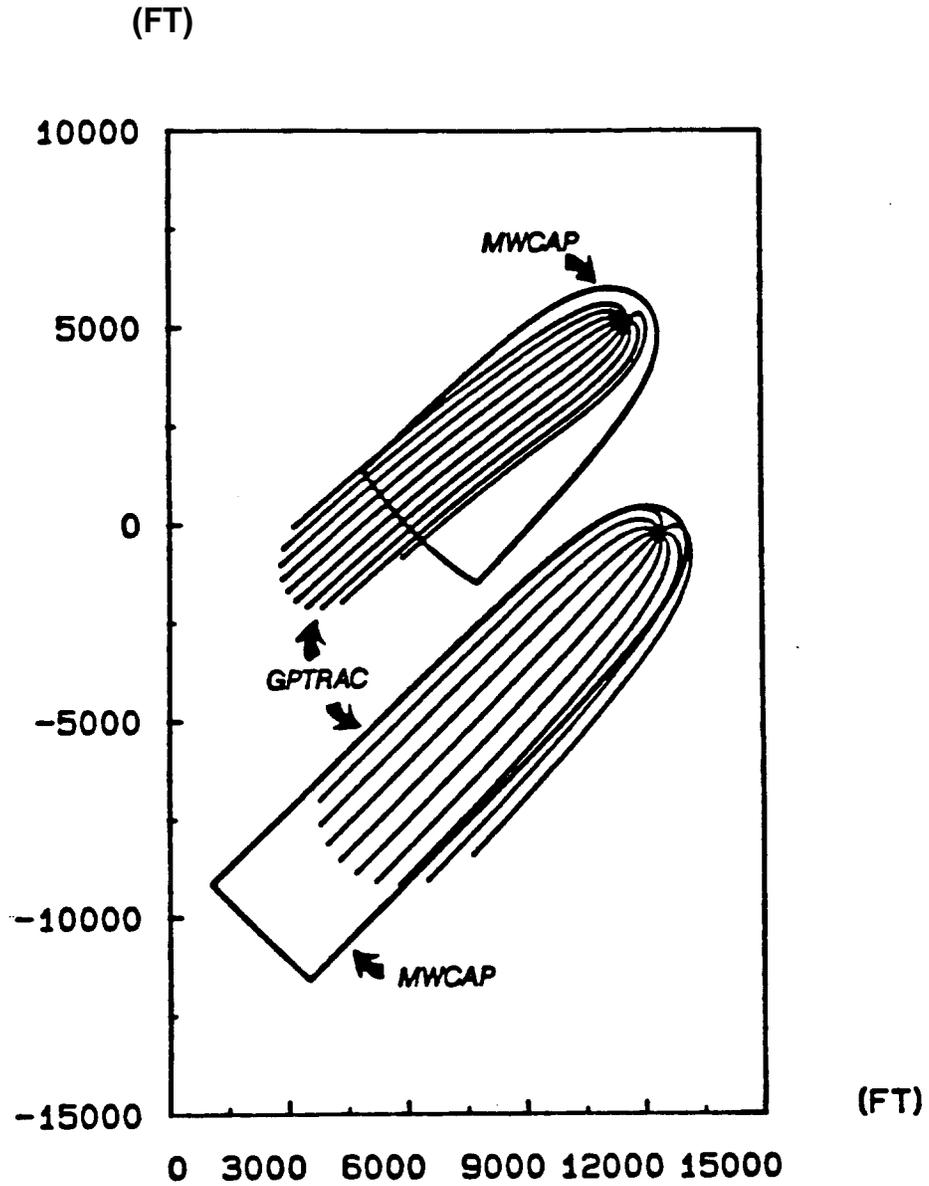
"averaged" valuc was required by GPTRAC. This approach leads to an interesting comparison of methods.

For the top well, the GPTRAC "average" transmissivity is higher than the MWCAP value. Therefore the 5-year GPTRAC capture zone is narrower and longer than the MWCAP S-year hybrid capture zone. For this well, the MWCAP capture zone is more conservative widthwise, but less conservative than the GPTRAC capture zone lengthwise.

For the bottom well the opposite is tree. The "average" GPTRAC transmissivity is lower for this well than was the MWCAP value. Therefore, the GPTRAC capture zone is more conservative than the MWCAP capture zone widthwise, but less conservative lengthwise.

8.3 Numerical Option

The numerical option of GPTRAC requires hydraulic heads at the nodes of a rectangular mesh as input. If head values are observed in the field or read from a map, they may be interpolated onto the nodal points of a grid using methods such as linear interpolation or kriging. More commonly, however, the head values supplied to GPTRAC will be the output of a finite difference or finite element ground-water flow model. In addition to nodal heads, GPTRAC requires the aquifer transmissivity (T), porosity (θ), and thickness (b). If the aquifer is heterogeneous, it may be divided into multiple zones of varying T, θ and/or b, and if it is anisotropic, each zone may have directional transmissivities T_x and T_y.

GPTRAC uses the above information, in conjunction with linear finite element or finite difference approximations, to determine the x and y velocity components of ground-water flow at the edges of each rectangular element or grid block Interlock or interelement hydraulic conductivities are computed by taking harmonic averages of the block or element hydraulic conductivities. If a finite element grid is used, the velocity components are also computed at the element centroids for the elements that share the well nodes. Pathlines of individual particles are delineated using particle tracking techniques based on semi-analytical and numerical integration. The computational procedure is described in detail in Appendix C.

t

8.3.1 Capabilities

The numerical option of GPTRAC can be used to delineate time-related capture zones. If required multiple pathlines starting at prescribed locations within the system can also be delineated. The number of pathlines used to delineate capture zones may be specified interactively by the user. Pathlines may be delineated using either forward or reverse particle tracking.

8.3.2 Assumptions and Limitations

Because the numerical GPTRAC option is based upon the availability of an observed or model calculated head field the assumptions and limitations associated with it are substantially less restrictive than those associated with the other WHPA model options. The first assumption is that the ground-water flow field is at equilibrium (steady state). The second limitation is that flow in the aquifer must be two-dimensional in the horizontal plane; vertical flow components arc neglected. Since GPTRAC does not obtain flow velocities from an analytical solution the aquifer need not be homogeneous.

8.3.3 Input Requirements

The input requirements for the GPTRAC numerical option are outlined in Table 8.2. Note that many of the variables may require iterative input depending upon the number of pumping wells, recharge wells, aquifer material zones forward-tracked pathlines, and reverse-tracked pathlines.

The most substantial input requirement for the GPTRAC numerical option that is different from the other WHPA model modules is the hydraulic head file. The structure of this file is illustrated in Figure 8.3. The head file should be a standard ASCII file with the format 5(I5,F1O.3). The first five spaces of each input field contain a node number, and the next ten spaces contain the head value associated with that node (head values may have a precision up to three decimal points). This pattern is repeated five times across each line of the input file. The utility program HEDCON, documented in Appendix E, is provided to assist users with the construction of GPTRAC head files.

The node number associated With each hydraulic head value is not used explicitly by the code, and therefore a dummy variable (e.g. set all node numbers to one) may be used if desired. However, the scheme of associating a node number with each head value provides a convenient method to assist users in visualizing the proper structure of the hydraulic head input file (Figure 83).

Table 8.2

Input Requirements for GPTRAC Numerical Option

Program Variable	Description
For each problem—	
IUNIT:	Default units of input parameters (feet and days or meters and days)
NPWELL:	Number of pumping wells within the study area
NRWELL:	Number of recharge (injection) wells within the study area
XMIN:	Minimum x-coordinate of study area (ft or m)
XMAX:	Maximum x-coordinate of study area (ft or m)
YMIN:	Minimum y-coordinate of study area (ft or m)
YMAX:	Maximum y-coordinate of study area (ft or m)
NZONES:	Number of aquifer zones that have different material properties (if aquifer is nonuniform)
NROWS and NCOLS, and XGRIDL(I), YGRIDL(J) for I=1, NCOLS and J=1, NROWS	Number of grid-line rows and columns, and (if non-uniform grid,) coordinates of each grid-line row and column
FILE1:	Input file name that contains head values for each node of the finite element or finite difference grid.
FILE2:	Input file name that contains the number of grid-line columns and rows and their coordinate values if file input option is selected.
NFPATH:	Number of forward-tracked pathlines
NRPATH:	Number of reverse-tracked pathlines
TMSIM:	Time period for which GPTRAC will be executed[a] (days)
TMCAPZ:	Time value assigned to time-related capture zones[a] (days)
For each pumping well (I=1, NPWELL) —	
XPWELL(I):	x-coordinate of well (ft or m)
YPWELL(I):	y-coordinate of well (ft or m)
QPWELL(I):	Well discharge rate[b] (ft^3/d or m^3/d)
NSTLIN(I):	Number of pathlines to be computed to delineate time-related capture zone (default = 20)

Table 8.2 (continued)

Input Requirements for GPTRAC Numerical Option

Program Variable	Description
For each injection well (I=1, NRWELL) —	
XRWELL(I):	x-coordinate of well (ft or m)
YRWELL(I):	y-coordinate of well (ft or m)
QRWELL(I):	Well recharge rate[b] (ft^3/d or m^3/d)
For each aquifer property zone (I=1, NZONES)[c] —	
XMINZO(I):	Minimum x-coordinate of zone (ft or m)
XMAXZO(I):	Maximum x-coordinate of zone (ft or m)
YMINZO(I):	Minimum y-coordinate of zone (ft or m)
YMAXZO(I):	Maximum y-coordinate of zone (ft or m)
TRANSX:	Transmissivity of zone - x direction[d] (ft^2/d or m^2/d)
TRANSY:	Transmissivity of zone - y direction[d] (ft^2/d or m^2/d)
BZO(I):	Saturated thickness of aquifer in zone (ft or m)
PORZO(I):	Porosity of aquifer in zone (dimensionless)
For each forward tracked pathline (I=1, NFPATH) —	
FSTART(I,1):	x starting coordinate (ft or m)
FSTART(I,2):	y starting coordinate (ft or m)
For each reverse tracked pathline (I=1, NRPATH) —	
RSTART(I,1):	x starting coordinate (ft or m)
RSTART(I,2):	y starting coordinate (ft or m)

[a]   A simulation time (TMSIM) different from the capture zone time (TMCAPZ) may be useful when arbitrary forward- or reverse-tracked pathlines are desired. These pathlines will represent the distance that a particle traveled for a time period equal to TMSIM.

[b]   The sign (+,-) of the well discharge or recharge rate does not need to be specified.

[c]   The first zonal area specified should be the entire study area. Therefore, it is most convenient to consider the largest zone to be zone 1, and then overlay the other zones on top of it. Zones of inactive cells should be given zero values for transmissivity.

[d]   The calculations in GPTRAC use the hydraulic conductivity of each material zone. Therefore, the transmissivity of each zone is divided by the thickness to obtain the conductivities, CONXZO(I) and CONYZO(I) for each zone I.

. **Figure 83**

Schematic Representation of Head Data File Format Required by GPTRAC
For Finite Element or Mesh-Centered Finite Difference Model Output With
Nodes Numbered in the y-Direction (a), or for Block-Centered Finite Difference Model
Output With Nodes Numbered in the x-Direction (b)

```
(4) 905.0      (8) 895.0          (12) 885.0      (16) 877.0

(3) |894.0     (7) |888.0         (11) |876.0     (15) |871.0

(2) |887.0     (6) |880.0         (10) |872.0     (14) |865.0

(1) |882.0     (5) |876.0          (9) |868.0     (13) |862.0
```

(1) = node number

1	882.0	2	887.0	3	894.0	4	905.0	5	876.0
6	880.0	7	888.0	8	895.0	9	868.0	10	872.0
11	876.0	12	885.0	13	862.0	14	865.0	15	871.0
16	877.0								

	1	2	3	4	5
1	905.0	895.0	885.0	877.0	864.0
2	894.0	888.0	876.0	871.0	861.0
3	887.0	880.0	872.0	865.0	860.0
4	882.0	876.0	868.0	862.0	858.0

1	882.0	2	876.0	3	868.0	4	862.0	5	858.0
6	887.0	7	880.0	8	872.0	9	865.0	10	860.0
11	894.0	12	888.0	13	876.0	14	871.0	15	861.0
16	905.0	17	895.0	19	885.0	19	877.0	20	864.0

(b)

Note that on the grid specification input screen the user is prompted for the number of grid-line columns and the number of grid-line rows. The number of grid-line columns is equal to the number of columns in the grid plus one, and the number of grid-line rows is equal to the number of rows in the grid plus one. The block-centered finite difference grid in Figure 8.3b has 5 columns and 4 rows, but it has 6 grid-line columns and 5 grid-line rows.

Many finite different codes (e.g., MODFLOW; McDonald and Harbaugh, 1988) usc formulations based upon a coordinate system where the y-axis is opposite that of a conventional Cartesian system. These codes assume an origin in the upper left-hand corner of the study area instead of the conventional lower left-hand corner location. Some postprocessing is required to rearrange the output from these codes to the format suitable for WHPA.

If the MODFLOW code is used, the POSTMOD program supplied with the code (if it was obtained from the International Ground Water Modeling Center) may be used to process the binary hydraulic head output file. POSTMOD has the capability to rearrange MODFLOW output to conform with a standard coordinate system where y-coordinates are measured from the lower left-hand comer rather than the upper left-hand comer of the modeled domain. The head file created using POSTMOD will have a x-coordinate, a y-coordinate and a head value on each line of the file. The HEDCON program supplied with the WHPA code may be used to convert the POSTMOD output file to a proper input format for GPTRAC.

The HEDCON program may also be used to construct GPTRAC input head files from data files that have nodal x- and y~coordinates and head values on each line, but which might be organized in no consistent fashion. Refer to Appendix E for detailed instruction on the capabilities and proper use of HEDCON.

83.4 Example Applications

Three examples that demonstrate the capabilities of the GPTRAC numerical option are presented in this section. The first two examples are hypothetical; the third example re-examines the Corning surficial aquifer previously analyzed using RESSQC.

8.3.4.1 Hypothetical Examples

The hypothetical aquifer used for the first two examples is shown in Figure 8.4. There are three distinct material zones within the aquifer. Zone 1 is isotropic and zones 2 and 3 are anisotropic (transmissivity is directionally dependent). Ambient ground-water flow is from north to south. The left and right sides of the aquifer are no-flow (barrier) boundaries. Two pumping wells discharging at 4,000 m^3/d and 3,000 m^2/d are screened over the entire aquifer depth of 20 m.

A hydraulic head field for the described hydrogeological scenario was obtained using a two-dimensional finite element ground-water flow and transport code called SAFTMOD (Huyakorn and Buckley, 1988). The steady-state head field computed by SAFTMOD, along with the aquifer geometry and the zonal hydraulic properties, were input to GPTRAC and the 100-day capture zone for each pumping well was delineated The input parameters for this example are presented in Table 8.3, and the capture zones are illustrated in Figure 8.5

The capture zones in Figure 8.5 have a complex shape and could not be delineated using the semi-analytical module. The top well located in zone 1 preferentially draws water from the region of high transmissivity; this is evidenced by the 'clustering" of pathlines that bend around the lower right-hand corner of zone 3. In general pathlines that enter low permeability materials will exhibit increased spacing between them as opposed to pathlines located in highly permeable materials. Note also that the pathlines refract at the material property interfaces. The capture zone for the top well is slightly larger than the capture zone of the bottom well primarily due to its larger pumping rate.

The results of the second example are presented in Figure 8.6. This example is identical to the first example, except that the pumping rate of the second well has been increased from 3,000 m^3/d to 5,000 m^3/d and its location was moved from zone 2 into zone 1 at x = 300 m and y = 333 m (Table 8.3). Again, it is readily apparent from Figure 8.6 that both wells tend to draw water from (and therefore have capture zones within) the zone of highest transmissivity.

For the second example, two initial locations from which particles were forward- and reverse-tracked for a period of 300 days were specified. The pathlines of these particles are indicated in Figure 8.6. The forward-tracked particle entered the first pumping well at some time less than 300 days. The reverse-tracked panicle travelled quite slowly during the 300 day period (as indicated by its short pathline) because it was released and tracked in the vicinity of the stagnation point formed by the bottom pumping well. If desired, additional panicles could have been released at arbitrary locations within the aquifer.

Figure 8.4

Hypothetical Aquifer and Hydraulic Properties Used
for First Two GPTRAC Numerical Examples
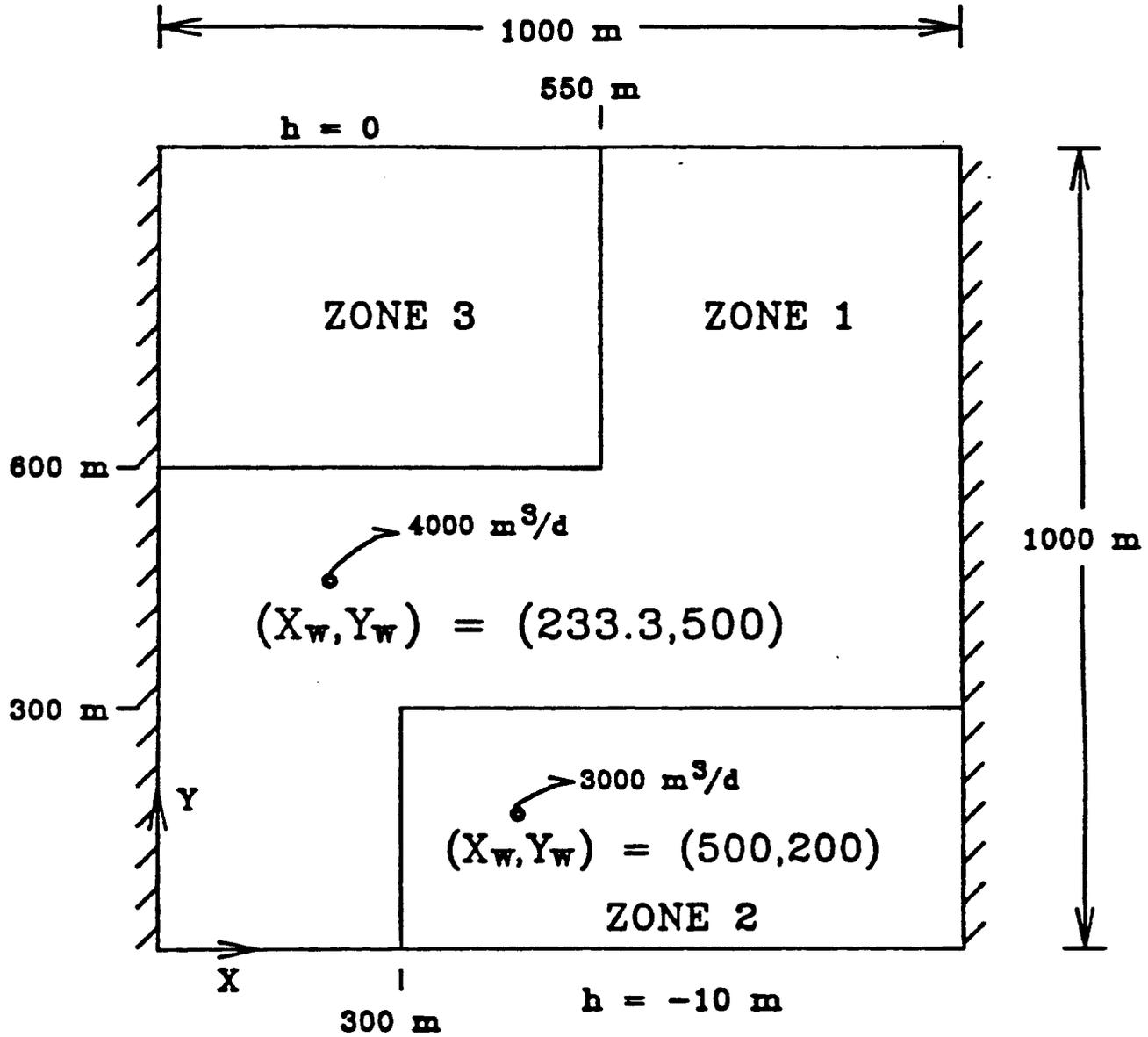
Zone No.	T_x	T_y	b	θ
1	2,000	2,000	20	0.25
2	1,000	200	20	0.20
3	500	200	20	0.15

Table 8.3

Input Parameters for GPTRAC Hypothetical Aquifer
(Examples One and Two)

EXAMPLE ONE

GPTRAC Numerical Option Using Rectangular Finite Element Model

Units = meters and days
Uniform Grid (Constant Spacings) - Yes
Uniform Aquifer Properties - No
Hydraulic Head Data File - TP8EX1

XMIN = 0.0   YMIN = 0.0
XMAX = 1000 YMAX = 1000

No. of Grid-line Rows = 31
No. of Grid-line Columns = 31
Nodes are numbered along y - axis (option O)
No. of Pumping Wells = 2
No. of Injection Wells = O
No. of Material Zones = 3

Zone No.	XMIN	XMAX	YMIN	YMAX	Tx	Ty	b	θ
1	0	1,000	0	1,000	2,000	2,000	20	0.25
2	300	1,000	0	300	1,000	200	20	0.20
3	0	550	600	1,000	500	200	20	0.15

Simulation Time = 300 days
Capture Zone Time = 100 days

Well No.	X	Y	Q	Capture Zone	No. of Pathlines
1	233	500	4,000	Yes	15
2	500	200	3,000	Yes	15

No. of Forward Pathlines = 0
No. of Reverse Pathlines = 0

Table 8.3 (continued)

Input Parameters for GPTRAC Hypothetical Aquifer
(Examples One and Two)

EXAMPLE TWO

Same as example 1 except for the following changes:

Hydraulic Head Data File - TP8EX2

Well No.	X	Y	Q	Capture Zone	No. of Pathlines
1	233	500	4,000	Yes	20
2	300	333	5,000	Yes	20

No. of Forward-Tracked Pathlines = 1
    Starting Location: X = 450, Y = 800

No. of Reverse-Tracked Pathlines = 1
    Starting Location: X = 175, Y = 175

Figure 8.5

**One-Hundred-Day Capture Zones for Two Pumping Wells in Hypothetical Aquifer**
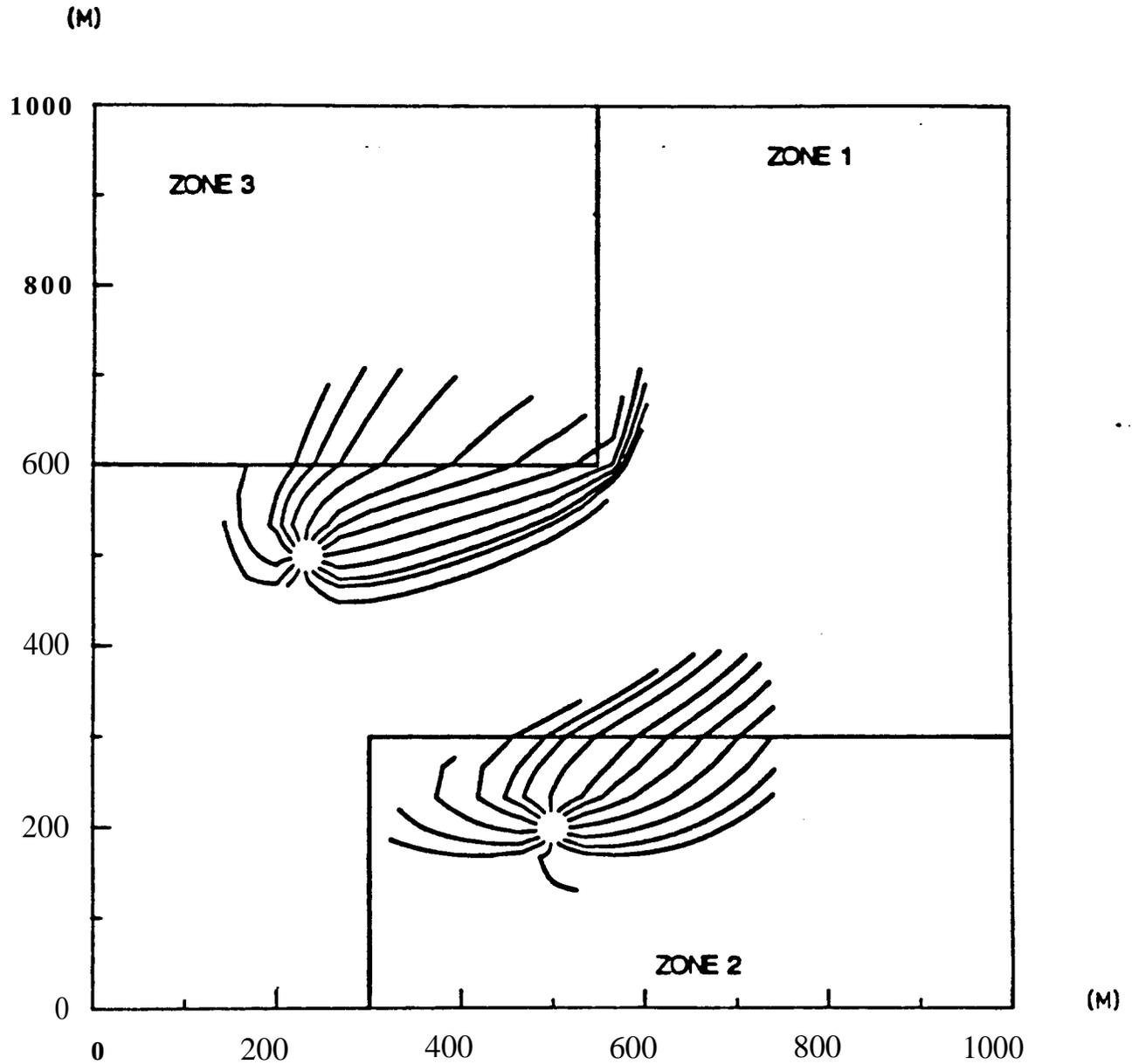
Figure 8.6

**One-hundred-Day Capture Zones for Two Wells and Three-Hundred-Day Reverse-
and Forward-Tracked Pathlines for Hypothetical Aquifer**
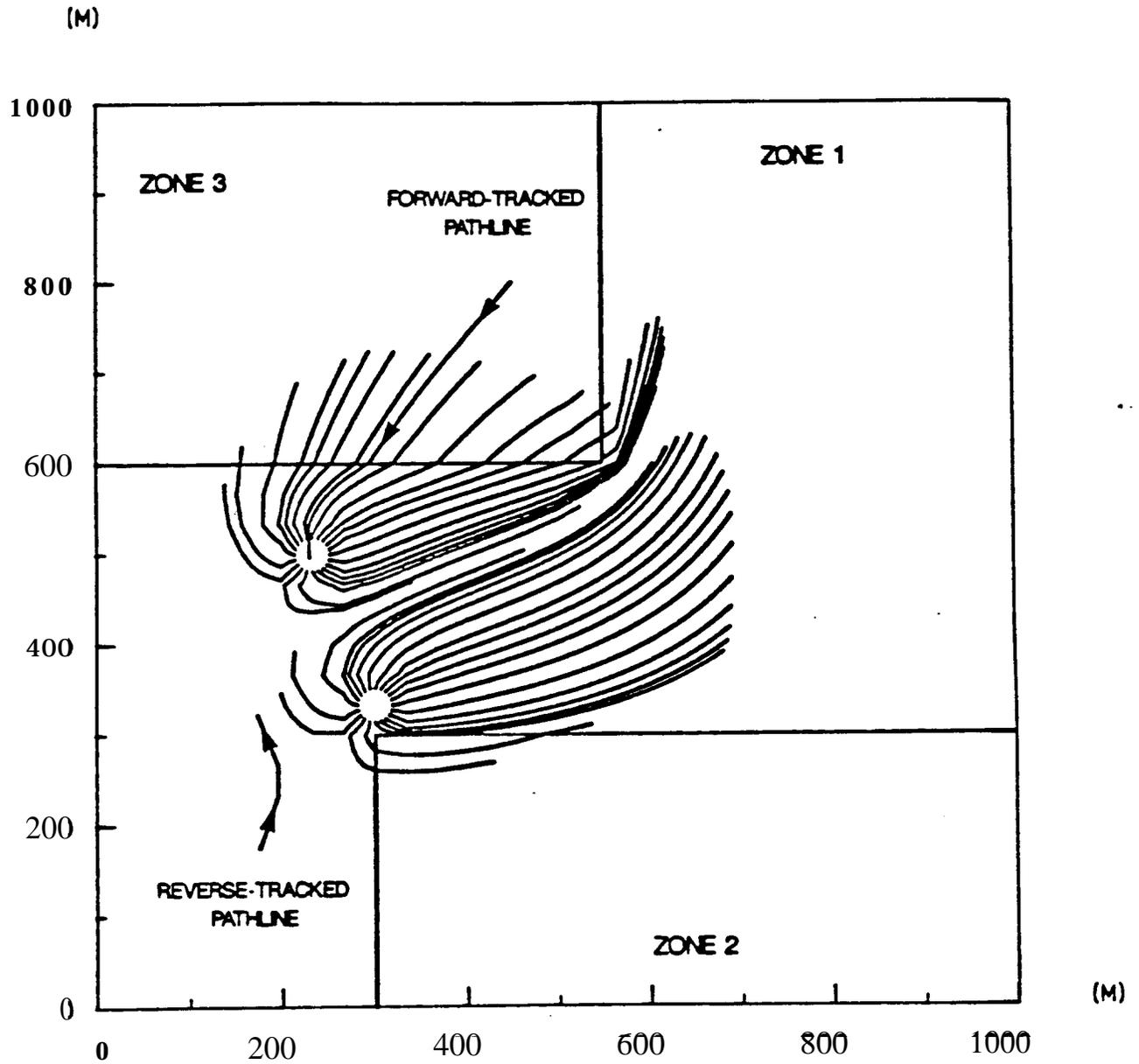
8.3.4.2 Corning Example

The final example is based on the results of a numerical ground-water flow simulation for the surficial aquifer in the vicinity of Corning, New York. Some background information for the Corning aquifer was provided in Section 6.5.2. The study area (Figure 8.7) is a subdomain of the region studied by Ballaron (1988).

The valley sediments in the vicinity of Corning consist of stratified glacial drift deposits that are primarily interbedded silty to clean sands and gravels. Relatively thin deposits of lacustrine clay, silt and fine sand exist over much of the Valley and separate a surficial, unconfined aquifer from a confined to semi-confined aquifer at depth. Two idealized cross sections through the study area are presented in Figure 6.4.

The surficial aquifer has an average saturated thickness of about 25 ft. No-flow boundaries were used where the surficial aquifer sediments pinch out or abut against the older, low permeability valley walls. Values for the prescribed hydraulic bead boundary nodes (Figure 8.8) were interpolated from the steady-state head map for the surficial aquifer presented in Ballaron (1988).

The approximate distribution of hydraulic conductivity for the surficial aquifer was also taken from Ballaron and is presented in Figure 8.8. An areal recharge rate of 0.00297 ft/d (13 in/yr) was used for the entire study area. Recharge from the Chemung River and leakage between the surficial and lower aquifer units were neglected. Ground-water flow in the aquifer was simulated using the USGS block-centered finite difference code MODFLOW (McDonald and Harbaugh, 1988). The grid consisted of 36 rows and 42 columns (37 g-rid-line rows and 42 grid-line columns). Each cell was 250 ft on a side.

The results of the first simulation for steady-state conditions are illustrated in Figure 8.9a. This is the steady-state head map that was used in the RESSQC examples section to obtain the hydraulic gradient and direction of ambient flow information for the Coming example.

For the second simulation, three pumping wells were assumed to fully penetrate the surficial aquifer. The location and rates of pumping for these wells, along with the steady-state head field predicted using MODFLOW are illustrated in Figure 8.9b.

Figure 8.7

**General Site Map and Modeling Area Boundary for Surficial
Aquifer in the Vicinity of Corning, NY**
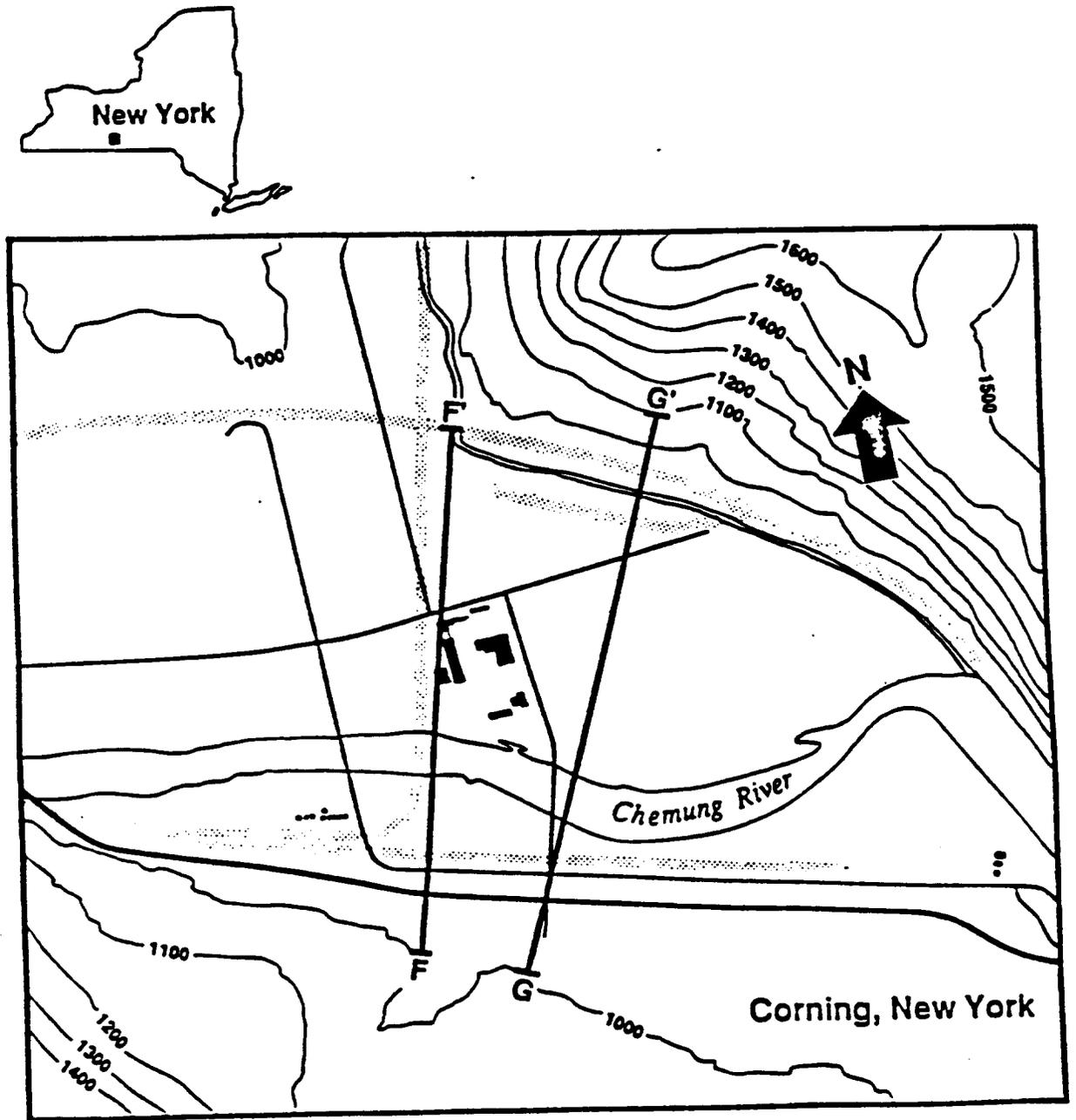
Figure 8.8

**Finite Difference Model Boundary Conditions and Distribution of
Hydraulic Conductivity for Surficial Corning Aquifer**

k = 1 FT/D

k = 30 FT/D

k = 150 FT/D

k = 400 FT/D
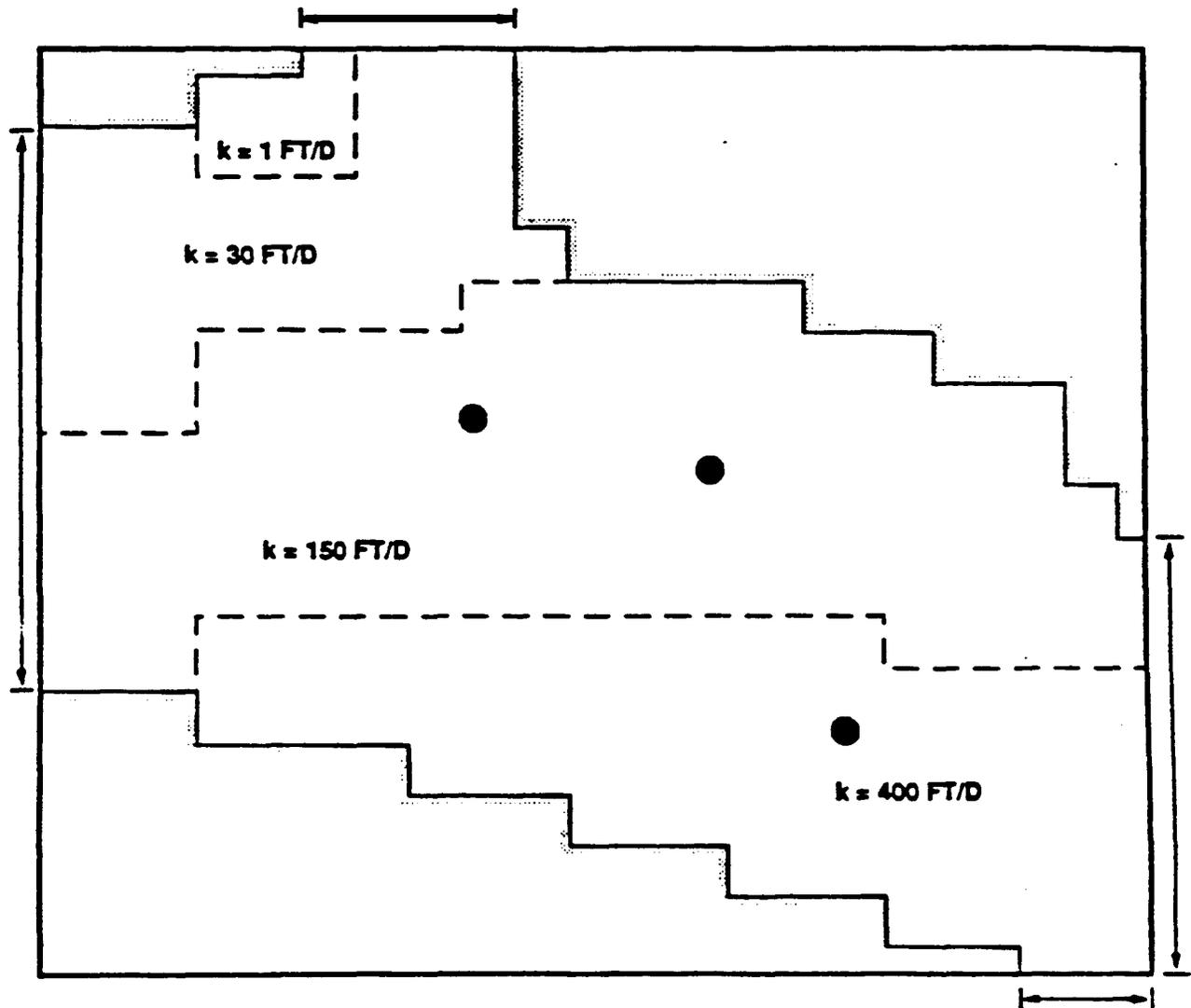
|←——→| Prescribed Head Boundary

No-Flow Boundary

– – – Hydraulic Conductivity Interface

● Pumping Well

0   1,750 ft

Scale
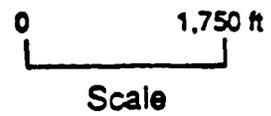
Figure 8.9

**Steady-State Head Field for Surficial Coming Aquifer Using MODFLOW
for (a) No Pumping Wells and (b) Three Pumping Wells**
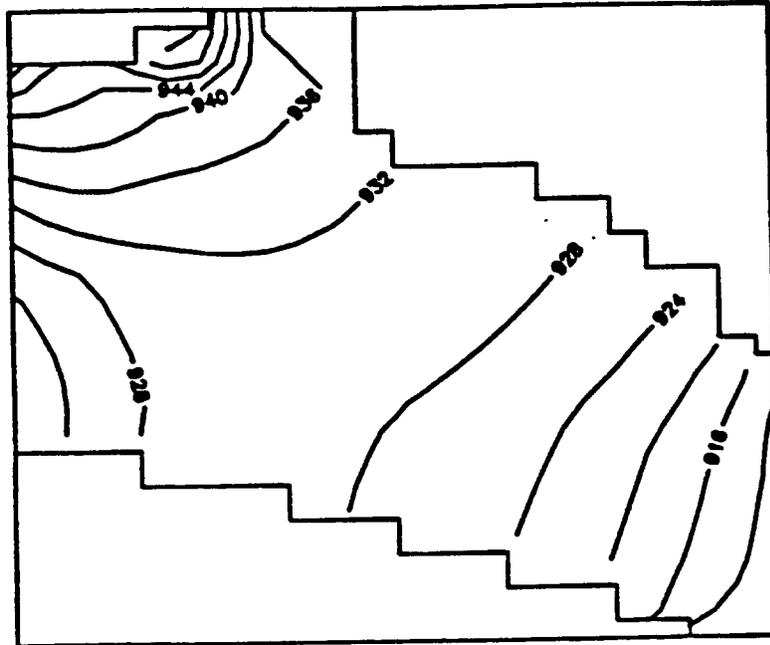
(a)
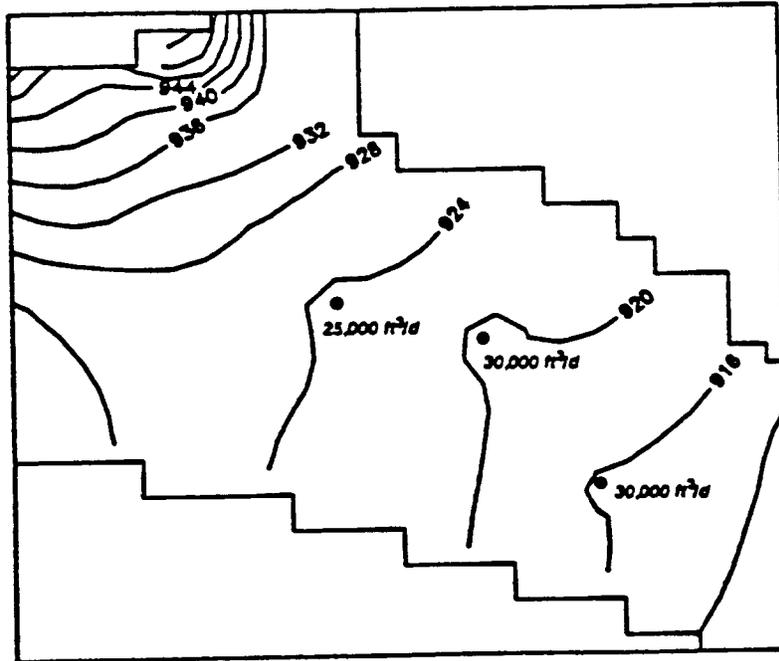
(b)

Once the head field for the second simulation was obtained using MODFLOW, the WHPA model was applied to delineate the 5-year capture zones for the three pumping wells. The required input for the GPTRAC numerical option is provided in Table 8.4, and the delineated capture zones are presented in Figure 8.10. The capture zones for this example are very complex due to the aquifer heterogeneities and well interference effects.

Note that since MODFLOW uses a coordinate system based upon an Origin in the upper left-hand corner of the study area some manipulation of the output head file was performed to obtain the head values ordered in a suitable fashion for input into WHPA. The standard POSTMOD program supplied with the MODFLOW code (when it is obtained from the International Ground Water Modeling center) was used to process the binary head file output by MODFLOW. The POSTMOD code has an option to produce an ASCII file in which the head values are ordered according to a standard coordinate system (i.e. origin in lower left-hand comer of study region). This file may then be used directly by numerous software plotting packages such as SURFER (Figure 8.9 was constructed using the ASCII file and SURFER). This ASCII file was further rearranged using the program HEDCON supplied with the WHPA code. One HEDCON program option is to create an input head file suitable for WHPA using an ASCII file output by POSTMOD.

By comparing the capture zones delineated using GPTRAC and RESSQC (Figures 8.10 and 6.6), the effects of areal recharge and aquifer heterogeneities on the Corning capture zones may be qualitatively assessed. The capture zones for wells 1 and 2 in the center of the study area are markedly similar. The RESSQC capture zones are larger in area] extent because recharge from local precipitation was neglected.

The capture zones for the third well are quite different due to aquifer heterogeneities. In Figure 8.10 this capture zone extends from the well almost due west; in Figure 6.6 this capture zone is aligned more with the angle of ambient flow (northwest). This effect is do "primarily to the fact that well 3 is located within a zone of high aquifer permeability and its effects on the capture zone could not be represented using RESSQC. For well 3, neglecting aquifer heterogeneities has very significant consequences.

Table 8.4

Input Parameters for GPTRAC Numerical Option for Corning Example Problem

Block-Centered Finite Difference Option

Units = feet and days
Uniform Grid (Constant Spacings) - Yes
Uniform Aquifer Properties -No
Hydraulic Head Data File - CRNMOD1.HED

XMIN = 0.0   YMIN = 0.0
XMAX = 10500   YMAX =9000

No. of Grid-line Rows = 37
No. of Grid-line Columns = 43
Nodes are numbered along x - axis (option 1)
No. of Pumping Wells = 3
No. of Injection Wells = O
No. of Material Zones = 20

Zone No.	XMIN	XMAX	YMIN	YMAX	Tx	Ty	b	θ
1	0	10,500	0	9,000	0	0	1	0.22
2	0	1,750	5,250	8,250	1,080	1,080	36	0.22
3	0	1,750	2,750	5,250	780	780	26	0.22
4	1,750	3,250	6,250	7,750	1,440	1,440	48	0.22
5	1,750	3,250	7,750	8,750	48	48	48	0.22
6	3,250	4,250	6,250	9,000	1,080	1,080	36	0.22
7	4,250	4,750	6,750	9,000	1,020	1,020	34	0.22
8	4,750	5,250	6,750	7,250	1,020	1,020	34	0.22
9	4,250	7,250	6,250	6,750	960	960	32	0.22
10	1,750	3,750	2,250	3,250	11,200	11,200	28	0.22
11	3,750	5,250	1,750	3,250	11,200	11,200	28	0.22
12	5,250	6,750	1,250	3,250	10,400	10,400	26	0.22
13	6,750	8,250	750	3,250	9,600	9,600	24	0.22
14	8,250	10,500	250	2,750	6,400	6,400	16	0.22
15	8,250	8,750	2,750	5,750	3,300	3,300	22	0.22
16	8,750	9,750	2,750	5,250	3,000	3,000	20	0.22
17	9,750	10,500	2,750	4,000	2,400	2,400	16	0.22
18	9,750	10,200	4,000	4,250	2,400	2,400	16	0.22
19	1,750	8,250	3,250	6,250	2,400	2,400	30	0.22
20	2,750	3,250	8,750	9,000	48	48	48	0.22

Simulation Time = 1825 days
Capture Zone Time = 1825 days

Table 8.4 (continued)

Input Parameters for GPTRAC Numerical Option for Coming Example Problem

Well No.	X	Y	Q	Capture Zone	No. of Pathlines
1	4,375	4,875	25,000	Yes	10
2	6,375	4,375	30,000	Yes	10
3	7,875	2,375	30,000	Yes	10

No. of Forward Pathlines = 0
No. of Reverse Pathlines = 0

Figure 8.10

Five-Year Capture Zones of Three Pumping Wells in the Vicinity of Corning, NY
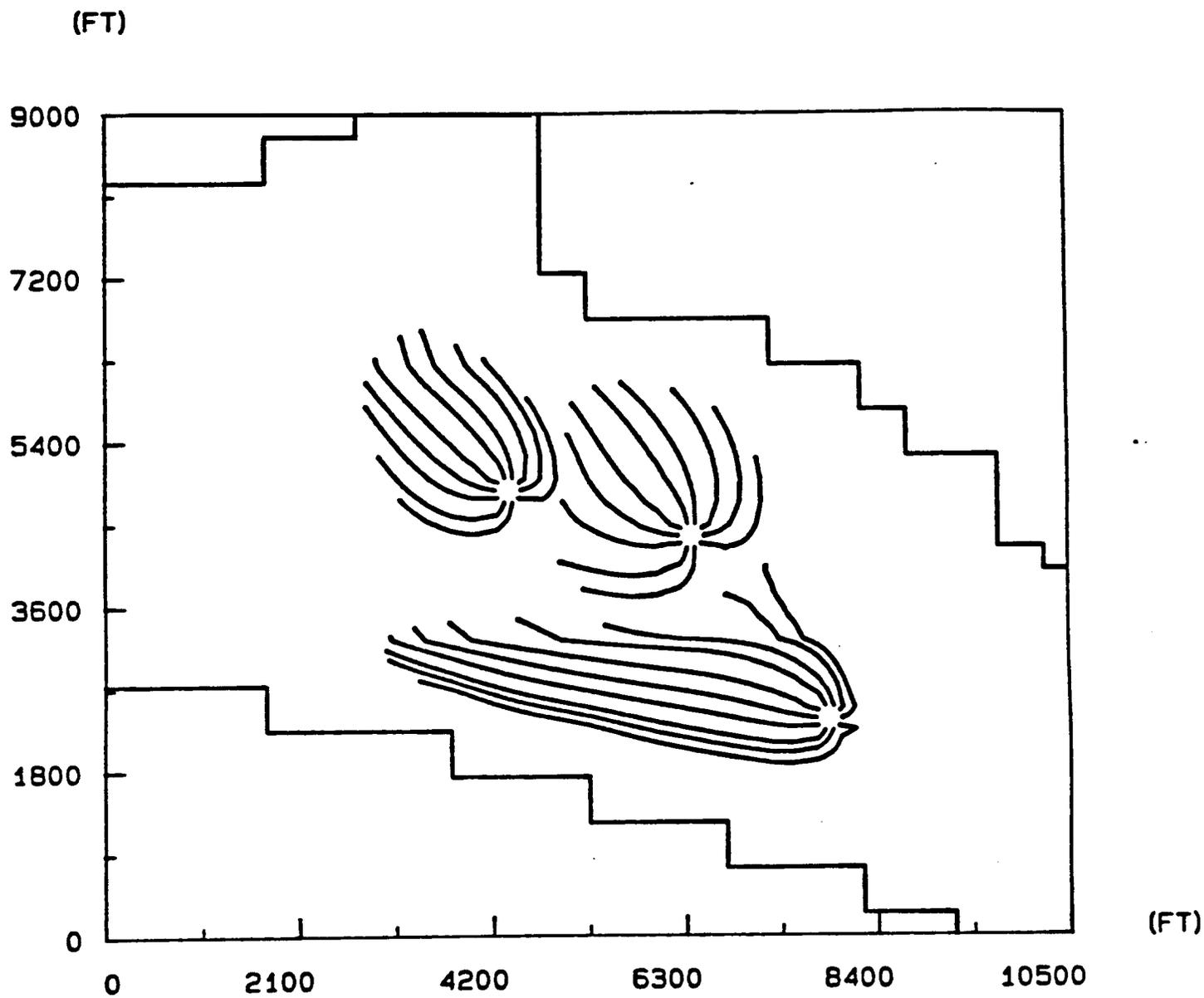
8.4 Comparison of Semi-Analytical and Numerical Options

In this section, both the semi-analytical and numerical options of GPTRAC are exercised with the intent of providing test examples that verify some additional analytical solutions available in the code for various aquifer and boundary conditions. In each example, capture zones obtained using the two modeling options are compared.

8.4.1 Strip Confined Aquifer Examples

This example involves strip confined aquifers bounded on two (parallel) sides. Three cases with different combinations of barrier and stream boundaries arc considered. For each case, the aquifer transmissivity and thickness are 1,000 ft^2/d and 50 ft respectively, and the effective porosity is 0.25. There is one well located at x=2,000 ft and y=l,200 ft and the pumping rate of the well is 3,000 ft3/d. Ambient ground-water flow is assumed to be zero. Figures 8.11a through 8.11c show capture zones computed using the semi-analytical module of GPTRAC for a very large time value, t=l0^6 days (to ensure a steady-state condition). Note that the three cases correspond to: (1) aquifer with two barrier boundaries, (2) aquifer with two stream boundaries, and (3) aquifer with a stream and a barrier boundary. In each case, the boundaries are parallel to the x-axis at y=O and at y=l,5OO ft. The three cases were also simulated using the numerical option of the code. For each case, a uniform finite element grid with ▲x=▲y= 100 ft was used, and zero drawdown conditions were imposed on the left and right hand side boundaries of the flow domain. Figure 8.12 illustrates the resulting capture zones. A comparison of the two sets of Figures (8.11 and 8.12) shows good agreement between the semi-analytical and the numerical solutions for each case.

8.4.2 Unconfined Aquifer Examples

Four unconfined flow examples with different values of pumping rate, recharge and hydraulic conductivity are presented in this section. In each case, there is one pumping well and the aquifer is assumed to be homogeneous and isotropic. The effective porosity of the aquifer is 0.25.

For the first case, an unconfined aquifer with a well pumping near a stream is considered. The well is located at x=350 ft and y=l,250 ft. The pumping rate is 5,000 ft^3/d. The hydraulic conductivity and initial saturated thickness of the aquifer are 20 ft/d and 48.12 ft, respectively. Ambient ground-water flow and areal recharge are assumed to be zero. Figures 8.13a and 8.13b are the 20,000-day capture zones computed using the

Figure 8.11

Strip Aquifer Simulations Using the Semi-Analytical GPTRAC Module for Two
Barriers (a), Two Streams (b), and a Sream and a Barrier (c)

(a)

(b)

(c)

. Figure 8.12

**Strip Aquifer Simulations Using the Numerical GPTRAC Module for Two
Barriers (a), Two Streams (b), and a Stream and a Barrier (c)**
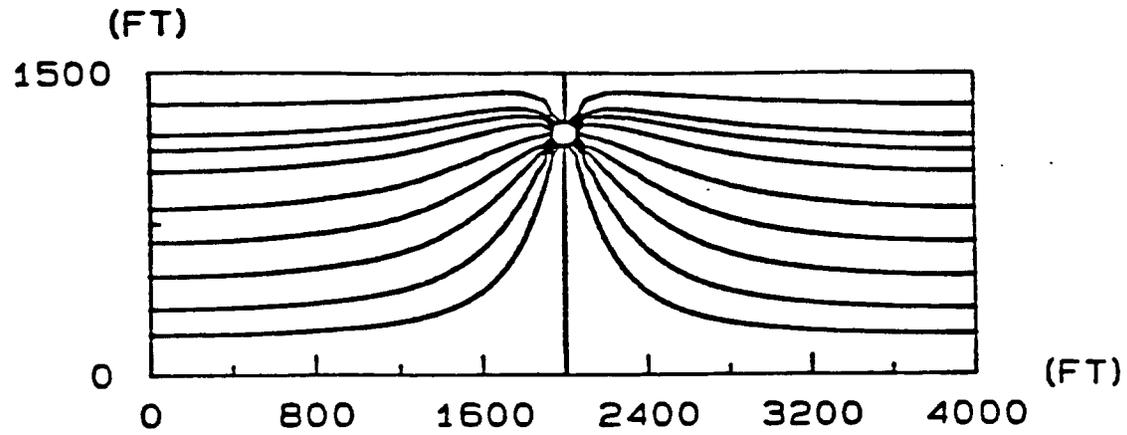
(a)
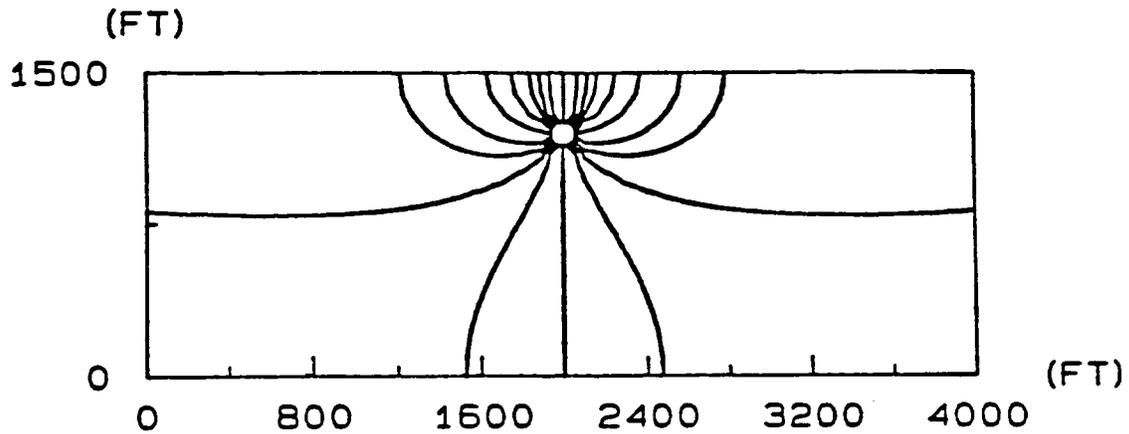
(b)
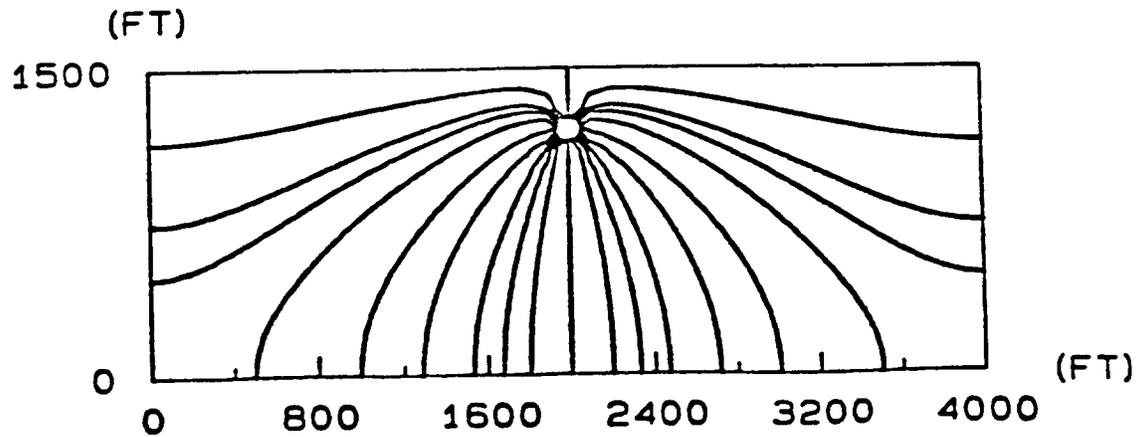
(c)

Figure 8.13

**Capture Zones Computed Using the Semi-Analytical (a) and Numerical (b)
GPTRAC Options for Unconfined Aquifer with Zone Recharge**
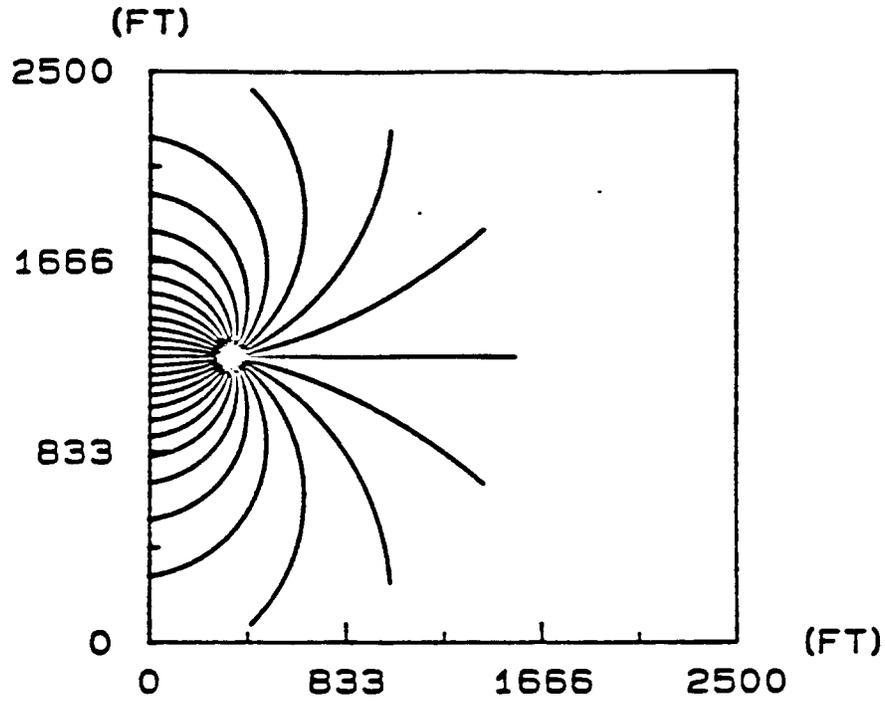
(a)
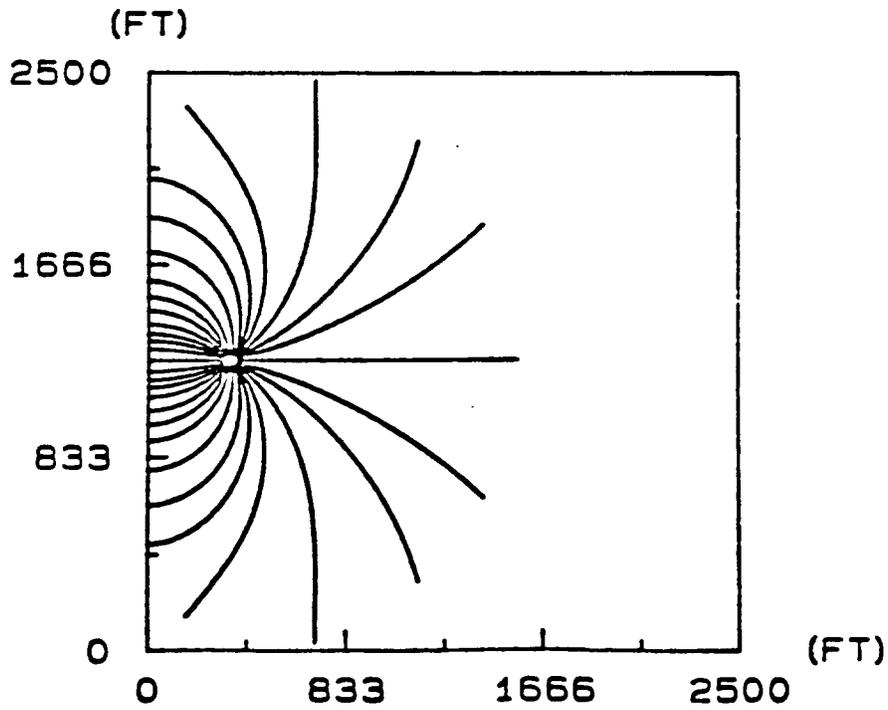
(b)

semi-analytical and numerical options, respectively. For the semi-analytical option, a stream boundary condition with a constant head value of 48.12 ft was imposed along the y-axis of the plot. For the numerical option a uniform rectangular grid with nodal spacings $\Delta x = \Delta y = 50$ ft was used. Nodal head values were obtained using a finite element flow model with a constant head boundary condition of h=48.12 imposed on each side of the rectangular domain. A comparison between Figures 8.13a and 8.13b shows an excellent agreement between the capture zones delineated using the semi-analytical and numerical GPTRAC options.

The second case concerns an unconfined aquifer with areal recharge of 0.0023 ft/d. (10.0 in/yr), and a well pumping rate of 20,000 ft^3/d. The remaining data and boundary conditions are the same as those for the previous case. Figures 8.14a and 8.14b illustrate the 2,000-day capture zones obtained using the semi-analytical and numerical options respectively. Again, the two solutions agree quite well.

For the third and fourth cases, the semi-analytical option of GPTRAC was used to model a well pumping in an areally infinite unconfined aquifer with recharge equal to 0.0023 ft/d and no ambient flow. The two cases were designed to demonstrate the effect of the reduction of hydraulic conductivity and saturated thickness of the aquifer on the extent of the capture zone. Figures 8.15a and 8.15b show the 4,000-day capture zones predicted by the GPTRAC semi-analytical model for hydraulic conductivity values of 20 and 2 ft/d respectively. Both capture zones correspond to the well pumping rate of 5,000 ft^3/d. Note that the two capture zones are circular and the low-conductivity capture zone (K=2 ft/d) has a slightly higher radius. The reason for this is that the decrease of hydraulic conductivity from 20 ft/d to 2 ft/d led to a reduction in saturated thickness (or increase in drawdown) in the inner portion of the flow region surrounding the well. This resulted in higher velocities for the same pumping rate.

Figure 8.15

Capture Zones Computed Using Semi-Analytical GPTRAC Module for an Unconfined
Aquifer with Zero Recharge and Ambient Flow and a Hydraulic Conductivity
of (a) 20 ft/d, and (b) 1 ft/d
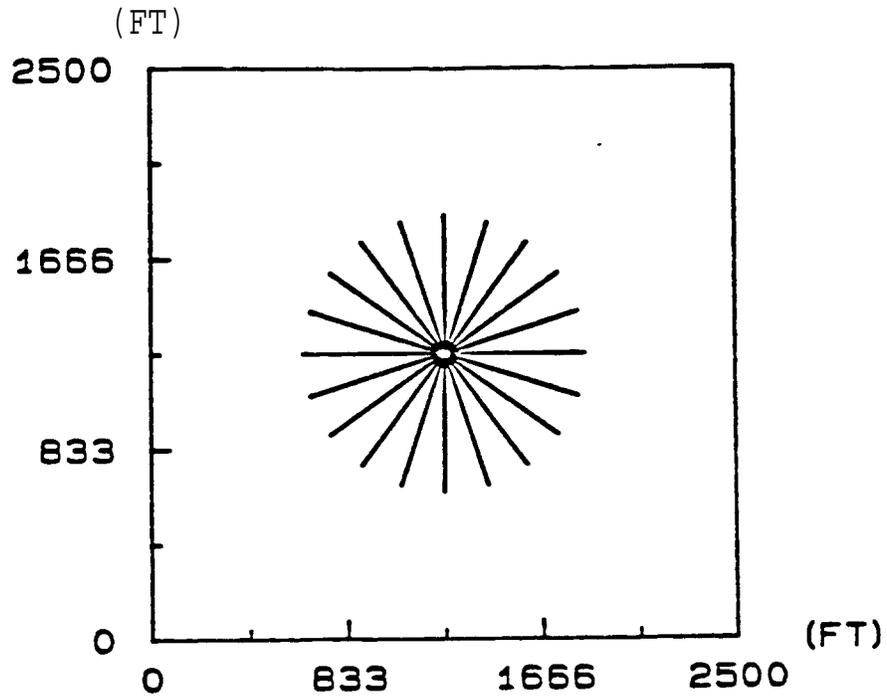
(a)
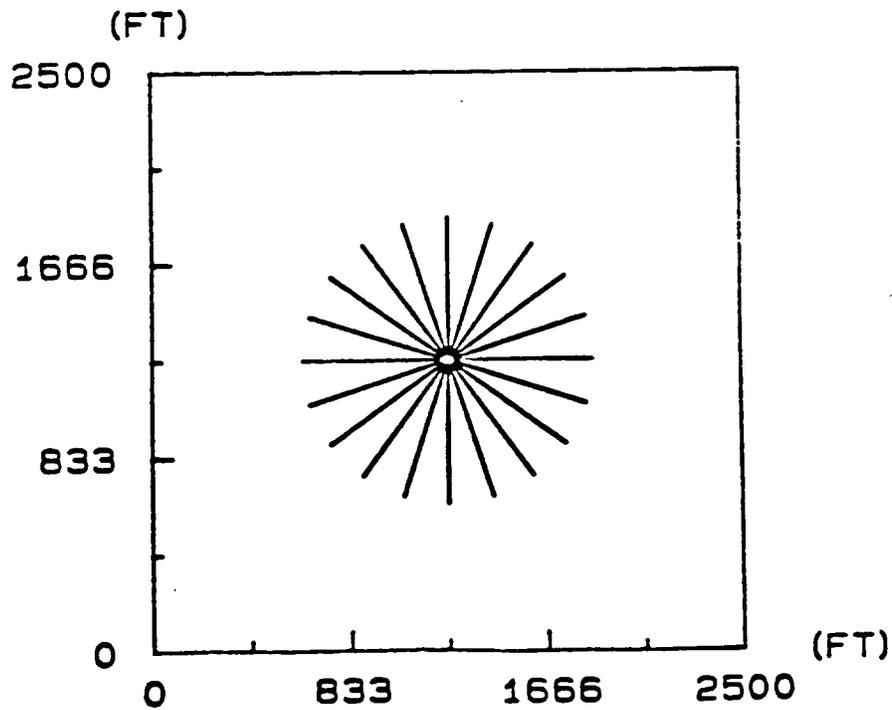
(b)

8.43 Leaky Aquifer Example

In this example, a semi-confined aquifer underlain by an impermeable (barrier boundary) and overlain by a semi-permeable aquitard layer is considered. When such an aquifer is pumped vertical leakage occurs through the aquitard. The top of the aquitard is assumed to be subject to a zero drawdown condition. For the case simulated the hydralic conductivity and thickness of the aquifer are 20 ft/d and 50 ft respectively, and the hydraulic conductivity and the thickness of the confining bed are 0.2 ft/d and 40 ft, respectively. The well is pumping near a stream at a rate of 20,000 ft^3/d. Depicted in Figures 8.16a and 8.16b are 10,000-day capture zones obtained using the semi-analytical and numerical GPTRAC options, respectively. Note that a zero drawdown condition was assumed on the boundary of a uniform rectangular finite element grid ($\Delta x = \Delta y = 50$ft). A comparison of Figures 8.16a and 8.16b shows very good agreement between the semi-analytical and numerical solutions to the problem.

Figure 8.16

**Capture Zones for Semi-Confined (Leaky) Aquifer Using the Semi-Analytical (a)
and Numerical (b) GPTRAC Modules**

(a)

(b)
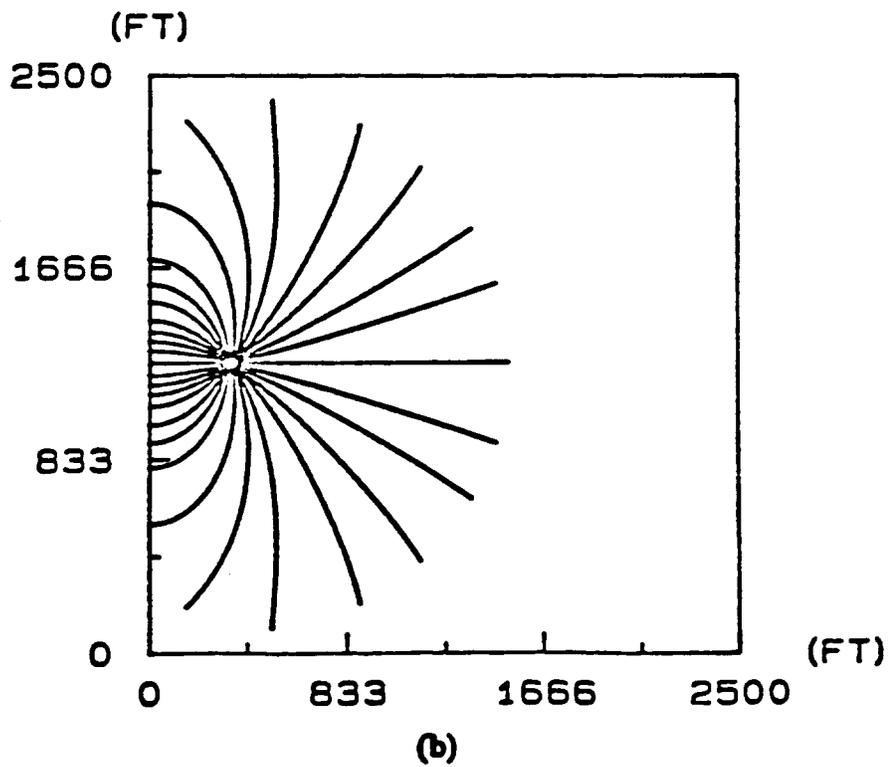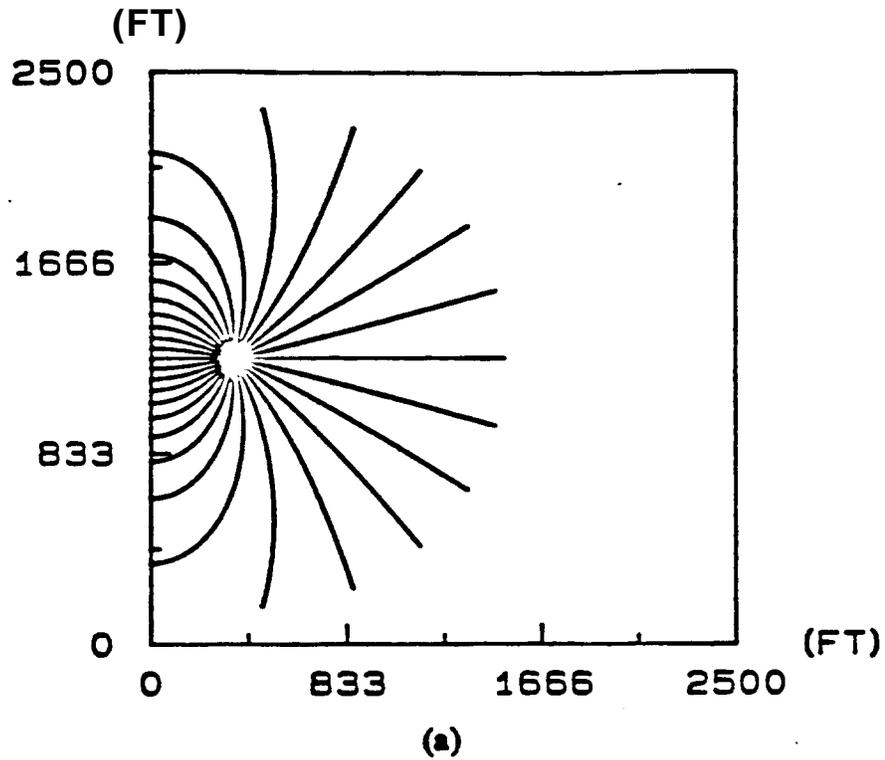
9.0 Uncertainty Analysis Module (MONTEC)

9.1 Introduction

The computational modules described previously delineate various types of capture zones for a variety of ground-water flow scenarios. Each module requires a number of user-specified input parameters such as transmissivity, porosity, etc. Typically, the values of these parameters are not known exactly due to measurement errors, data limitations, and/or inherent spatial and temporal variability. Often, no tests have been performed to determine the aquifer hydraulic properties for a given site, and the values used will be an "educated guess" on the part of the delineator.

If the uncertainties associated with one or more input variables are deemed significant, it may be appropriate to express the variable(s) in a random context. Random variables may be thought of as variables with more than one potential value, and therefore they are described by probability distributions. The most likely value that a random variable will assume is the mean of its associated probability distribution. The variance of a probability distribution is a measure of the range of values that the corresponding random variable may assume.

If one or more input variables of the capture zone model are considered random, then Monte Carlo analysis may be used to assess the effect of the uncertain input parameters on the model output (capture zones). For reasons discussed in Section 9.4.1, only time-related capture zones for a single pumping well in a homogeneous, isotropic, confined or semi-confined aquifer with steady and uniform ambient ground-water flow may be analyzed using the Monte Carlo option.

9.2 Uncertainty Analysis Objectives

The objective of the Monte Carlo approach is to estimate the uncertainty in capture zone size and shape given the uncertainty in the model input parameters. Alternatively, the objective is to estimate the cumulative probability distribution of the capture zone boundary

given the probability distribution of the input parameters. Thus, if R represents some measure of the capture zone size and $\underline{X}$ represents the vector of all model inputs:

$$R = W(\underline{X}) .\tag{9.1}$$

where W represents the WHPA model. Note that only some of the components of $\underline{X}$ may vary in an uncertain way, i.e., they may be random variables defined by a probability distribution. Thus, the goal is to calculate the cumulative distribution function $F_R(R')$ given a probabilistic characterization of $\underline{X}$. $F_R(R')$ is defined as

$$F_R(R') = \text{Probability } (R \leq R')\tag{9.2}$$

where R' is a given capture zone extent.

9.3 The Monte Carlo Technique

Given a set of values for each of the model input parameters, $X_1, X_2 \cdots X_n$, the WHPA model computes the capture zone boundary R:

$$R = W(X_1, X_2, X_3 \cdots X_n)\tag{9.3}$$

Application of the Monte Carlo simulation procedure requires that at least one of the input variables, $X_1 \cdots X_n$, be uncertain and that the uncertainty be represented by some probability distribution. The method involves the repeated generation of pseudo-random values of the uncertain input variable(s) (drawn from the known distribution and within the range of any imposed bounds) and the application of the model using these values to generate a series of capture zones. The term pseudo-random (hereafter referred to as random) number is used because truly random numbers can not be generated on the computer; the computer is only capable of generating sets of numbers that exhibit the characteristics of a given probability distribution. The capture zones are then statistically analyzed to yield a cumulative probability distribution. Thus, the various steps involved in the application of the Monte Carlo simulation technique are:

1. Selection of representative probability distributions for the input variables that are to be considered uncertain.

2. Generation of a random number from each of the distributions selected in (l). These values represent a possible set of values (a realization) for the input variables.

3.   Application of the WHPA model to compute a capture zone.

4.   Repeated application of steps (2) and (3) for a specified (large) number of iterations.

5.   Presentation of the series of output values generated in step (3) as a cumulative probability distribution function (CDF).

6.   Analysis and application of the cumulative probability distribution as a tool for decision making.

The number of Monte Carlo iterations that must be conducted is problem specific, but in general a minimum of at least several hundred iterations should be used (see section 9.4.2).

9.4 Application of Monte Carlo Technique to Capture Zone Analysis

9.4.1 Methodology

Figure 9.1 illustrates the methodology used to link the Monte Carlo method to the WHPA model. Figure 9.la represents one realization for a time-related capture zone about a pumping well. The capture zone would be obtained by running MONTEC for a single iteration subsequent to the generation of a random number for each of the uncertain input variables.

Because MONTEC will calculate many capture zones during a Monte Carlo run, the shape and areal extent of each capture zone needs to be saved so that a comparison of all of the capture zones can be made. A series of radial 1ines, with the well as their common origin, are used to accomplish this task. Each line has associated with it a unique angle, α_i. The length of each radial line segment and its corresponding angle compose a piecewise constant representation of the capture zone. Therefore, for each capture zone generated, the radial distance from the well to the capture zone boundary for n lines at each α_i (i = 1,n) is saved by the code. The total number of values saved is N x n, where N is the number of Monte Carlo runs.

Figure 9.1

Monte Carlo Method **Applied to Capture Zone Analysis
Series of Radial Lines Used to Save Capture** Zone **Boundary (a)
and Cumulative Distribution Function For One Radial Line (b)**
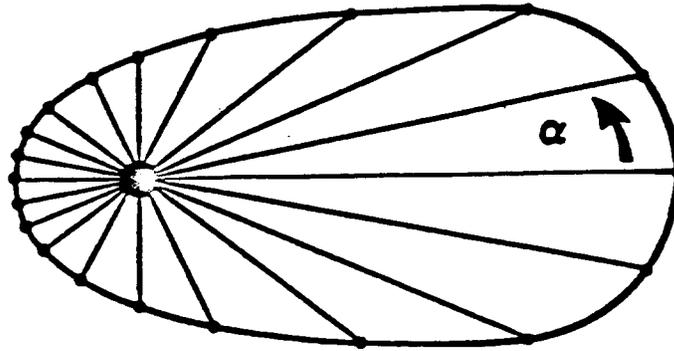
(a)
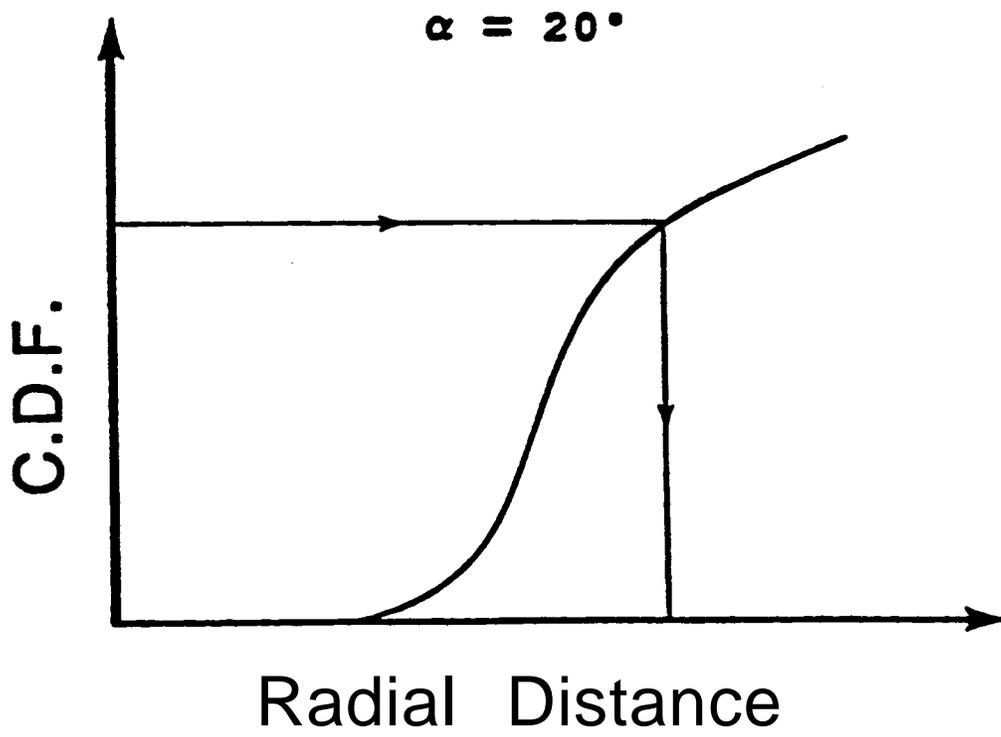
(b)

Once N capture zones have been generated by MONTEC, the N distances saved for each radial line arc sorted into ascending order. The resulting tabulation is the experimental cumulative distribution function (CDF) for each line. A sample CDF, which corresponds to the radial line defined by α_i in Figure 9.1a is shown in Figure 9.lb.

Once the CDF is obtained, any percentile of radial distance may be chosen. For example, the 85th percentile radial distance implies that 85 percent of the radial distances for the current line are less than or equal to that value. The 85th percentile capture zone would be determined by finding the 85th percentile distance for each radial line, and then connecting the endpoints of each line after plotting them at the appropriate angles.

One can see from Figure 9.la that the quality of the "preservation" of each capture zone depends upon the number and spacing of the radial lines. In addition the number of lines required to preserve a capture zone increases with the complexity of the capture zone shape. However, it is inconvenient to use large numbers of radial lines due to increased storage and computational requirements. For these reasons, the Monte Carlo option of the WHPA model may only be used for simple WHPA delineation scenarios. The following restrictions apply to use of the MONTEC module:

- Only the capture zone for a single pumping well in a confined or semi-confined aquifer may be analyzed using the Monte Carlo technique. The capture zone type must be time-related.

- The aquifer must be infinite in area] extent (effects of nearby stream or barrier boundaries may not be assessed).

- The portion of MONTEC that calculates capture zones is similar to MWCAP, and therefore most of the restrictions applicable to MWCAP are applicable to MONTEC as well.

9.4.2 Input Requirements

The input requirements for MONTEC are essentially the same as those of MWCAP for the case of a single, time-related capture zone for a well pumping in an aquifer of infinite areal extent (no boundaries). Additional input requirements are the number of Monte Carlo runs (NRUN), the desired capture zone percentile(s) (PERCEN; up to five may be specified), and the statistical attributes (mean and standard deviation) of the probability density functions (PDF's) assigned to the uncertain input variables. Note that MONTEC may also handle aquifers subject to leakage through a confining bed, whereas MWCAP can not.

A maximum of 1,000 Monte Carlo runs maybe specified. In general, it is recommended that for all final analysis the maximum number of iterations be used. For screening purposes, a smaller number of Monte Carlo iterations may be sufficient. For several example problems analyzed using MONTEC it was observed that the Monte Carlo capture zones obtained using 200-500 iterations were almost identical to those obtained using 1,000 iterations. Users that have access to a powerful PC such as the 80386 series machines will be able to run a Monte Carlo problem with a large number of iterations within several hours. Users with less computing power (e.g. an IBM XT class PC) may have to wait overnight for results. Note that proper selection of the number of pathlines delineated and the maximum spatial step length are very important when MONTEC is used.

The input variables that may be considered uncertain are

- Well discharge rate
- Hydraulic conductivity
- Hydraulic gradient
- Effective porosity
- Aquifer thickness
- Confining layer hydraulic conductivity
- Confining layer thickness

Any one, some combination of, or all of the above parameters may be represented as a probability distribution during a Monte Carlo run.

9.4.2.1 Distribution Types

If one or more input variables is considered uncertain, the probability distribution type of the variable(s) must be specified. There are six distribution types to choose from in the WHPA model:

- Normal
- Lognormal
- Exponential
- uniform
- Log10 uniform
- Empirical

The normal, exponential and uniform distributions are commonly used in practice and a description of each may be found in any introductory statistics text. The lognormal and log10 uniform distributions involve a mathematical transformation of the original data. The result of the mathematical transformation, referred to as the transformed data, follows a specified probability distribution that the untransformed (original) data does not. The two transformations are defined as:

$$\text{Lognormal:} \quad Y \; = \; \ln(X) \tag{9-4}$$

$$\text{Log10 uniform:} \quad Y = \text{Log10}(X) \tag{9-5}$$

where in denotes natural log, $\log_{lo}$ is logarithm to the base 10, X is an untransformcd random variable, and Y is a transformed random variable. The variable Y will have a normal distribution when the lognormal transformation applies, and a uniform distribution when $\log_{lo}$ uniform transformation applies. The untransformed random variable X represents the original data prior to any logarithm operations.

When a normal or uniform random number is generated from one of the logarithm distributions in the Monte Carlo module, the generated value must be transformed from the transformed space back to untransformed space. This is accomplished through the inverse transforms defined by:

$$\text{Lognormal:} \qquad \mathbf{X} \;=\; \exp(Y) \tag{9-6}$$

$$\text{Log1O uniform:} \qquad \mathbf{X} \;=\; 10^{(Y)} \tag{9-7}$$

where exp denotes the exponential. Note that Y is the random value generated by MONTEC, but X is the value that is used by the WHPA model.

The empirical distribution is a set of coordinates that define an observed cumulative distribution function (CDF) for a random process. The y-axis of the CDF has a range of 0-1 and represents the probability that any value X will be less than or equal to y. The x-axis of the CDF represents values of the random variable of interest.

The normal and lognormal distributions require the user to specify the mean and standard deviation of the distribution. Note that for the lognormal distribution the mean and standard deviation are entered in untransformed space, and the transformation of these parameters to log space is made by the code using

$$\mu_T = \ell n \mu_U - 0.5 \, (\sigma_T^2) \tag{9-8}$$

and

$$\sigma_T^2 = \ell n \, (\sigma_U^2 / \mu_U^2 + 1) \tag{9-9}$$

where μ_U and σ_U are the mean and standard deviation in untransformed space, and μ_T and σ_T are the mean and standard deviation in log space, respectively.

The uniform and log10 uniform distributions require minimum and maximum values. The log10 uniform distribution bounds are input in untransformed space. The exponential distribution requires only one parameter; the mean of the distribution. For the empirical distribution, the user must input the coordinates of the cumulative distribution function (minimum 2 pairs, maximum 50 pairs) which is subsequently treated as a piecewise linear curve.

Once the distribution type for each uncertain input variable has been specified, the MONTEC module generates a random number for each varab!e for each Monte Carlo run. If the generated value lies outside any imposed bounds (see next section), the number is regenerated. The random number generation routines used in MONTEC are documented in McGrath and Irving (1973).

9.4.2.2 Distribution Bounds

The user may assign limiting upper and lower values that a random variable may assume if the variable is represented by the normal, lognormal or exponential distribution types. Upper and lower bounding values are inherent in the definitions of the other distribution types. All upper and lower bounds are input in untransformed space.

Extreme caution should be used when specifying limiting values for distributions that have none by definition.   If the bounds lie too close to the mean of the distribution, the available sampling space may be too limited and the nature of the statistical distribution will not be preserved during the sampling (random number generation) process. Bounding values should be used only to avoid physically unrealistic scenarios that could be caused by an extreme value generated for a random variable. For example, if well discharge is characterized using a normal distribution an upper bound might be specified for Q such that complete dewatering of the aquifer in the vicinity of the well would not occur.

The upper and lower bounding values imposed automatically by MONTEC are as follows:

- Well discharge must be greater than zero
- Hydraulic conductivity must be greater than zero
- Hydraulic gradient must be greater than or equal to zero
- Porosity must be greater than zero and less than one
- Aquifer thickness must be greater than zero
- Aquitard hydraulic conductivity must be greater than zero
- Aquitard thickness must be greater then zero

9.4.2.3 Statistical Correlations Between Input Parameters

If more than one input variable is considered uncertain, statistical correlations that may exist between variables are neglected. Each random variable is assumed to be independent of every other random variable during the random number generation process. This assumption is based primarily upon practical rather than technical considerations. In practice, it is generally extremely difficult due to data limitations to derive statistical correlations (covariances) between input parameters.

However, statistical correlations between aquifer parameters certainly exist. For example, it follows from Darcy's Law that hydraulic conductivity, aquifer thickness and hydraulic gradient are correlated with one another since per unit width of aquifer

$$\mathbf{Q} \ = \ Ti \tag{9-10a}$$

where

$$T \ = \ Kb \tag{9-10b}$$

Therefore high values of T are associated with small values of i, and high values of i (steep gradients) are associated with small T values. Furthermore, the variable T is a direct function of K and b.

These correlations may pose a problem if statistical independence between variables is assumed. For a given Monte Carlo run, there may be a significant probability that a low value of i will be generated in conjunction with a low value of the product Kb. Such a situation might be unreasonable in light of the previous discussion.

To avoid extremely unrealistic hydrogeological scenarios, an automatic check based upon drawdown at the pumping well was implemented into MONTEC. If the maximum allowable drawdown specified by the user is exceeded the current set of random values generated by the code is ignored and a new set is generated until the drawdown criterion is met. Hydraulic parameter combinations that lead to excessive drawdowns at the well during a Monte Carlo run are output to the file DD.LST (drawdown list).

Drawdown at the pumping well is calculated using the Theim equation:

$$s = \frac{Q}{2\pi\, Kb}\, \ell n\left(\frac{R_e}{r}\right) \tag{9-11}$$

where s is drawdown from the initial piezometric surface at radial distance r from the pumping well, R_e is the radial distance from the well at which there is no drawdown (the radius of influence of the well), and Q, K and b are as defined previously. For each Monte Carlo run the values of Q, K and b are known. Because drawdown at the well is being calculated, r corresponds to the effective radius of the well bore. In order to calculates, the only remaining unknown variable is R_e.

Unfortunately, there is no sound quantitative method to estimate R_e. This parameter is often estimated from experience or actual field observation. Two approximate methods for estimating R_e arc implemented in MONTEC. The method used by the code depends upon the selected aquifer type (confined or leaky-confined).

Because R_e is related to the recharge processes that supply ground water to the well, the following method is used to estimate **R_e** in MONTEC when the confined aquifer option is selected. Using equation (9-1O) and the relation

$$Q = qW \tag{9-12}$$

where W is the width of aquifer required to supply the total recharge to a well pumping at rate Q, R_e is calculated from

$$\mathbf{R_e} = 0.5\,\mathbf{W} = 0.5\,\frac{Q}{Kbi} \tag{9-13}$$

Fortunately, R_e and r appear in the form of a log function in equation (9-11), and therefore even a large error in the estimation of one of these parameters does not appreciably affect

the drawdown computed using equation (9-11). The drawdown check is not made if there is no ambient ground-water flow (i =0).

If the leaky-confined aquifer option is used in MONTEC, R_e is obtained from

$$R_e = 1.23 \, \lambda \tag{9-14}$$

and

$$\lambda^2 = \frac{b'bK}{K'} \tag{9-15}$$

where λ is a characteristic length of the leaky aquifer called the leakage factor (Bear, 1979), b' is the thickness of the semi-permeable confining unit K' is the hydraulic conductivity of the semi-permeable confining unit and the other variables are as defined previously. In this case, the pumping rate of the well, Q, will be equal to the volume of leakage per unit time supplied to the aquifer within the circle defined by radius R_e. In this case the drawdown calculation does not depend on the presence of ambient ground-water flow.

The maximum drawdown that may not be exceeded is input by the user; an appropriate value for this parameter must be derived on a case-by-case basis. It might be obtained from field observation (e.g. the maximum drawdown observed in a well in a particular region), or from theoretical considerations (e.g. the piezometric surface can not drop below the well bottom or some other datum such as the base of an overlying confining unit). If the maximum allowable drawdown is set to zero, which is the default value, the drawdown check is not conducted.

The procedure of eliminating certain variable sets due to excessive drawdown will indirectly induce correlation between model parameters. For example, combinations of low T and low i values create large drawdowns, and therefore the elimination of parameter sets in which this condition occurs tends to allow only combinations of low T with high i and high Twith low or high i. Note that if the maximum allowable drawdown is set to a large value, the condition of complete independence between parameters will again exist because the drawdown criterion will never be exceeded.

9.4.2.4 Data Analysis

The data required to derive the probability distributions for uncertain input variables can be obtained from a variety of sources. The most obvious source of data is field tests conducted in the aquifer under study. For example, if 50 aquifer tests have been conducted for a region of interest, standard statistical techniques might be used to estimate a probability distribution type for hydraulic conductivity. A lognormal distribution might be found and this distribution type along with its mean and standard deviation, could be input into MONTEC (note that a lognormal distribution is commonly observed for the hydraulic conductivity of an aquifer).

In general it is uncommon that enough field data exists to obtain estimates of PDFs via traditional methods. Additional sources of data may become available if the WHPA delineator is willing to make certain assumptions. For example, suppose that a delineator would like to determine the l0-year capture zone for some municipal water supply wells located in a shallow, river-valley aquifer. The delineator would like to consider hydraulic conductivity to be a random variable because no hydraulic conductivity values estimated from field tests are available in the vicinity of the wells. However, there are other not too-distant aquifers similar in morphology (stream valley settings, similar thicknesses, similar aquifer materials, etc.) for which many hydraulic conductivity estimates are available. If the assumption is made of some equivalence between aquifers due to similar physical characteristics, the measurements made in the surrounding a quifers maybe used to obtain a PDF of hydraulic conductivity for the aquifer of interest.

Barring a reasonable quantitative means of obtaining sample PDFs, a distribution type may be chosen using qualitative professional judgement. Often the uniform distribution i s used if a 'guess" at the distribution type is made. A uniform random variable has an equal likelihood of assuming any value between the specified upper and lower limits of the distribution The lower and upper distribution limits correspond to the minimum and maximum parameter values thought to be reasonable for the given site. Other distributions (e.g., normal) may be hypothesized as well.

9.4.3 output

Output of the MONTEC module consists of a capture zone that corresponds to any specified percentile value (85th,90th, etc.) The 90th percentile capture zone implies that there is a 90 percent chance that the "actual" capture zone boundary for the well will be less than or equal to the areal extent of the delineated capture zone. Conversely, there is a 10 percent chance that the actual capture zone may exceed the bounds of the delineated capture zone. Up to five percentiles may be specified in the MONTEC preprocessor, and

the outline of each corresponding capture zone will be computed and plotted. The percentile value used for WHPA delineation purposes is a policy decision; however, generally values of 90 or 95 percent are used when uncertainty analysis is applied in a regulatory framework.

The capture zones produced by MONTEC may have slightly distorted shapes due to the piecewise linear representation used (Figure 9.2). The distortionwill generally be minor, and the actual shape of the capture zone is usually discernable.

In addition to the standard output file MONTEC.OUT, the MONTEC module automatically creates three additional files that may be of interest to the user. These files and their contents are listed below.

CAPTUR.VAR	-	Contains the MONTEC input parameters Q, K, i, b, K', b', and θ generated for each Monte Carlo iteration.
RANBND.LST	-	Contains a listing of the generated random values that were rejected because they did not lie within any imposed bounds. File will be empty if no lower and upper bounds are set.
DD.LST	-	Contains a listing of input parameter combinations that caused excessive drawdown at the pumping well (as determined by the maximum permitted drawdown input parameter).

9.5 Example Applications

Two hypothetical Monte Carlo problems were run to illustrate the capabilities of the Monte Carlo option. Note that the MONTEC module is substantially more computationally intensive than the other WHPA model modules. The first example problem ran in about 20 minutes on a Dell 80386-20 mgHz PC and in about 1.5 hours on an Everex 80286-12 mgHz PC. The second example ran in about 1 hour and 20 minutes on the Dell 80386 machine. Both machines were equipped with math coprocessor. Run times would be substantially longer on an IBM XT model PC.

9.5.1 Hypothetical Example 1

For the first example problem, the input parameters well discharge, effective porosity and aquifer thickness were considered uncertain. The input required by MONTEC is listed in Table 9.1. Since this is only a hypothetical example, the maximum allowable drawdown was set to a large value (40 m). The three percentiles specified were the 5th, 90th and 99th.

Figure 9.2

Distorted Shape of MONTEC Capture Zone
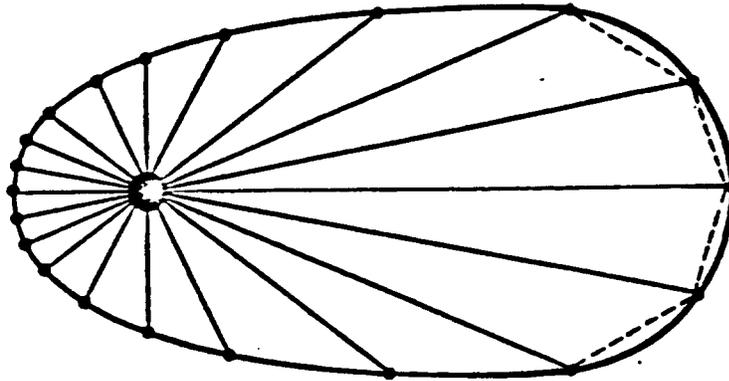
Legend:

— Actual Capture Zone

--- Capture Zone Outline Saved by MONTEC

Table 9.1

Input Parameters for First MONTEC Example

Aquifer Type: Confined

Units: Meters and Days

Problem Boundaries: XMIN = YMIN = 0.0 m
                     XMAX = YMAX = 5,000 m

Maximum Step Length: 50 m

Well Location: x = 750 m; y = 2,500 m
Well Radius : 0.25m

Angle of Ambient Flow: 180^0

Maximum Permissible Drawdown: **40m**

No. of Monte Carlo Runs: 1,000

No. of capture zone percentiles to be solved for: 3

Percentile Values: 5, 90, 99

Monte Carlo Variables:

Parameter	Distribution Type	Mean	Standard Deviation	Lower Bound	Upper Bound
Well Discharge	Normal	3,000 m^3/d	500 m^3/d	0	0
Hydraulic Conductivity	Constant	15 m/d	--	--	--
Gradient	Constant	0.0015	--	--	--
Porosity	Uniform	--	--	0.2	0.25
Thickness	Empirical*	--	--	--	--

*   Empirical distribution for thickness

Thickness	CDF
40 m	0.0
50 m	0.5
62 m	0.8
70 m	1.0

Capture Zone Time = 3,650 days (10 years)
Number of Pathlines = 20

Note in Table 9.1 that the well discharge has a normal distribution with the upper and lower bounds on the distribution set equal to zero. When the lower and upper bounds of a distribution are set to zero, MONTEC does not check the random number generated prior to each iteration to ensure that it lies within the specified bounds.

A uniform distribution with lower and upper bounds of 0.2 and 0.25 respectively was specified for aquifer porosity. Therefore, for each Monte Carlo iteration, the random value generated for porosity had an equal likelihood of lying anywhere within the range 0.2-0.25.

The empirical distribution used for aquifer thickness is listed at the bottom of Table 9.1. Reading the table, one finds that the smallest possible value of aquifer thickness is 40 m, there is a 50 percent chance that, the aquifer thickness is less than or equal to 50 m, and so on. Such a distribution might be derived for a particular site using available well logs for the region.

The 5th, 90th and 99th capture zone percentiles are plotted in Figure 9.3. The 5th and the 99th percentile capture zones lie near the smallest and largest Monte Carlo capture zones respectively. obviously, the 90th percentile capture zone lies between these two extremes.

9.5.2 Hypothetical Example 2

The second Monte Carlo example is loosely based on statistical distributions of flow parameters derived for the Quadra Sand, British Columbia (Smith, 1981). The hypothetical setting is a stratified sand aquifer with a single pumping well withdrawing water for public supply at the rate of 1 mgd (1.34×10^5 ft^3/d). The aquifer ranges in thickness from 80-120 ft. The spatial variability of hydraulic properties is ignored and the statistical distributions are viewed as representing the uncertainty associated with parameters describing a homogeneous aquifer. The uncertain input parameters are hydraulic conductivity, effective porosity and aquifer thickness. Table 9.2 is a summary of the MONTEC input for this example.

The 50th, 80th and 95th capture zone percentiles for this example are presented in Figure 9.4. The most striking feature of these capture zones is their atypical pear shape. This shape results from the composite effects of averaging many different capture zones of various shapes and sizes.

Figure 9.3

**5th, 90th, and 99th Percentile Capture Zones For The
First Hypothetical Example Computed Using MONTEC**
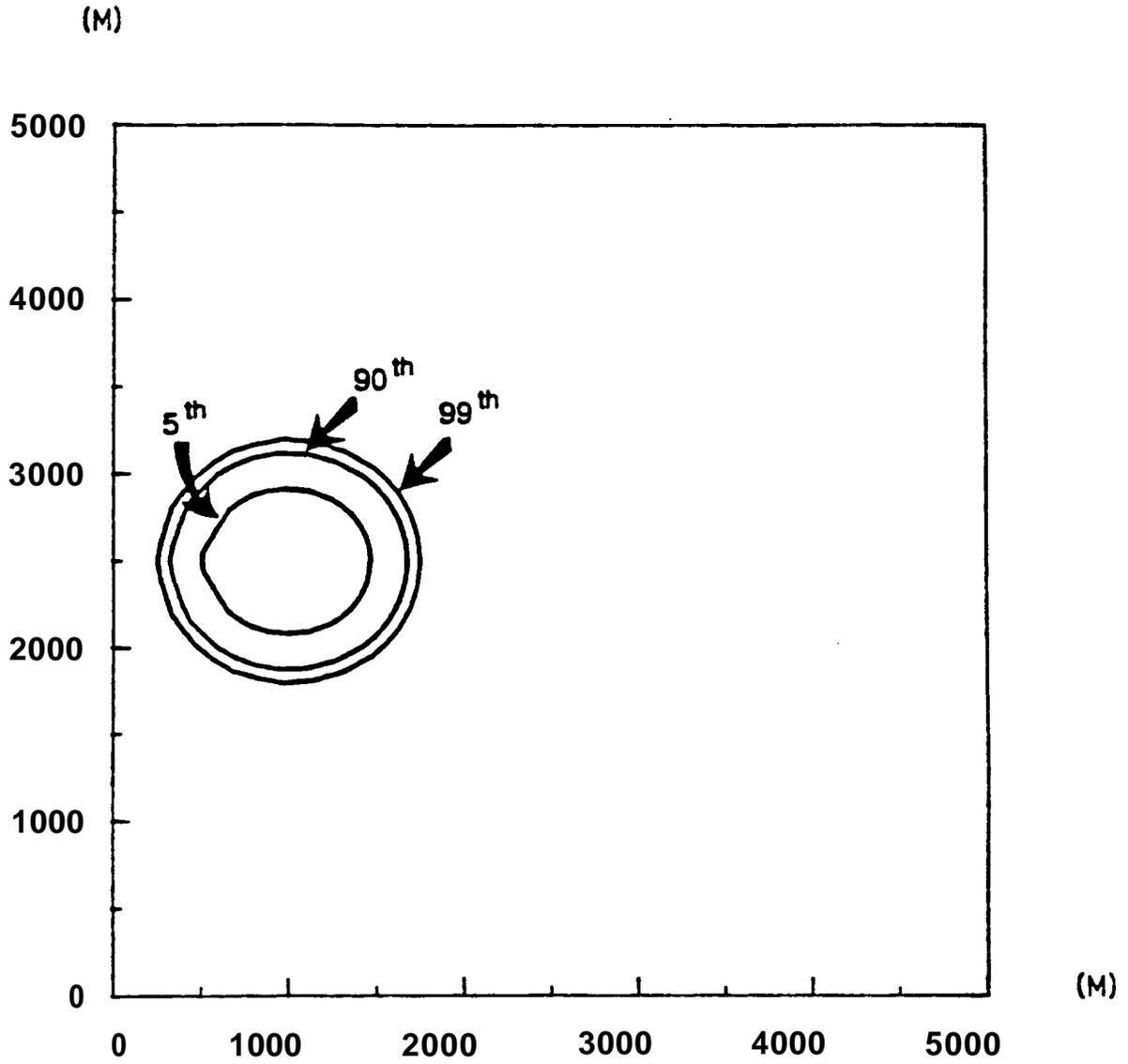
Table 9.2

Input Pammeters For Second MONTEC Example

Aquifer Type: Confined

Units: Feet and Days

Problem Boundaries: XMIN = YMIN = 0.0 ft
$\qquad\qquad\qquad\quad$ XMAX = YMAX = 10,OOO ft

Maximum Step Length: 50 ft

Well Location: x = 2000 ft; y = 5,000 ft
Well Radius : 1 ft

Angle of Ambient Drawdown 180^0

Maximum Permissible Drawdown: 100 ft

No. of Monte Carlo Runs: 1,000

No. of capture zone percentiles to be solved for: 3

Percentile Values: 0.5, O.8 0.95

Monte Carlo Variables:

Parameter	Distribution Type	Mean	Standard Deviation	Lower Bound	Upper Bound
Well Discharge	Constant	134,000 ft³/d	--	--	--
Hydraulic Conductivity	Lognormal	142 ft/d	50 ft/d	--	--
Gradient	Constant	0.002	--	--	-
Porosity	Lognormal	0.43	0.03	0	0
Thickness	Uniform	--	--	80 ft	120 ft

Capture Zone Time = 3,650 days (10 years)
Number of Pathlines = 40

Figure 9.4

**The 5Oth, 80th, and 95th Capture Zone Percentiles Calculated Using
MONTEC For The Second Hypothetical Example**
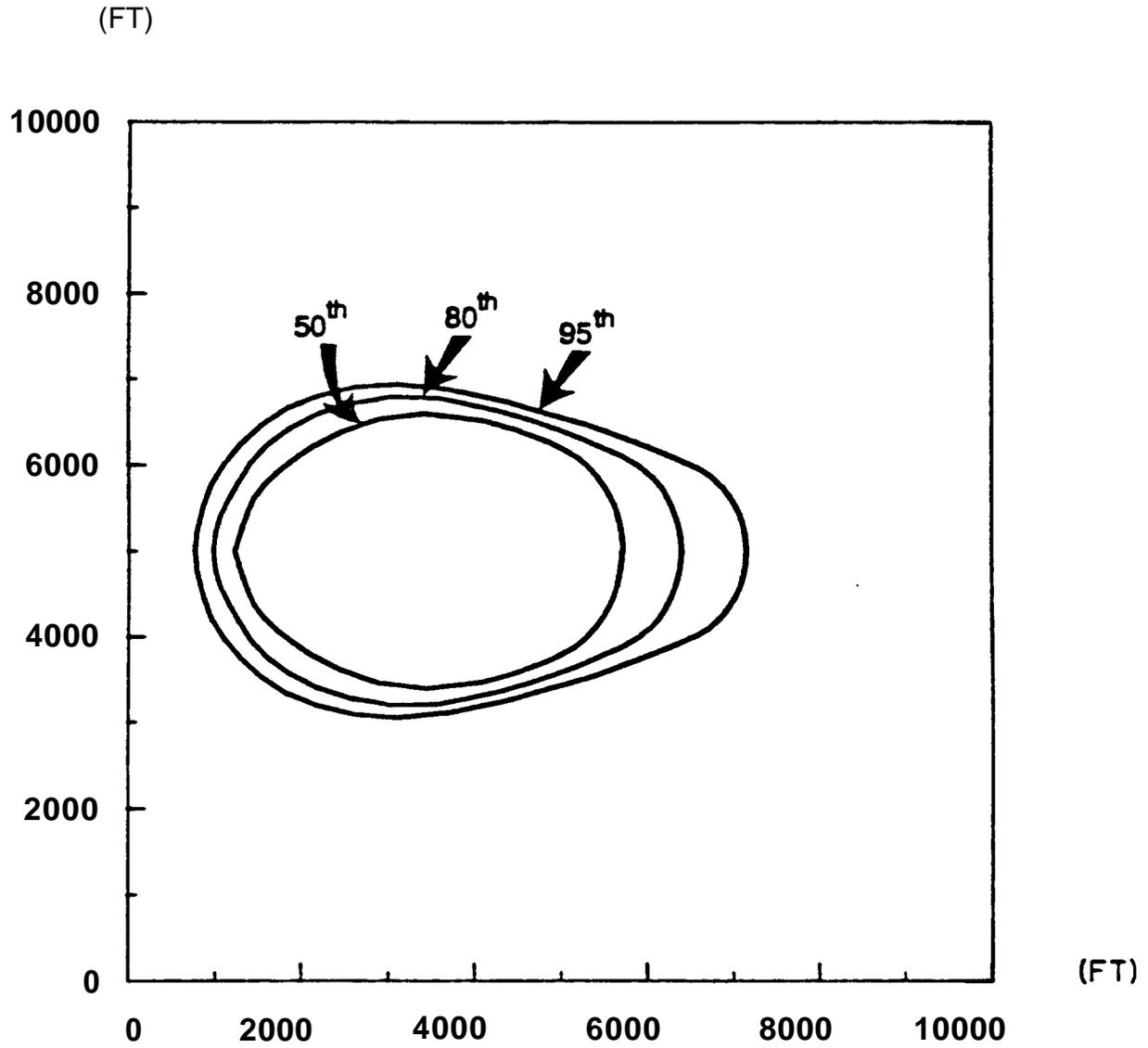
To illustrate the cause of the pear shapes more clearly, two additional capture zones were delineated using MWCAP (recall. that much of the MONTEC module is based upon the MWCAP module). The smallest and the largest transmissivity values generated during the 1,000 MONTEC iterations were used as input for the first and second MWCAP runs respectively. The values were extracted from the standard MONTEC output file CAPTUR.VAR. All of the input parameters for each MWCAP run arc presented m Table 9.3.

Figure 9.5 portrays the MWCAP results. For the run that used the low value of transmissivity as input a nearly circular capture zone was delineated while an oblong capture zone resulted from using the high value of transmissivity as input. These capture zones may be conceptualized as the two "extreme" or 'end-member" capture zones delineated during the MONTEC run. The origin of the pear shape becomes immediately apparent when the circular and elongated capture zones are visually laid one atop the other. Note that the pear shape will only occur when input parameters that effect the determination of ambient ground-water flow (i.e. hydraulic conductivity, aquifer thickness, and hydraulic gradient) are considered uncertain.

To demonstrate the semi-confined aquifer option in MONTEC the second example was rerun using the leaky aquifer option. The input for this run was the same as that presented in Table 9.2 with the exception that the hydraulic conductivity and thickness of the confining bed were also specified as uniform random variables with bounds of 0.1-0.001 ft/d and 10-25 ft respectively. The results of this run are presented in Figure 9.6. A comparison of Figures 9.4 and 9.6 shows the general effect of decreased capture zone size due to leakage through the confining bed over the zone of influence of the well.

Table 9.3

MWCAP Input Parameters For Two Monte Carlo End-Member Capture Zones

For Each Run:

Units = ft and days

XMIN=0   YMIN = 0
XMAX = 10,000   YMAX = 10,000

Step Length = 50
No. of Pumping Wells = 1

Input Parameter	Run No. 1	Run No. 2
X Coordinate	2,000	2,000
Y Coordinate	5,000	5,000
Discharge	134,000	134,000
Transmissivity	4,218	41,840
Hydraulic Gradient	0.002	0.002
Angle of Ambient Flow	180°	180°
Porosity	0.43	0.43
Aquifer Thickness	87	109
Boundary Type	None	None
Distance from Well to Boundary	N/A	N/A
Boundary Angle	N/A	N/A
Capture Zone Type	Time-Related	Time-Related
Travel Time Value	3,650	3,650
No. of Pathlines	20	12
Capture Zone Plotting	Yes	Yes

Figure 9.5

Capture Zones Delineated Using MWCAP for (a) Lowest Randomly Generated Transmissivity Value and (b) Highest Randomly Generated Transmissivity Value

(a)

(b)
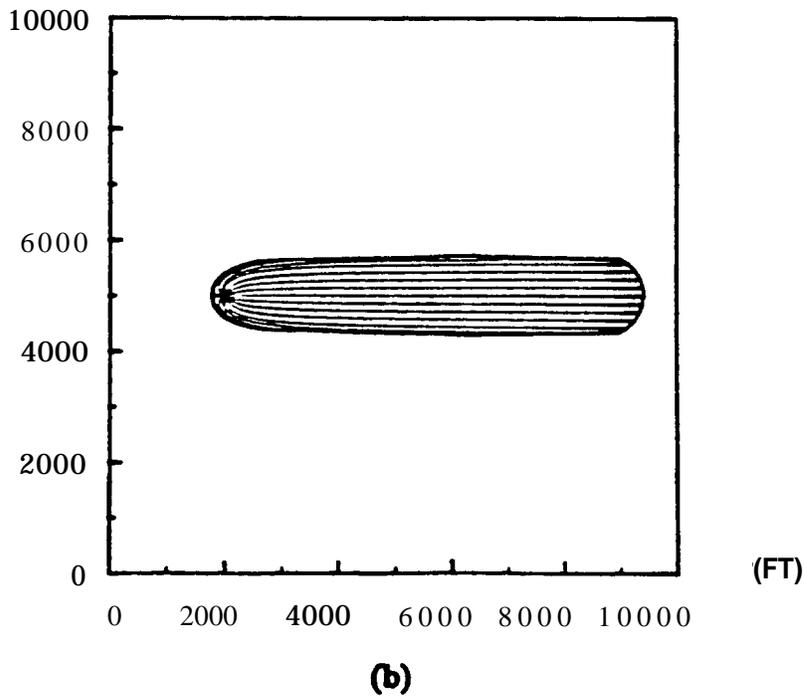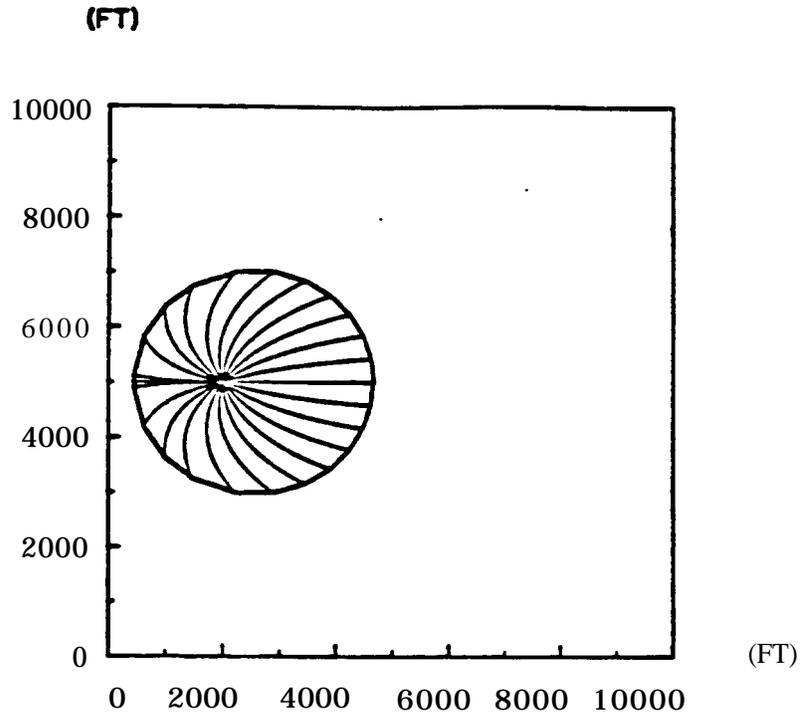
Figure 9.6

**The 50th, 80th and 95th Capture Zone Percentiles Calculated Using MONTEC
for the Second Hypothetical Example with Vertical Leakage**
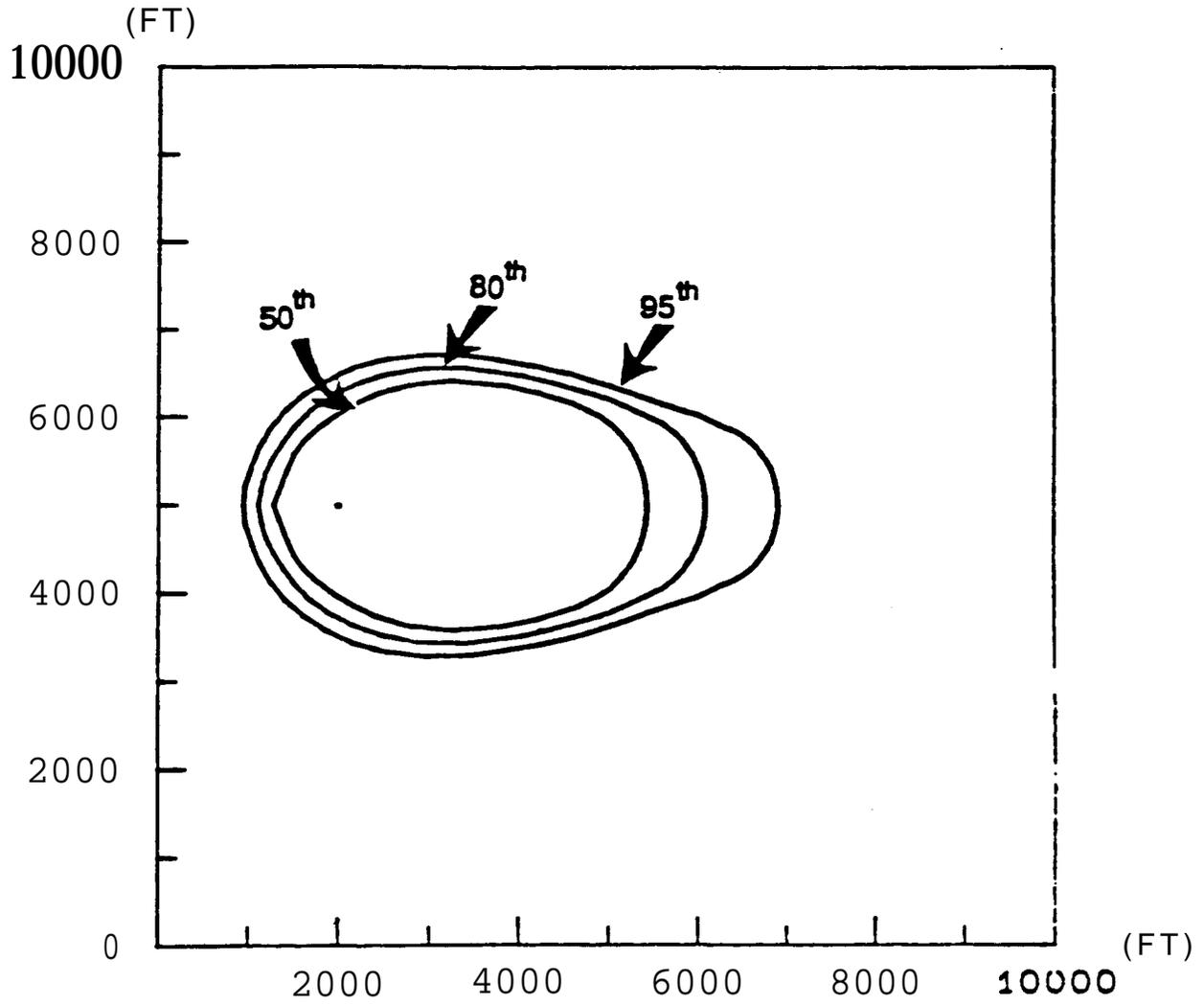
10.0 Problem Conceptualization vs. Reality: Potential for Abuse

1O.1 Introduction

In order to understand what the capture zones output by the WHPA model truly represent the effects that the input parameters and the underlying model assumptions have on capture zone morphology must be understood. The effect of the model input parameters and the underlying model assumptions on capture zone size and shape is the topic of this chapter. The majority of the material presented herein is applicable to the RESSQC MWCAP, MONTEC and GPTRAC semi-analytical modules. The GPTRAC numerical module is limited only by the capabilities of the numerical model used to obtain the input hydraulic head field.

10.2 Effects of Input Parameters on Capture Zone Morphology

The effects of the input parameters transmissivity (T), aquifer thickness (b), hydraulic gradient (i), aquifer porosity (θ), well discharge (Q_w), and the angle of ambient flow (a) on capture zone morphology may be assessed using Darcy's Law and the mass balance equation. Darcy's Law may be written

$$Q = KiA \tag{10.1}$$

where Q is discharge, K is the hydraulic conductivity of the porous medium, and A is the cross-sectional area of flow. If Q is assumed to represent the discharge per unit width of aquifer, it holds that

$$Q = Kbi(1) \tag{10.2}$$

or

$$Q_a = Ti \tag{10.3}$$

where Q_a is the ambient ground-water flow per unit width of aquifer. The average pore water velocity (seepage velocity) for a fluid particle moving through the porous medium may be written as

$$v = q/\theta \tag{10.4}$$

where $q = Q/A = Ki$ is called the specific discharge or Darcy velocity.

The equation of mass balance maybe written

$$I-O = \Delta S \tag{105}$$

where

$\quad I =$ inflow per unit time
$\quad O =$ outflow per unit time
$\quad \Delta S =$ change in storage per unit time

Equation 10.5 may be applied to any hydrologic system. For the hydrogeologic systems to which the WHPA model is applicable, I represents ground-water recharge moving into the aquifer (i.e., ambient ground-water flow, induced infiltration from streams, injection well recharge, areal recharge, leakage from an overlying confining unit), and O represents ground-water discharge from the aquifer (i.e., well discharge, ground-water discharge to streams, ambient ground-water flow that is not captured by the pumping well(s)). Because the flow fields considered are assumed to be at steady-state, the AS term is equal to zero. Therefore, the mass balance equation for the WHPA model may be written

$$I = O \tag{10.6}$$

Equation 10.6 implies that water discharged from the aquifer by the pumping well(s) must be obtained from a combination of ambient ground-water flow within the aquifer, induced infiltration from streams, and injection well recharge.   Figure 10.1 is a schematic representation of a mass balance analysis for a simple hydrogeologic system.

With equations 10.1, 10.3, 10.4 and 10.6 in hand the effects of T, b, i, θ, Q_w and a on capture zone morphology can be assessed. First of all, consider an aquifer of infinite areal extent (no barrier or stream boundaries) with no recharge wells. If a pumping well exists in the aquifer, its Q_w must be derived entirely from the ambient ground-water flow.

Figure 10.1

Mass Balance Analysis For Simple Hydrogeological System

GENERAL SYSTEM

$$O \longleftarrow \boxed{\Delta S = 0} \longleftarrow I$$

$$I = 0$$

Aquifer with uniform ambient flow

Q_O Q_I Q_O Q_I

Plan View $Q_I = Q_O$ Cross Section
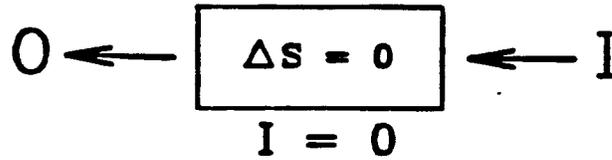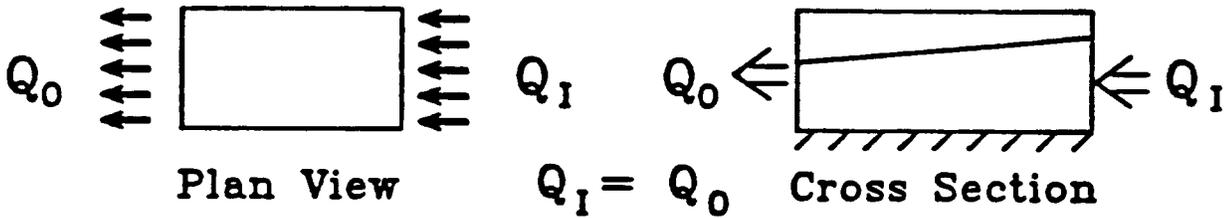
Aquifer with uniform ambient flow and pumping well

Q_O Q_2 Q_1 Q_3 Q_I Q_O Q_I

Plan View $Q_I = Q_O$ Cross Section
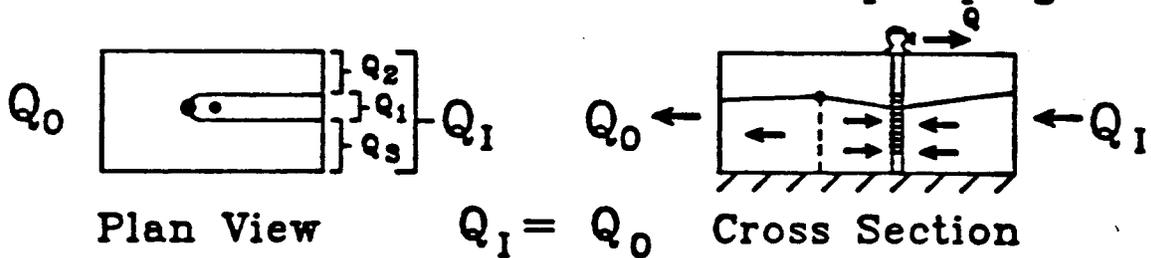
$$Q_O = Q_I - Q_W$$

$$\text{AND: } Q_I = Q_1 + Q_2 + Q_3$$

$$Q_W = Q_1$$

$$Q_O = Q_2 + Q_3$$

Therefore, as Q_w increases the capture zone must expand in all directions to capture a larger portion of the ambient aquifer flow, Q_a. Conversely, as Q_w decreases the areal extent of the capture zone will decrease.

From equation 10.3 one can see that the ambient ground-water flow per unit width of aquifer is the product of T and i. Therefore, for a constant Q_w increasing T and/or i will decrease the capture zone size because the well can derive a larger portion of water from each unit aquifer width confined within the capture zone. Decreasing T and/or i will increase the areal extent of the capture zone. The capture zone for a given scenario will not change if T and i are adjusted in opposite directions in such a way that Q_a remains constant.

The above generalizations hold if a stream or barrier boundary exists within the aquifer. If a stream boundary is in close enough proximity to the well, it will act as a source of water to the well and the areal extent of the capture zone will be smaller than it would otherwise be. In addition the stream may act as a limiting condition on the capture zone extent. If a barrier boundary is in close enough proximity to the well, it will act as a barrier to ground-water recharge to the well and the areal extent of the capture zone will be larger than it would be otherwise. The orientation of the barrier boundary in conjunction with the angle of ambient flow will dictate the direction in which the capture zone must expand.

Steady-state capture zones are not dependent upon porosity, θ, or thickness, b. For the time-related capture zone solutions, θ and b do not affect the position or orientation of the pathlines; they only affect the velocity of the fluid flow along each pathline. Equation 10.4 indicates that fluid velocity is inversely proportional to porosity (i.e., decreasing porosity increases fluid velocity). Therefore, when solving for time-related capture zones, decreasing the porosity will have the same effect as increasing the time for which the pathlines are delineated and vice versa; the same is also true for b. Note that the increased seepage velocity due to decreasing θ or b leads to more conservative capture zones because the capture zone will become larger for a given time.

The aquifer parameters T and i will also effect the velocity of ground-water flow. Recall that $K = T/b$. Equations 10.1 and 10.4 indicate that if θ remains constant, the seepage velocity will increase or decrease in direct proportion with K and/or i. However, unlike porosity, K and i will also effect the location and orientation of pathlines because they determine the ambient flow rate, Q_a.

For steady-state capture zones decreasing T or i will lead to more conservative capture zones for a well pumping at a constant rate Q_w. However, for time-related capture zones simple generalizations should not be made regarding the effect of these parameters. Although increasing T or i may lead to higher seepage velocities and therefore larger time-related capture zones, the increased ambient flow rate will tend to limit the areal extent of the capture zone.

The effect of one final input parameter, a, is readily apparent. A capture zone will always orient itself so that it extends upgradient in the direction opposite to that of ambient flow (i.e., if α = 45° (NE), the bulk of the capture zone will extend in the direction of 225° (SW)). Many interesting capture zone shapes may occur when a stream or barrier boundary exists within the ambient flow field (Figure 10.2).

For the sake of simplicity, the effects of areal recharge and vertical leakage on capture zones in unconfined and leaky-confined aquifers, respectively, were not addressed in the preceding discussion. The general effect of these processes, obviously, is to decrease the capture zone size. In the case of a leaky confined aquifer, larger values of the confining bed hydraulic conductivity (K'), and smaller values of the confining bed thickness (b'), lead to greater quantities of leakage supplied to the aquifer through the confining bed and therefore smaller capture zones.

10.3 Effects of Boundary Conditions on Capture Zones

The presence of a boundary condition in the proximity of a pumping well can dramatically alter the shape and areal extent of the well's capture zone. The boundary condition options incorporated in the WHPA model are designed to simulate those that often occur in the field. However, in many cases encountered the boundary conditions as formulated in the WHPA model may not adequately represent the natural system, and therefore their use may lead to erroneous conclusions regarding capture zone size and shape. Whenever the stream or barrier boundary conditions are applied, the user must be aware of the underlying assumptions and how they affect capture zone morphology.

Of the two boundary types available, the stream boundary condition assumptions are the most likely to be violated. Figure 10.3a is a schematic diagram of how the WHPA model simulates a stream boundary; the stream is assumed to fully penetrate the aquifer and therefore can provide water to the aquifer over the entire saturated thickness, b. With this conceptualization, the capture zone may expand along the stream boundary axis, but may never extend across the stream.

Figure 10.2

Miscellaneous Capture Zones

(M)

4000

3200

2400

STREAM
BOUNDARY

1600

BARRIER
BOUNDARY

800

0

0   800   1600   2400   3200   4000

(M)

(M)
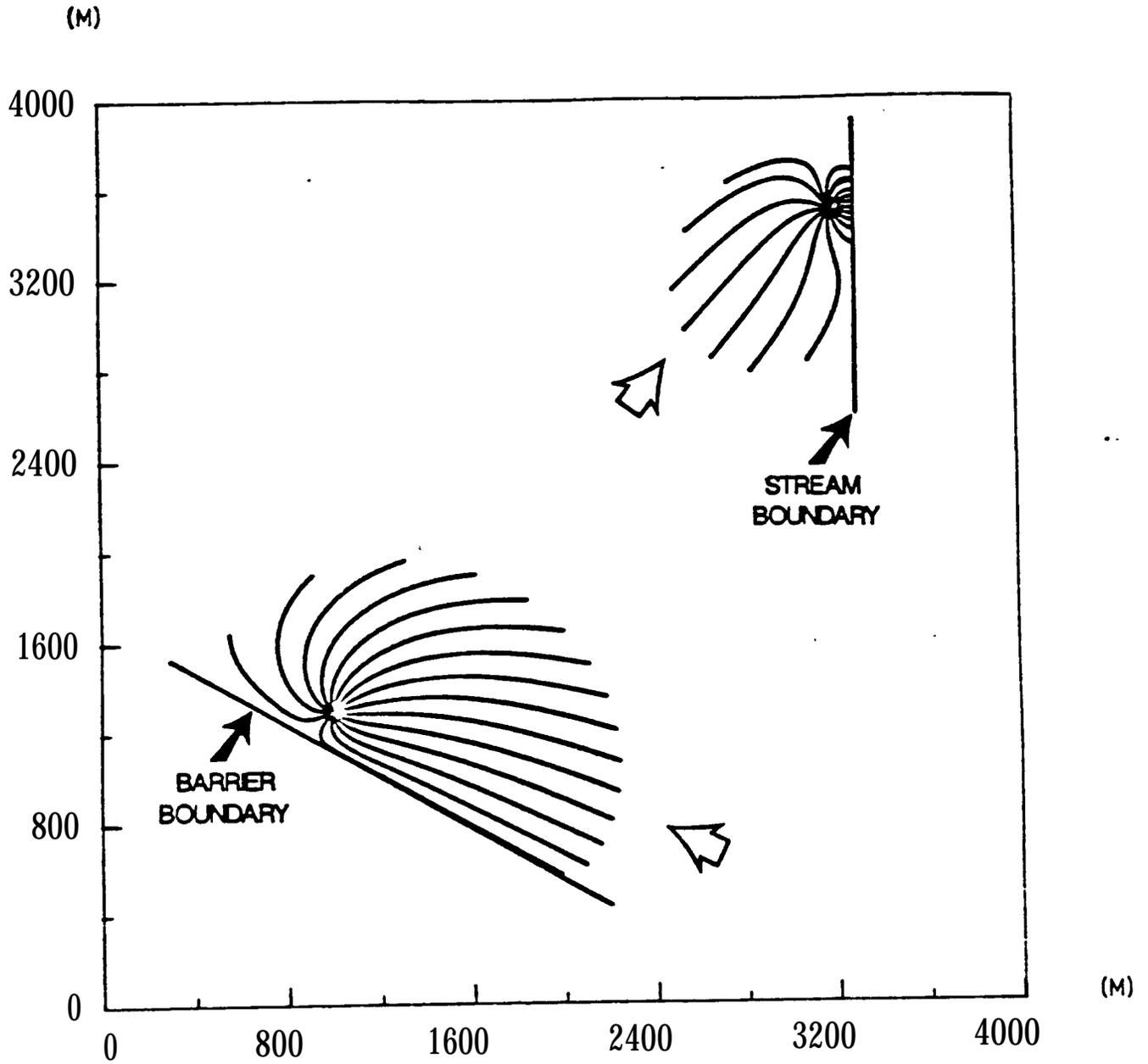
Figure 10.3

Stream Boundary As Represented by the WHPA Model **(a), and**
Stream Boundary As Often Encountered in Practice (b)
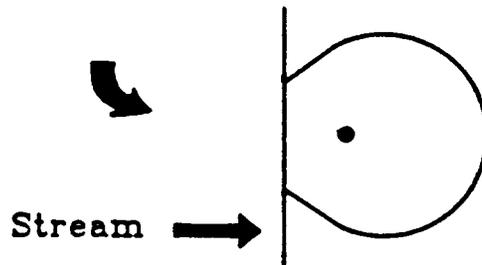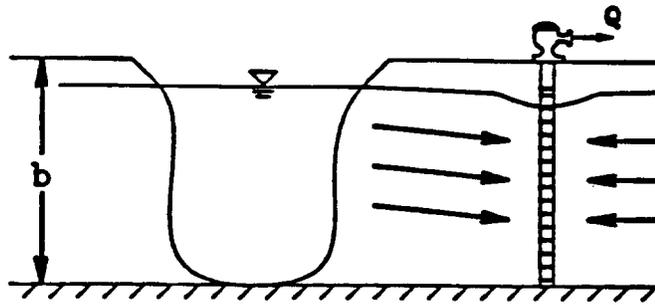

(a)
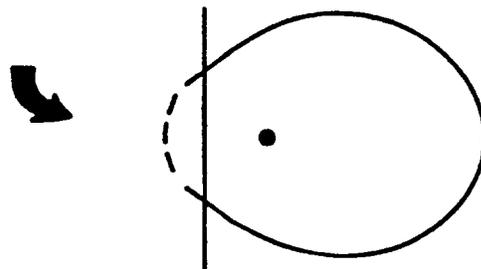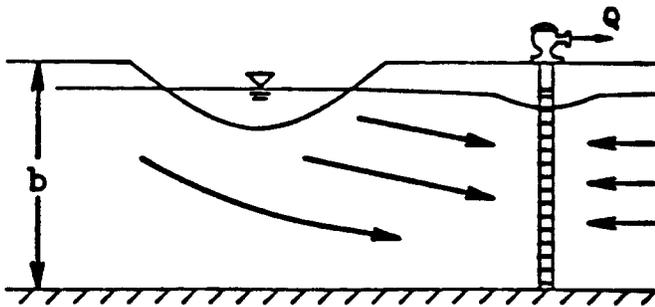
(b)

Figure 10.3b diagrams the stream boundary condition as it is often observed in practice. Note that the stream is partially penetrating it does not exist over the entire depth of the aquifer. In such a case the well may be pumping at a larger rate than that which can be sustained by induced infiltration from the stream into the aquifer. When such a situation occurs, the capture zone will extend across the stream boundary, and the pumping well will draw a component of recharge from the opposite side of the stream. The occurrence, or potential for occurrence, of this phenomena should be carefully examined whenever the stream boundary condition is used. Morrissey (1987) has examined this problem in detail.

The assumption of a fully penetrating barrier boundary is less apt to be violated in practice than is the fully penetrating stream assumption. Figure 10.4a is a schematic diagram of how the WHPA model simulates a barrier boundary, the impermeable rock formation is assumed to extend, and therefore act as a barrier to flow, over the entire saturated thickness of the aquifer. With this conceptualization the capture zone may never extend across the boundary face.

In some instances, the barrier boundary may not fully penetrate the aquifer and the capture zone may actually extend across the boundary face (Figure 10.4b). Detailed geological and hydrogeological data would have to be available to identify this situation.

Whenever a stream or barrier boundary condition is partially penetrating, a potentially significant vertical component of flow is introduced into the flow system. The WHPA model is designed to simulate horizontal two-dimensional flow and therefore the effects of partially penetrating boundaries can not be assessed using the model. Even if the model is run assuming that no boundary is present the resulting capture zone may still not be conservative. In order to rigorously assess the effects of partially penetrating boundaries, a numerical model should be used.

10.4 Analysis of Simulation Results

All capture zones output from the WHPA model should be viewed in light of the assumptions applied (e.g., steady flow, homogeneous aquifer, etc.). Although the model assumptions may not allow an exact representation of many hydrogeological systems, the assumptions will often be close enough to reality so that a reasonable capture zone solution may be obtained. When one or more model input parameters are thought to be significantly uncertain, the Monte Carlo module (MONTEC) can be used or a sensitivity analysis can be performed by altering the input parameter values in a series of WHPA model runs and overlaying the resulting capture zones.

Figure 10.4

**Barrier Boundary As Represented by the WHPA Model (a), and
Barrier Boundary That May Be Encountered In Practice (b)**

Barrier
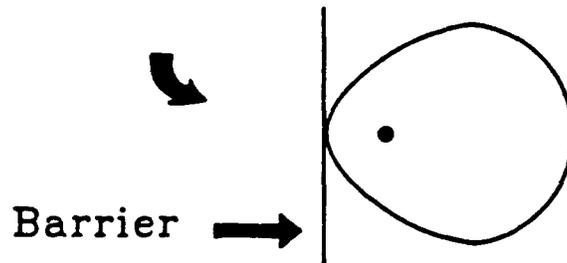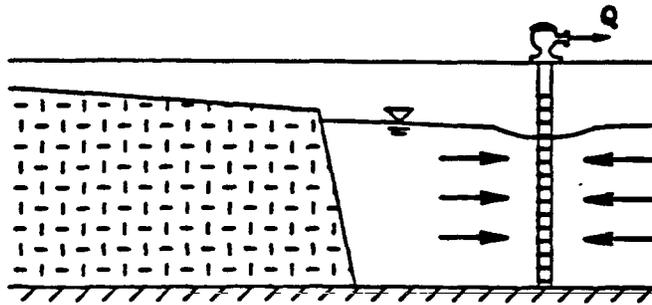
(a)
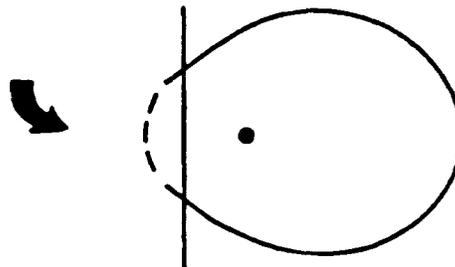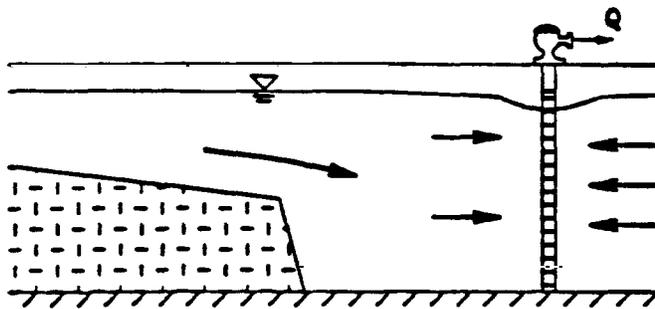
(b)

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Appendix A

Theoretical Development and Implementation of RESSQC Module

A.1 Introduction

In this appendix analytical solutions used in the RESSQC module are presented. These solutions are derived from simple applications of the complex potential theory of fluid dynamics. The analytical solutions implemented in RESSQC may be constructed using three fundamental component solutions. These components are: (1) the uniform flow solution (2) the point source/sink solution; and (3) the finite radius source/sink in uniform flow solution. The various components can be combined or superposed to derive a more complex overall solution of the ground-water flow system. The basic assumptions used in developing the analytical solutions in RESSQC are as follows:

- The aquifer is homogeneous, isotropic, and of constant saturated thickness.

- The flow of ground water in the aquifer is two-dimensional in a horizontal plane and is at a steady state.

The fundamentals of complex potential theory as applied to ground-water flow problems are outlined below. The notation used here is consistent with that used by Javandel et al. (1984) in their presentation of the original RESSQ code.

Let ϕ and ψ denote two functions known as the velocity potential function and stream function, respectively. These functions satisfy the following pair of Laplace's equations:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \qquad\qquad (A.1)$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = 0 \qquad\qquad (A.2)$$

where x and y are Cartesian coordinates in a horizontal areal plane. Equations (A.l) and (A.2) can be used to describe steady-state two-dimensional ground-water flow if the following definitions are adopted:

$$q_x = -\frac{\partial \phi}{\partial x} = -\frac{\partial \psi}{\partial y} \qquad\qquad (A.3)$$

$$q_y = -\frac{\partial \phi}{\partial y} = \frac{\partial \psi}{\partial x} \qquad\qquad (A.4)$$

where q_x and q_y arc components of Darcy velocity of ground-water flow along the x and y directions, respectively. Note that the ground-water seepage velocity is defined as the ratio of Darcy velocity to porosity of the aquifer.

In view of Equations (A.l) - (A.4), which represent the Cauchy-Riemann condition of a complex analytic function the two functions ϕ and ψ can be considered as being the real and imaginary parts of the analytic function W defined as

$$W = \phi + i\psi \qquad\qquad (A.5)$$

where $i = \sqrt{-1}$.

With the above definition, the complex potential funtion, W, can be used to provide simple representations of various two-dimensional flow patterns. The real part of W, which is ϕ, can be used to produce equipotential lines (or lines of constant hydraulic head values) in the flow field. Using Darcy's law, the velocity potential ϕ, and the hydraulic head, h are related by $\phi = Kh$ On the other hand the imaginary component of W, which is ψ, can be used to produce streamlines (or flow lines). Each streamline corresponds to a constant value of ψ.

A.2 Analytical Solutions Used in RESSQC

A.2.1 Uniform Flow

A uniform ambient ground-water flow in a direction making an angle a with the positive x-axis (Figure Ala) may be represented by:

$$W = -UZ(\cos\alpha - i\sin\alpha) \qquad \text{(A.6)}$$

where U is the magnitude of the Darcy velocity, and Z is a complex variable defined as

$$Z = x + iy \qquad \text{(A.7)}$$

Combining Equations (A.6), (A.5), and (A.7) yields

$$\phi + i\psi = -U(x+iy)(\cos\alpha - i\sin\alpha) \qquad \text{(A. 8)}$$

from which the following expressions for ϕ and ψ arc obtained:

$$\phi = -U(x\cos\alpha + y\sin\alpha) \qquad \text{(A.9)}$$

$$\psi = U(x\sin\alpha - y\cos\alpha) \qquad \text{(A. 10)}$$

Components of the Darcy velocity are obtained by differentiation of (A.9). Thus,

$$q_x = -\frac{\partial\phi}{\partial x} = U\cos\alpha \qquad \text{(A. 11)}$$

$$q_y = -\frac{\partial\phi}{\partial y} = U\sin\alpha \qquad \text{(A. 12)}$$

A.2.2 Point Sources and Sinks

The flow field resulting from a point source (e.g., a fully penetrating recharge well) located at (x_o, y_o) maybe described by the following complex potential function (A.lb):

Figure A.1

Fundamental Flow Fields.
Uniform Flow Field (a), and
Radial Flow Fields (b)

(a)

(b)

$$W = -\frac{Q}{2\pi b} \ell n \ (Z-Z_o) \qquad (A.13)$$
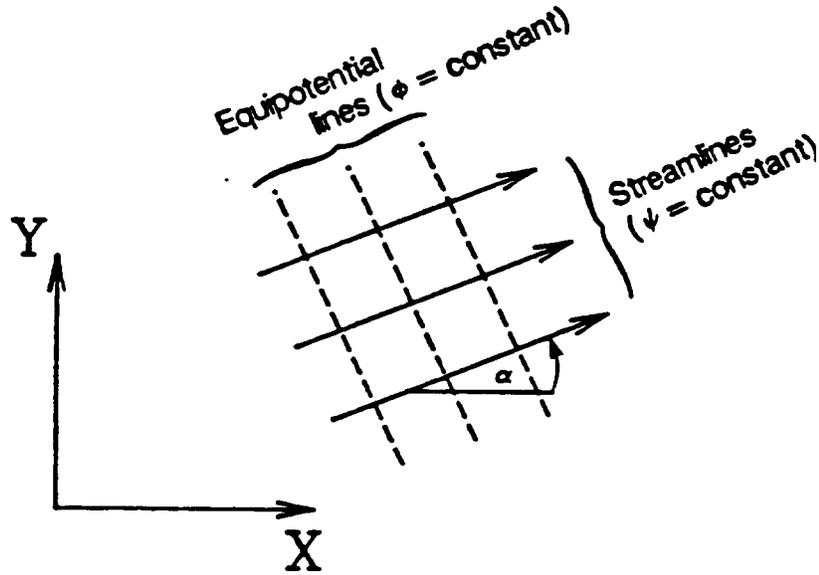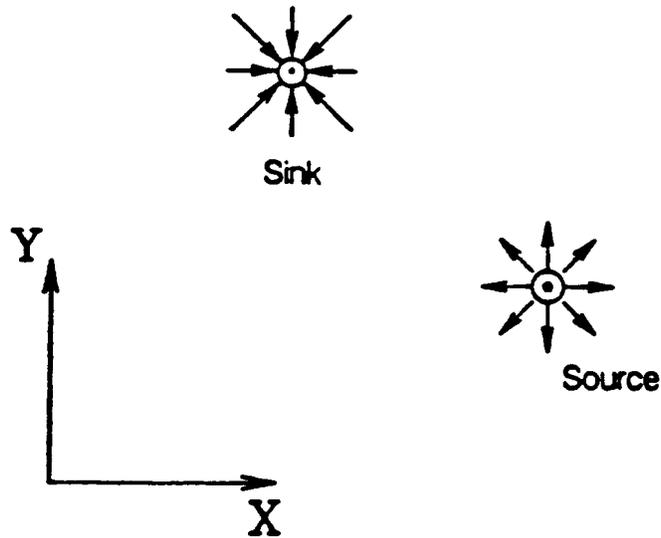
where

$$Z_o = x_o + iy_o \qquad (A.14)$$

Substituting for complex numbers Z and Z_o m (A.13), the velocity potential and stream function for the specified source may be obtained as follows:

$$W = \phi + i\psi = -\frac{Q}{2\pi b} \ell n \ (Z-Z_o) \qquad (A.\ 15)$$

$$\phi + i\psi = -\frac{Q}{2\pi b} \ell n \ [(x-x_o)^2 + (y-y_o)^2]^{\frac{1}{2}}$$

$$- i \frac{Q}{2\pi b} \tan^{-1} \left[\frac{y-y_o}{x-x_o} \right] \qquad (A.\ 16)$$

Thus

$$\phi = -\frac{Q}{4\pi b} \ell n \ [(x-x_o)^2 + (y-y_o)^2] \qquad (A.\ 17)$$

$$\psi = -\frac{Q}{2\pi b} \tan^{-1} \left[\frac{y-y_o}{x-x_o} \right] \qquad (A.\ 18)$$

The Darcy velocity components, q_x and q_y, arc given by

$$q_x = -\frac{\partial\phi}{\partial x} = \frac{Q}{2\pi b} \left[\frac{(x-x_o)}{(x-x_o)^2 + (y-y_o)^2} \right] \qquad (A.\ 19)$$

$$q_y = -\frac{\partial\phi}{\partial y} = \frac{Q}{2\pi b} \left[\frac{(y-y_o)}{(x-x_o)^2 + (y-y_o)^2} \right] \qquad (A.20)$$

The above analytical solution describes the radial flow field emanating from the source located at (x_o, y_o). Replacement of Q by -Q has the effect of reversing the flow direction The resulting flow field then correspond to that of a converging radial flow field toward a point sink located at (x_o, y_o).

A.2.3 Finite Radius Source in Uniform Flow

In a situation where a source of contamination covers a large area, representing it by a point in the two-dimensional flow field may be inaccurate. A more realistic representation of this case is to treat it as a circular source whose radius is computed such that the area of the circle equals the area of the actual contaminant source. Physically, the idealized circular source may represent either a surface impoundment a waste pond or a lagoon that discharges leachate into the ground-water system.

Consider a particular case where such a source operates at a constant head m an aquifer with ambient flow in the positive x-direction. The center of the source is located at the origin of the coordinate axes, and the source is assumed to be a fully penetrating source of radius r_o. The complex velocity potential describing the resulting flow field may be expressed as

$$W = -Uz + \frac{Ur_o^2\, \bar{z}}{|z|^2} - \frac{Q_p}{2\pi b}\, \ln z + C \qquad (A.21)$$

where Q_p is the rate of outflow from the finite-radius source, $\bar{z}$ and $|z|$ are the conjugate and the modulus of Z, respectively, C is a constant and the remaining symbols are as defined previously.

The expressions for potential and stream functions, ϕ and ψ, can be obtained by separating the real and imaginary parts of W. The resulting expressions are given by

$$\phi = -Ux + \frac{Ur_o^2 x}{x^2 + y^2} - \frac{Q_p}{4\pi b}\, \ln (x^2+y^2) + c_1 \qquad (A.22)$$

$$\psi = -Uy + \frac{Ur_o^2 y}{x^2 + y^2} - \frac{Q_p}{2\pi b}\, \tan^{-1}\left[\frac{y}{x}\right] + c_2 \qquad (A.23)$$

where c_1 and c_2 are constants. C_2 maybe set equal to zero and c_1 is determined by imposing that ϕ satisfies the boundary condition of $\phi = H_o$ at the boundary of the source where $r = r_o$. Thus, c_1 is evaluated as being equal to $H_o + \frac{Q_p}{4\pi b}\, \ln r_o^2$. The expression for ϕ then becomes

$$\phi \ = \ -Ux + \frac{Ur_o^2 x}{x^2 + y^2} - \frac{Q_p}{4\pi b} \quad \ell n \left[\frac{x^2 + y^2}{r_o^2} \right] + H_o \qquad (A.24)$$

The Darcy velocity components, q_x and q_y, are obtained by differentiating (A.24) and reversing the signs:

$$q_x \ = \ U + Ur_o^2 \left[\frac{x^2 - y^2}{(x^2+y^2)^2} \right] + \frac{Q_p}{2\pi b} \frac{x}{x^2 + y^2} \qquad (A.25)$$

$$q_y \ = \ Ur_o^2 \left[\frac{2xy}{(x^2+y^2)^2} \right] + \frac{Q_p}{2\pi b} \frac{y}{x^2 + y^2} \qquad (A.26)$$

A.2.4 Combination of Uniform Flow with Point Sources and Sinks

In a general situation where there arc groups of discharging and recharging wells operating simultaneously in an aquifer with ambient ground-water flow, the resulting flow field can be constructcd by means of superposition. The overall complex velocity potential, W, of such a system is given by adding the uniform flow component to the source and sink components. The general expression of W may be written as

$$W \ = \ -UZ \ (\cos\alpha - i\sin\alpha) + \sum_{j=1}^{N} \frac{Q_j}{2\pi b} \ \ell n \ (Z-Z_j)$$

$$- \sum_{k=1}^{M} \frac{Q_k}{2\pi b} \ \ell n \ (Z-Z_k) \qquad (A.27)$$

where Q_j is the flow rate of discharging well j (located at $Z=Z_j$), Q_k is the flow rate of recharging well k (located at $Z=Z_k$), N and M are the numbers of discharging and recharging wells, respectively, and the remaining symbols are as defined previously.

As before, the expressions for potential and stream functions, ϕ and ψ, can be obtained by separating the real and imaginary parts of W. These expressions are given by

$$\phi = -U\ (x\cos\alpha + y\sin\alpha) + \sum_{j=1}^{N} \frac{Q_j}{4\pi b}\ \ell n\ [(x-x_j)^2 + (y-y_j)^2]$$

$$- \sum_{k=1}^{M} \frac{Q_k}{4\pi b}\ \ell n\ [(x-x_k)^2 + (y-y_k)^2] \qquad (A.28)$$

$$\psi = U\ (x\cos\alpha + y\cos\alpha) + \sum_{j=1}^{N} \frac{Q_j}{2\pi b}\ \tan^{-1}\left[\frac{y-y_j}{x-x_j}\right]$$

$$- \sum_{k=1}^{M} \frac{Q_k}{2\pi b}\ \tan^{-1}\left[\frac{y-y_k}{x-x_k}\right] \qquad (A.29)$$

The Darcy velocity components, q_x and q_y, are obtained by differentiating (A.28):

$$q_x = -\frac{\partial\phi}{\partial x} = U\cos\alpha - \sum_{j=1}^{N} \frac{Q_j}{2\pi b}\ \frac{(x-x_j)}{(x-x_j)^2 + (y-y_j)^2}$$

$$+ \sum_{k=1}^{M} \frac{Q_k}{2\pi b}\ \frac{(x-x_k)}{(x-x_k)^2 + (y-y_k)^2} \qquad (A.30)$$

$$q_y = -\frac{\partial\phi}{\partial y} = U\sin\alpha - \sum_{j=1}^{N} \frac{Q_j}{2\pi b}\ \frac{(y-y_j)}{(x-x_j)^2 + (y-y_j)^2}$$

$$+ \sum_{k=1}^{M} \frac{Q_k}{2\pi b}\ \frac{(y-y_k)}{(x-x_k)^2 + (y-y_k)^2} \qquad (A.31)$$

Additional composite potential fields can be generated through various combinations of the fundamental component solutions given in the previous sections.

A.3 Pathline and Capture Zone Delineation Algorithms

The RESSQC module performs the computation of pathlines by tracing the movement of individual fluid particles through the ground-water flow system. (Because steady-state flow is assumed the term pathline and streamline can be used interchangeably. The term 'streamline" is normally defined as a line that is tangent at a given instant to the velocity vector at each point upon it.) By tracing multiple streamlines, contaminant frontal positions and capture zones may be delineated. The computational procedures are described in the following subsections.

A.3.1 Pathline Computation

For a given particle, the pathline computation begins with the evaluation of particle velocity at the starting position. For water particles, the seepage (or average pore water) velocity components in the x and y directions are evaluated using the following formulas:

$$v_x = q_x/\theta \tag{A.32}$$

$$v_y = q_y/\theta \tag{A. 33}$$

where $v_=$ and v_y are the seepage velocity components, q_x and q_y are components of the Darcy velocity obtained using the analytical solution described previously, and θ is the aquifer porosity.

For contaminant (or solute) particles, the velocity components, v_{cx} and v_{cy}, are computed as follows:

$$v_{cx} = q_x/\theta R \tag{A.34}$$

$$v_{cy} = q_y/\theta R \tag{A.35}$$

where R is a is a physical parameter called the retardation factor that accounts for the adsorption of solute onto the rock matrix= If there is no adsorption the value of R is 1. In the general case involving adsorption R is given by

$$R = 1 + \rho_b k_d/\theta \tag{A. 36}$$

where ρ_B is the bulk density of the porous medium (aquifer material), and k_d is the distribution coefficient.

Consider the situation involving a water particle moving through the flow system. The pathline of the particle can be traced by solving the following pair of differential equations:

$$\frac{dx}{dt} = v_x = q_x/\theta \tag{A.37a}$$

$$\frac{dy}{dt} = v_y = q_y/\theta \tag{A.37b}$$

Subject to the initial conditions:

$$x(t=0) = x_o \tag{A.38a}$$

$$y(t=0) = y_o \tag{A.38b}$$

where (x_o, y_o) is the initial location (stinting position) of the particle.

The solution of the above equations is obtained through numerical integration. In RESSQC the Euler integration scheme is used to determine a new position of the particle for each specified time increment At. According to this scheme, given that at time t the particle is at the point (x_j, y_j), then its new position at time $t+\Delta t$ is determined from

$$x_{j+1} = x_j + (q_x/\theta)\ \Delta t \tag{A. 39a}$$

$$y_{j+1} = y_j + (q_y/\theta)\ \Delta t \tag{A. 39b}$$

Thus, starting from the initial position of the particle at t=O, one can use equations (A.39a) and (A.39b) repetitively to determine successive locations of the particle at later time values. The accuracy of such a forward integration procedure depends on the size of the time step, Δt.

In RESSQC, an automatic control of the time step value is made by limiting $\Delta \ell$, the incremental displacement length along the pathline. The value of $\Delta \ell$ is determined in the calculation process such that the following criteria are satisfied:

1. $\Delta \ell$ must not exceed ΔL, the maximum prescribed step length input by the user.

2. The velocity direction change over the displacement length must not be greater than a prescribed tolerance. More precisely, the magnitude of angular acceleration must not exceed 1. When this criterion is violated, $\Delta \ell$ is reduced by 1/2. The angular acceleration, $\dot{\omega}$, is computed from

$$\dot{\omega}^2 = [(v_{xN}/|v_N|) - (v_{xP}/|v_P|)]^2$$

$$+ [(v_{yN}/|v_N|) - (v_{yP}/|v_P|)]^2 \qquad (A.40)$$

where v_{xN} and v_{yN} are the seepage velocity components at the new point, v_{xP} and v_{yP} arc the seepage velocity components at the previous point and $|v_N|$ and $|v_P|$ are the magnitude of seepage velocity at the new and previous points, respectively.

3. The selected value of $\Delta \ell$ must satisfy a velocity convergence criterion within 5 iterations. The iteration is done by checking the average of the velocities at the previous and tentative points on the pathline against the velocity used to compute the tentative point If this differs by more than 1 percent of the magnitude of the averaged velocity, then that average is used to compute a new tentative point and the iteration is repeated. If convergence is not achieved within 5 iterations, the value of $\Delta \ell$ is reduced by 1/2.

Using the algorithm described above, the code draws the flow pattern in the aquifer by tracing the pathlines that emanate from specified starting locations. Each starting location may correspond to the location of an injection well a production well, or simply a point from which a single pathline (or streamline) is to be traced. In the case of an injection well, the flow rate and radius of the well need to be specified in conjunction with the number of pathline to be calculated for the well. If the flow rate is not specified the code assumes a zero default value and only one pathline is traced from the specified starting point. Production wells are distinguished from injection wells via different input specifications. In the original RESSQ code presented by Javandel et al. (1984), neither

pathline nor capture zone delineation is performed for production wells. This limitation is removed in RESSQC which is the modified code presented in this report. In RESSQC, pathlines and capture zone boundaries can also be delineated for production wells by reversing the velocity field before particle tracking is performed.

A.3.2 Front Tracking and Capture Zone Delineation

Tracking of contaminant fronts surrounding an injection well (or an areal contaminant source modeled as a circle of finite radius) can be made by keeping record of the travel times of contaminant particles released from the boundary of the well (or circular source). RESSQC requires the user to specify as input the travel time values at which the fronts are to be calculated. At each prescribed travel time value, the terminal points of all pathlines that originate from the contaminant source are identified. The frontal position can then be drawn by joining these terminal points in a sequential order. Time-related capture zones for production wells are also delineated by RESSQC using a similar approach. In this case, reverse pathlines of water particles are traced from the well bore of each production well. The travel times taken by these particles to move along their pathlines are recorded. At each prescribed capture zone time, the terminal points of all pathlines are identified. The capture zone boundary is drawn by joining these terminal points sequentially.

A.4 Code Structure and Dimension Limits of RESSQC Module

Table A.l is a list of program segments (subroutines) that compose the RESSQC module. The dimension limits of RESSQC arrays are listed in Table A.2

A.5 Differences Between RESSQC and the Original RESSQ Code

Three major changes were incorporated into the original RESSQ code of Javandel et al. 1984:

1.   The code was modified to allow the delineation of capture zones as well as contaminant fronts.   If reverse tracking is to be performed, the velocity components $v_=$ and $\mathbf{v_y}$ are multiplied by -1. Use of the adsorption coefficient is not permitted with this new option.

Table A.l

Description of RESSQC Subroutines
(Subroutines Listed In Alphabetical Order)

Subroutine Name	Description
FLOW	Traces the path of a streamline. Streamlines terminate at pumping wells (contaminant fronts), at injection wells (capture zones), or at the model boundary.
PRINTWL	Prints the well information to output file.
READW	Reads the input parameters associated with each recharge/pumping well from the input file.
RESSQ2	Continuation of main program. Reads some input parameters from file, initializes variables, calls subroutines to calculate streamlines, and writes results to output file.
SORT1	Sorts the values of the time-related capture zones or contaminant fronts into ascending order.
SORT2	Sort the array TARR and NWARR first by the number of the well of arrival, then by the number of the well of departure, and finally by the time of arrival.
TESTAR	Checks if the current particle location is within distance DL (maximum allowable step length) of a production well (contaminant fronts) or injection well (capture zones).
VXVY	Computes the ground-water flow velocity vector at any given point (x,y).
WEED	Weeds out every other point in the trace of a streamline starting with the fourth point in order to obtain enough room in the XL and YL arrays to save the entire streamline.

Table A.2

Dimension Limits For RESSQC Arrays

Array Name	Dimension	Description
BETA	140	Angle of first pathline to leave the well
DATE	7	Contaminant front or capture zone time values.
INDW	140	Contains flag for each well to indicate whether or not contaminant fronts or capture zones should be plotted.
ITRW	140	Ratio of number of pathlincs to number plotted.
NAMEW	140	Character array containing the name of each pumping and injection well.
NPATH	140	Number of pathlines to be computed to delineate contaminant fronts or capture zones.
NWARR	140	Well of arrival of pathline.
QW	140	Flow rate into/from the wall(s).
RADW	140	Well radii.
TARR	140	Time of arrival of pathline in pumping well (contaminant fronts) or injection well (capture zones).
XF	(2,140,140)	Coordinates of contaminant fronts or capture zone boundaries.
XL	7,000	X-coordinates of pathline.
XW	(2,140)	Well coordinatcs.
YL	7,000	Y-coordinatcs of pathline.

2. The code was "undimensionalized". The units for all model input parameters used by RESSQC must be" consistent (e.g. all length values might be in feet and all time values might be in days). RESSQ has internal conversion factors so that parameters must have a "practical" or "CGS" system of units.

3. The common block structure of RESSQ was changed in RESSQC so that the storage space for CHARACTER, INTEGER, and REAL data is separated and Fortran EQUIVALENCE statements are no longer used.

In addition to these major changes, several smaller changes were incorporated so that RESSQC would conform to the overall WHPA model structure. For example, the plotting output for pathlines is written to the file WHPA.PLT instead of TAPE7, and several format statements have been altered.

Appendix B

Theoretical Development and Implementation of MWCAP Module

B.1 Introduction

The MWCAP module is designed especially for the efficient delineation of capture zones of individual production wells. Three types of capture zones can be delineated. These include (1) steady-state capture zones (open-ended capture zones that correspond to infinite travel time), (2) time-related capture zones (closed capture zones that correspond to specified values of travel time), and (3) hybrid capture zones (combined capture zones formed by closing a steady-state capture zone with a time-related upstream boundary). MWCAP uses potential function analytical solutions to determine the locations of stagnation points. The stagnation points are used as control points in delineating capture-zone boundaries. The computational procedure is based on the fundamental analytical assumption of steady-state two-dimensional flow in a homogeneous aquifer of constant saturated thickness. In addition, MWCAP assumes that well interferences due to simultaneous pumping have negligible effects on capture zones of the individual wells.

Three major cases are considered by MWCAP. These cases concern (1) an aquifer without a lateral boundary (infinite areal-extent aquifer), (2) an aquifer with a stream boundary, and (3) an aquifer with a barrier boundary. Much of the material presented here follows the work of Newsom and Wilson (1988) and Lee and Wilson (1986). It should be noted however, that the present notation differs somewhat from the previous works in terms of the definitions of potential and stream functions and the convention for identifying the ambient flow angle.

B.2 Analytical Solutions Used in MWCAP

B.2.1 Aquifer Without Lateral Boundary

For this simple case, the expression of the potential function ϕ, for a pumping well in uniform ambient flow may be written as

$$\phi = -U(x\cos\alpha + y\sin\alpha) + \frac{Q}{4\pi b} \ln [(x-x_o)^2 + (y-y_o)^2] \qquad (B.1)$$

where U is the Darcy velocity of the ambient flow, a is the angle of ambient flow measured counter-clockwise from the positive x-axis, Q is the well discharge rate, b is the aquifer thickness and x_o and y_o are the x and y coordinates of the well respectively.

If the coordinate system is oriented such that the origin is at the well and the x-axis is parallel to the flow direction then (B.1) reduces to

$$\phi = -Ux + \frac{Q}{4\pi b} \ln [x^2+y^2] \qquad (B.2)$$

Using equation (B.2), the following expressions for Darcy velocity components are obtained:

$$q_x = -\frac{\partial \phi}{\partial x} = U - \frac{Q}{2\pi b} \left[\frac{x}{x^2+y^2} \right] \qquad (B.3)$$

$$q_y = -\frac{\partial \phi}{\partial y} = -\frac{Q}{2\pi b} \left[\frac{y}{x^2+y^2} \right] \qquad (B.4)$$

From equations (B.3) and (B.4), it follows that there is one stagnation point (where $q_x = q_y = 0$), and its coordinates (x_s, y_s) are given by

$$x_s = Q/(2\pi bU) \qquad (B.5a)$$

$$y_s = 0 \qquad (B.5b)$$

Two streamlines pass through this stagnation point. These are the dividing streamlines which separate the capture zone of the well from the rest of the aquifer. Both dividing streamlines can be traced by releasing two particles in the neighborhood of each stagnation point. The coordinates of these neighborhood points, points A and B, are set such that

$$(x_A, y_A) = (x_s - \epsilon, \epsilon)$$
(B. 6a)

and

$$(x_B, y_B) = (x_s - \epsilon, -\epsilon)$$
(B. **6b**)

where ϵ is a small positive number. This approach is used by MWCAP to locate the two bounding streamlines representing the boundary of the steady-state capture zone. An analytical expression for the two dividing streamlines can be obtained as follow.

First the expression for stream function for this case is written as

$$\psi = -Uy + \frac{Q}{2\pi b} \tan^{-1}\left[\frac{y}{x}\right]$$
(B.7)

which can be rearranged in the form

$$\eta_D = \left[\frac{2\pi b}{Q}\right]\psi = -\left[\frac{2\pi b U}{Q}\right] y + \tan^{-1}\left[\frac{y}{x}\right]$$
(B.8)

where η_D is a dimensionless stream function. The values of η_D corresponding to the two dividing streamlines are π and $-\pi$, respectively. Substituting these values into (B.8) gives the equations for these streamlines. Thus one obtains

$$y = \pm \frac{Q}{2bU} + \frac{Q}{2\pi bU} \tan^{-1}\left[\frac{y}{x}\right]$$
(B.9)

$$x \rightarrow \infty, \frac{y}{x} \rightarrow 0 \text{ and } \tan^{-1}(0) = 0$$

Equation (B.9) indicates that the water-dividing streamlines approach asymptotically (i.e. as x -> ∞) the lines y = ± Q/2bU.

B.2.2 Aquifer With Stream Boundary

Although the previous analytical solution is fairly simple, it is limited to the situation where the well is far enough removed from any physical boundaries so that the effects of these boundaries on the capture zone are negligible. A more general solution that accounts for the presence of a nearby stream boundary is also available and implemented into MWCAP. For this case, the potential function, ϕ, is obtained using image well theory.

Consider the flow system shown in Figure B.1. To satisfy the stream boundary condition (zero drawdown along the stream), an image pumping well is introduced at the location (x,y) = (40). The resulting expression of potential function ϕ is given by

$$\phi = -U(x\cos\alpha + y\sin\alpha) + \frac{Q}{4\pi b}\left[\ell n\frac{(x-d)^2 + y^2}{(x+d)^2 + y^2}\right] \qquad (B.10)$$

Differentiating (B.1O) gives the following expressions for Darcy velocity components:

$$q_x = -\frac{\partial\phi}{\partial x} = U\cos\alpha + \frac{Q}{4\pi b}\frac{\partial F}{\partial x} \qquad (B.11)$$

$$q_y = -\frac{\partial\phi}{\partial y} = U\sin\alpha + \frac{Q}{4\pi b}\frac{\partial F}{\partial y} \qquad (B.12)$$

where

$$\frac{\partial F}{\partial x} = -\left[\frac{2(x-d)}{(x-d)^2 + y^2} - \frac{2(x+d)}{(x+d)^2 + y^2}\right] \qquad (B.13)$$

$$\frac{\partial F}{\partial y} = -\left[\frac{2y}{(x-d)^2 + y^2} - \frac{2y}{(x+d)^2 + y^2}\right] \qquad (B.14)$$

Figure B.1

Schematic Flow System For MWCAP Stream Boundary Formulation
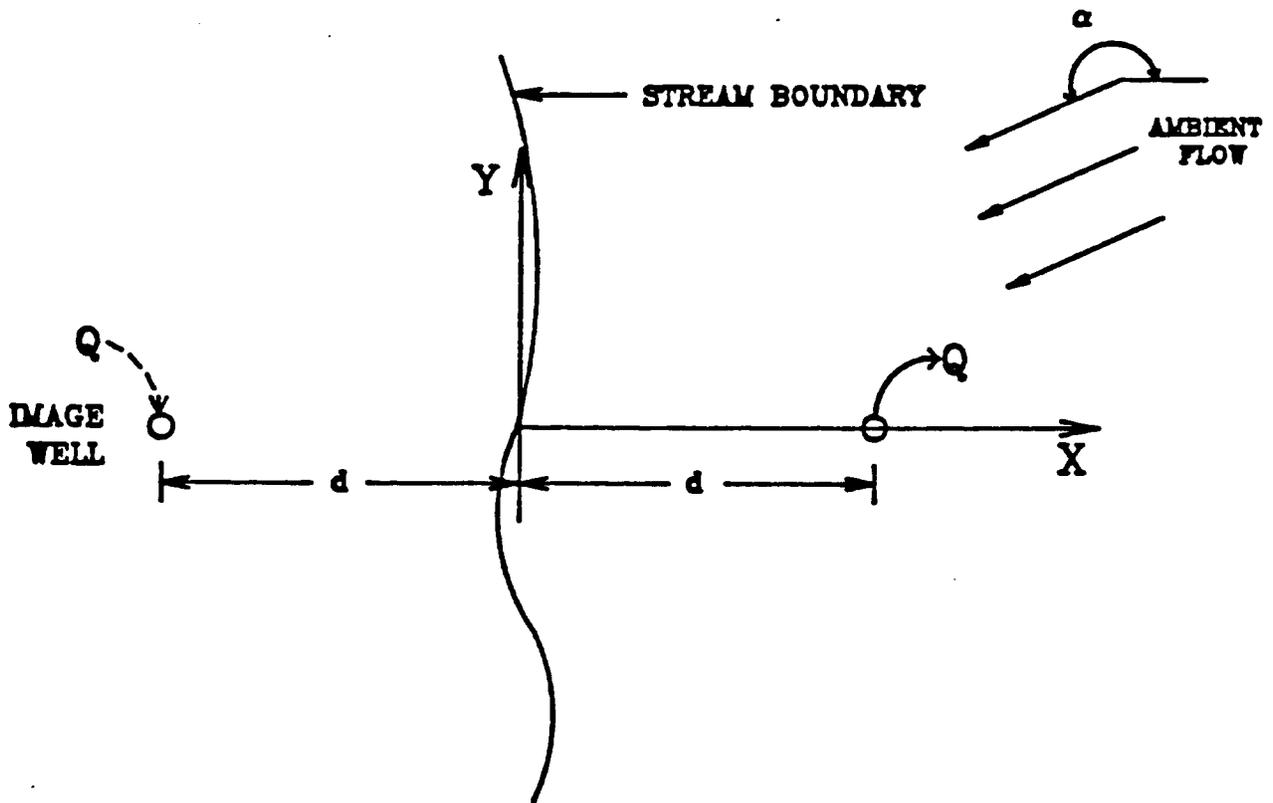
A general expression for stagnation-point coordinates can be derived by differentiating the complex velocity potential, W, (referred to in Appendix A) and setting it to zero. For the particular case considered here, the expression of W is given by

$$W = -U(\cos\alpha - i\sin\alpha)Z + \frac{Q}{2\pi b} \ln \left[\frac{Z-d}{Z+d} \right] \tag{B.15}$$

where $Z = x + iy$, and $i = \sqrt{-1}$. Since W is an analytic function, its derivative is given by

$$\frac{dW}{dZ} = -U(\cos\alpha - i\sin\alpha) + \frac{Q}{2\pi b(Z-d)} - \frac{Q}{2\pi b(Z+d)} \tag{B.16}$$

Setting $dW/dZ = 0$ at $Z = Z_s$ and solving for Z_s gives

$$Z_s = \pm d [1 + \beta(\cos\alpha + i\sin\alpha)]^{\frac{1}{2}} \tag{B.17}$$

where β is a dimensionless parameter defined as

$$\beta = \frac{Q}{\pi d U b} \tag{B.18}$$

and

$$Z_s = x_s + iy_s \tag{B.19}$$

where (x_s, y_s) are stagnation point coordinates.

For the special case where the ambient ground-water flow is parallel to the negative x-axis $(\alpha = 180^0)$, and equation (B.17) reduces to

$$Z_s = \pm d [1 - \beta]^{\frac{1}{2}} \tag{B.20}$$

which, upon combination with (B.19), leads to three following possibilities (see Figure B.2).

(1) when $\beta < 1$, only one stagnation point exists on the x-axis and its x-coordinate is given by

$$x_s = d [1 - \beta]^{\frac{1}{2}} \tag{B.21}$$

Figure B.2

## Typical Pumping Well Capture Zones for a Well Near A Stream In an Aquifer With Ambient Flow:
a) Pumping Rate Below Critical Value; b) Pumping Rate at Critical Value; c) Pumping Rate Above Critical Value
(from Lee, 1986)

a) Small $Q < Q_0$
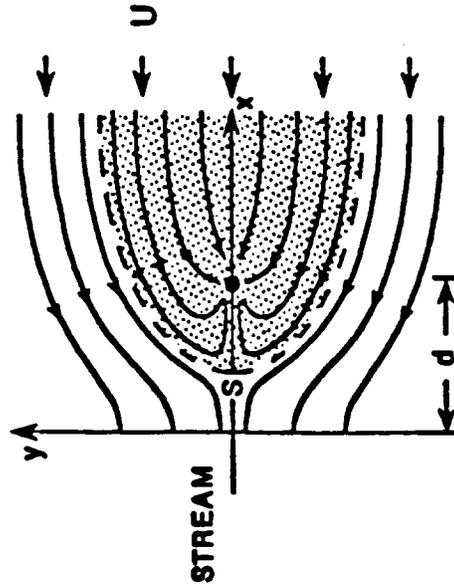
b) Critical $Q = Q_0$
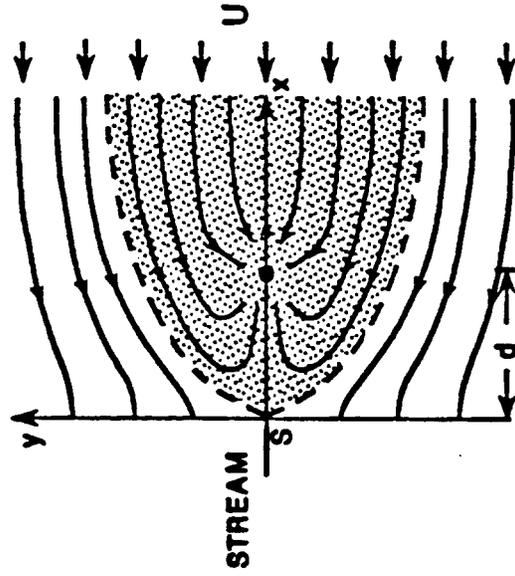
c) Large $Q > Q_0$
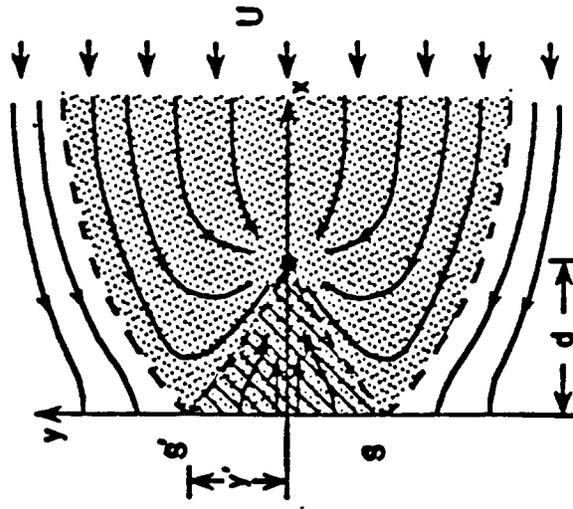
LEGEND

CAPTURE ZONE

SWEPT ZONE

Note that the other (negative) solution for x_s is unrealistic because it is outside the flow domain. This case of $\beta < 1$ corresponds to Figure B.2a. As can be seen, the capture zone does not intercept the stream because the pumping rate Q is smaller than the critical value Q_c ($Q_c = \pi dUb$). Thus the stream does not contribute recharge to the well.

(2) When $\beta = 1$, there is also one stagnation point but it is located at the origin of the coordinate axis. This value of β is the critical value above which the stream will begin to contribute to the flow of the well. The case of $\beta = 1$ corresponds to Figure B.2b. As can be seen, the stagnation point contacts the stream when $Q = Q_c$.

(3) when $\beta > 1$, two stagnation points exist. They are both located on the y axis. Their y-coordinates arc given by

$$y_s = \pm d [\beta - 1]^{\frac{1}{2}} \tag{B.22}$$

This case corresponds to Figure B.2c. As depicted when the pumping rate Q exceeds the critical value, Q_c, the stream contributes to the well flow. The shaded part of the capture zone is called the stream capture zone; within this region the flow lines emanate from the stream.

In a general situation where the direction of ambient flow is such that both $\cos\alpha$ and $\sin\alpha$ are nonzero, the stagnation point coordinates (x_s, y_s) must be determined from Equation (B.17) by taking the complex root. It can be shown that the general expressions for x_s and y, are given by

$$x_s = (\frac{d^2}{2})^{\frac{1}{2}} [\gamma \pm (1 + \beta\cos\alpha)]^{\frac{1}{2}} \tag{B.23a}$$

$$y_s = \pm (\frac{d^2}{2})^{\frac{1}{2}} [\gamma \pm (\beta\cos\alpha + 1)]^{\frac{1}{2}} \tag{B. 23b}$$

where

$$\gamma = (1 - 2\beta\cos\alpha + \beta^2)^{\frac{1}{2}} \tag{B.24}$$

Physical consideration leads to the conclusion that the number of stagnation points cannot exceed 2. Furthermore, the values of x_s and y_s that are acceptable must satisfy the following constraints: (1) both x_s and y_s must be real and $x_s \geq 0$, and (2) at (x_s,y_s) the velocity must be zero. These constraints are used to determine the cornet solution for x_s and y_s.

B.2.3 Aquifer With Barrier Boundary

Another senario that may be addressed using MWCAP is the case of an aquifer with a barrier boundary (Figure B.3). For this case, the expression of the potential function is obtained once again using image well theory. An image discharging well is introduced at $(x,y) = (-d,0)$. The resulting expression of the potential function ϕ, is given by

$$\phi = -U(x\cos\alpha + y\sin\alpha) + \frac{Q}{4\pi b}\{\ell n[(x-d)^2 + y^2]$$

$$+ \ell n[(x+d)^2 + y^2]\} \tag{B.25}$$

Differentiation of Equation (B.25) gives the following expressions for Darcy velocity components:

$$q_x = -\frac{\partial\phi}{\partial x} = U\cos\alpha + \frac{Q}{4\pi b}\frac{\partial F}{\partial x} \tag{B.26}$$

$$q_y = -\frac{\partial\phi}{\partial y} = U\sin\alpha + \frac{Q}{4\pi b}\frac{\partial F}{\partial y} \tag{B.27}$$

where

$$\frac{\partial F}{\partial x} = -\left[\frac{2(x-d)}{(x-d)^2 + y^2} + \frac{2(x+d)}{(x+d)^2 + y^2}\right] \tag{B.28}$$

$$\frac{\partial F}{\partial y} = -\left[\frac{2y}{(x-d)^2 + y^2} + \frac{2y}{(x+d)^2 + y^2}\right] \tag{B.29}$$

Figure B.3

Schematic Flow System For MWCAP Barrier Boundary Formulation
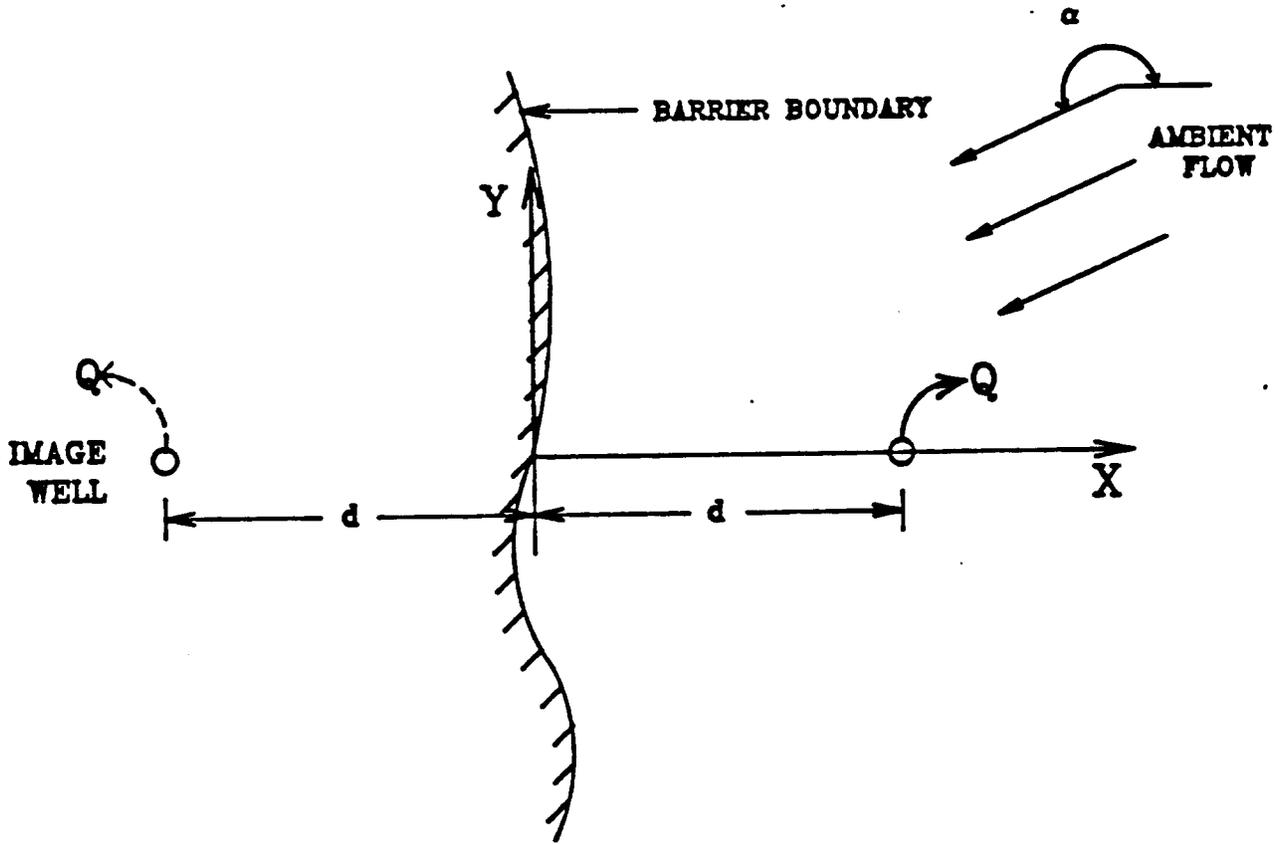
Note that the given potential function ϕ, yields a non.zero velocity at the barrier boundary (x= O). Indeed the values of q_x and q_y correspond to the x and y components of ambient flow velocity, respectively. This indicates that the barrier boundary simulated is not an impermeable boundary but rather a semi-permeable boundary across which there is ambient flow.

As before, a general expression for the stagnation point coordinates can be derived by differentiating the complex velocity potential, W, which is given by

$$W \;=\; -U(\cos\alpha - i\sin\alpha)Z + \frac{Q}{2\pi b} \ln [Z^2 - d^2] \qquad (B.30)$$

Differentiation of equation (B.30) gives

$$\frac{dW}{dZ} \;=\; -U(\cos\alpha - i\sin\alpha) + \frac{Q}{2\pi b} \left[\frac{2Z}{Z^2 - d^2} \right] \qquad (B.31)$$

Setting dW/dZ = O at Z = Z_s and solving for ~ one obtains

$$Z_s \;=\; \frac{\beta d \exp(i\alpha \pm [\beta^2 d^2 \exp(2i\alpha) + 4d^2]^{\frac{1}{2}}}{2} \qquad (B.32)$$

where β is defined by Equation (B.18), and $Z_s = x_s + iy_s$. From Equation (B.32), it can be shown that the stagnation point coordinates are given by

$$x_s \;=\; \frac{1}{2} [\beta d \cos\alpha \pm (\gamma/2)^{\frac{1}{2}} (1 + \cos\xi)^{\frac{1}{2}}] \qquad (B.33)$$

$$y_s \;=\; \frac{1}{2} [\beta d \sin\alpha \pm (\gamma/2)^{\frac{1}{2}} (1 - \cos\xi)^{\frac{1}{2}}] \qquad (B.34)$$

where

$$\cos\xi \;=\; (\beta^2 d^2 \cos 2\alpha + 4d^2)/\gamma \qquad (B.35)$$

For the special case where the ambient flow is parallel to the negative x-axis ($\alpha = 180^0$), Equations (B.33) and (B.34) reduce to

$$x_s = \frac{1}{2} [-\beta d \pm (\beta^2 d^2 + 4d^2)^{\frac{1}{2}}] \tag{B.36}$$

$$y_s = 0 \tag{B.37}$$

Since x_s must not be negative, there is only one feasible solution corresponding the stagnation point located on the positive x-axis at

$$x_s = \frac{1}{2} [-\beta d + (\beta^2 d^2 + 4d^2)^{\frac{1}{2}}] \tag{B.38}$$

In a general situation where the direction of ambient flow is not necessarily parallel to the x-axis, the feasible solutions for x_s and y_s can be determined from Equations (B.33) and (B.34) using the set of constraints described previously for the ease of an aquifer with a stream boundary.

B.3 Capture Zone Delineation Algorithms

General algorithms for delineating three types of capture zones have been incorporated into the MWCAP module. In a general situation involving multiple wells or a well field, these algorithms are formulated in terms of local coordinates and applied to the individual wells. The local coordinate system is set up for each well and related to the global coordinate system of the overall problem by means of a coordinate transformation matrix. The procedure for setting up a local coordinate system is simply to orient the local x-axis in the direction opposite to that of ambient ground-water flow. The local y-axis is oriented at 90^0 and counterclockwise to the local x-axis.

B.3.1 Steady-State Capture Zones

The delineation of steady-state capture zones is performed in a straightforward manner by performing pathline tracking of particles released from the neighborhood of each stagnation point Typical patterns of capture zones that can be expected for the situation of an aquifer with a stream boundary and various ambient flow angles are depicted in Figure B.4. Note that in case b of the figure where $\alpha = 240^0$ and the capture

Figure B.4

Typical Steady-state Capture Zones That Can Be Expected For The Situation Of An Aquifer With A Stream Boundary And Various Angles Of Ambient Flow (Newsom and Wilson, 1988).
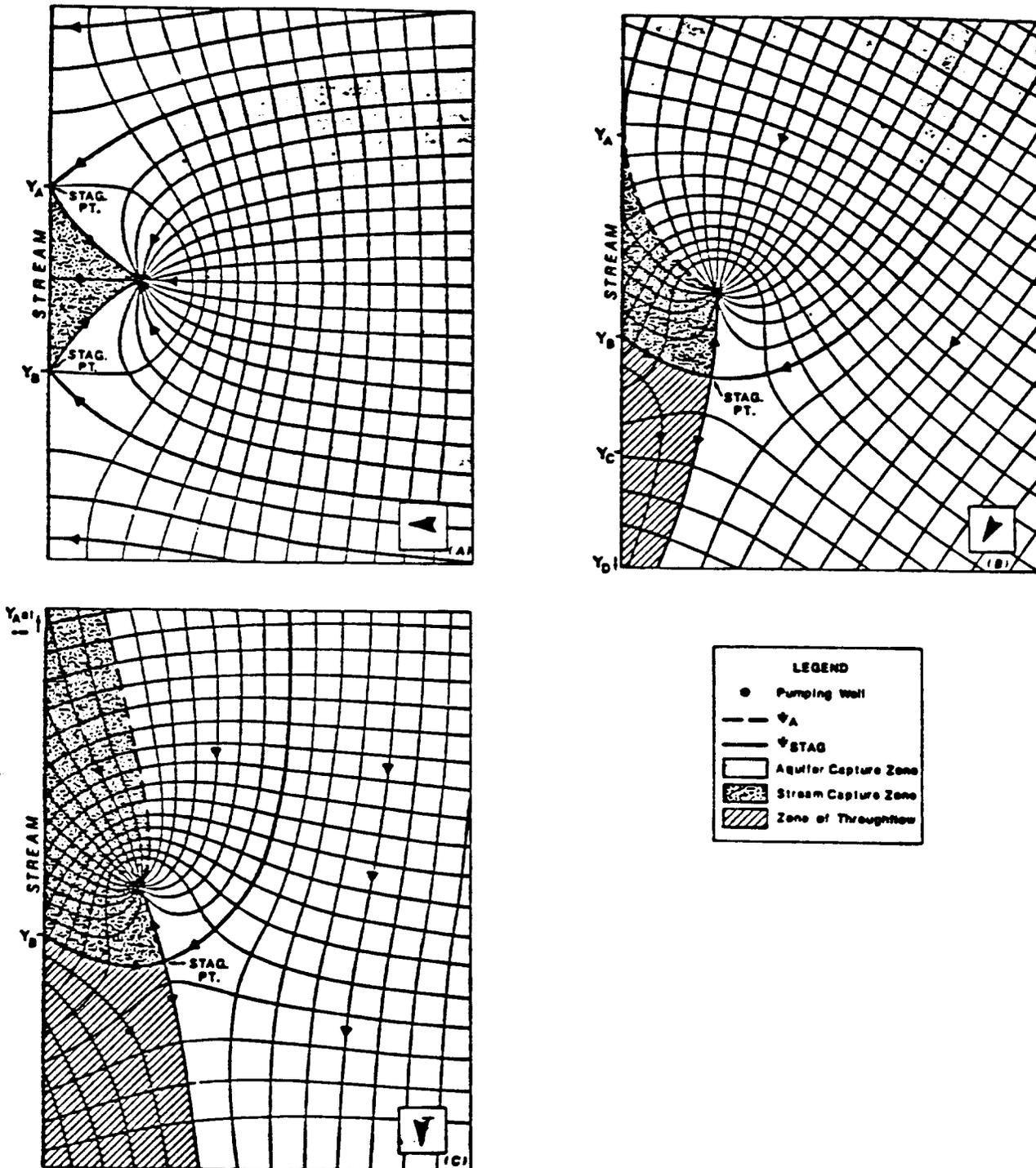
zone boundary becomes tangential to the stream boundary, it is necessary to identify point A (the critical tangent point). Once this point is located two additional panicles can be released from its neighborhood to trace the boundary segments of the capture zone. The location of A can be determined using the following expression of stream function derived from (B.15):

$$\psi = Ux\sin\alpha - Uy\cos\alpha + \frac{Q}{2\pi b}\left[\tan^{-1}\left(\frac{y}{x-d}\right) - \tan^{-1}\left(\frac{y}{x+d}\right)\right] \qquad (B.39)$$

At point A, $x_A = 0$ and Equation (B.39) reduces to

$$\psi = -Uy\cos\alpha - \frac{Q}{\pi b}\left[\tan^{-1}\left(\frac{y}{d}\right)\right] \qquad (B.40)$$

Differentiation of Equation (B.40) with respect to y and setting the derivative to zero yields the following equation for y_A:

$$-U\cos\alpha - \frac{Q}{\pi b}\left(\frac{d}{d^2 + y_A^2}\right) = 0 \qquad (B.41)$$

which can be rearranged in the form:

$$y_A = d\left(-1 - \frac{\beta}{\cos\alpha}\right)^{\frac{1}{2}} \qquad (B.42)$$

where $\beta = Q/\pi dUb$. To obtain a feasible solution from (B.42), we must have

$$-\frac{\beta}{\cos\alpha} \geq 1 \qquad (B.43)$$

The algorithm for tracing a pathline from a given swing position is now presented. This algorithm which is used in MWCAP, is different from that used in the RESSQC module. Refer to Figure B.5 as a guide for the following discussion.

Suppose the particle is currently located at point i. Its tentative (future) position is first calculated from

$$x_{i+1} = x_i + v_{ix}\Delta t = x_i + \Delta x_i \qquad (B.44a)$$

Figure B.5

Iterative Predictor-Corrector Particle Tracking Procedure
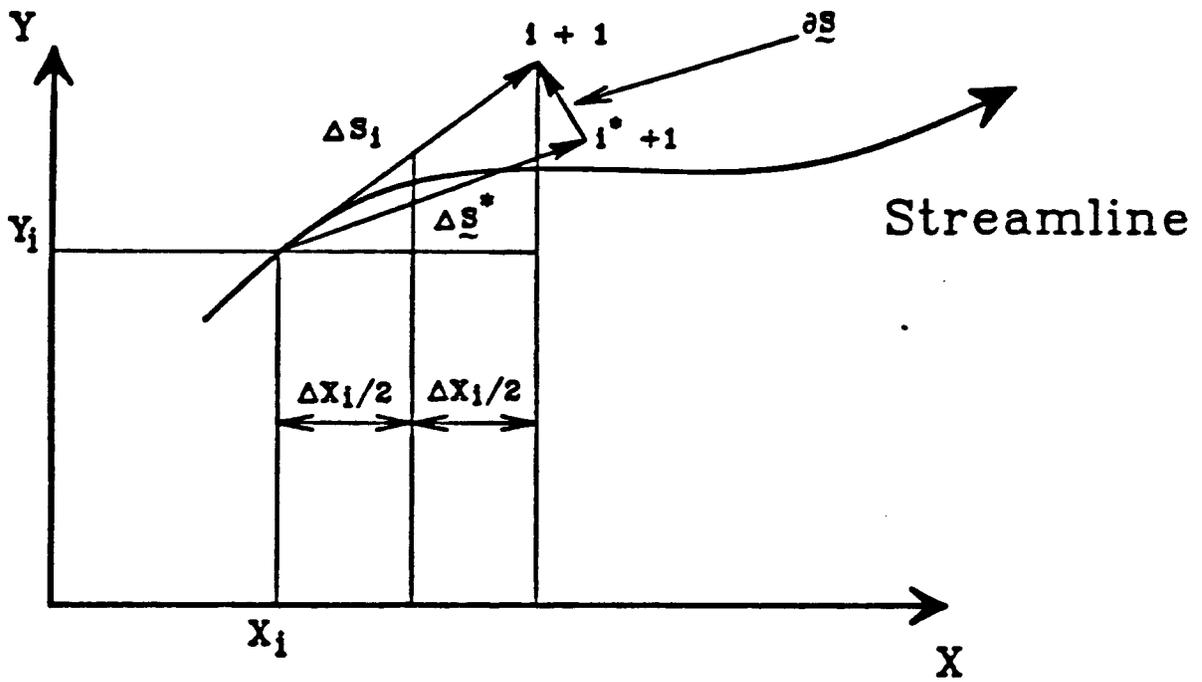
$$Y_{i+1} = Y_i + v_{i,y}\Delta t = Y_i + \Delta Y_i \tag{B. 44b}$$

where v_{ix} and v_{iy} are seepage velocity components evaluated at point i. The initial value of At is calculated from At $= \Delta \ell_{max}/|v|$, where $\Delta \ell_{max}$ is the maximum prescribed spatial step length and $|v|$ is the magnitude of the velocity at point i.

Next a modified velocity vector is computed. Its components are determined from

$$v_{i+\frac{1}{2},x} = v_x (x_i + \Delta x_i/2, y_i + \Delta y_i/2) \tag{B.45a}$$

$$v_{i+\frac{1}{2},y} = v_y (x_i + \Delta x_i/2, y_i + \Delta y_i/2) \tag{B.45b}$$

The modified velocity is then used to compute a corrected tentative position of the particle.

$$\overset{\bullet}{x}_{i+1} = x_i + v_{i+\frac{1}{2},x} \Delta t = x_i + \overset{\bullet}{\Delta x_i} \tag{B.46a}$$

$$\overset{\bullet}{y}_{i+1} = y_i + v_{i+\frac{1}{2},y} \Delta t = y_i + \overset{\bullet}{\Delta y_i} \tag{B.46b}$$

The next step is to check if the corrected particle position is sufficiently close to the previous predicted position. The checking is performed by evaluating the magnitude of incremental displacement vector $\partial \underline{s}$ (Figure B.5).

$$\partial \underline{s} = \Delta \underline{s}^* - \Delta \underline{s}_i \tag{B.47}$$

If $|\partial \underline{s}|/|\Delta \underline{s}|$ is greater than a prescribed tolerance, then the value of At is reduced by " and the calculation is repeated with the reduced time increment. The iteration is continued until the error is within the specified tolerance.

B.3.2 Time-Related Capture Zones

A time-related (transient) capture zone is constructed by MWCAP using a procedure similar to that used by RESSQC In essence, a series of water particles are placed at sequential locations along the perimeter of a small circle representing the well boundary. These particles are then allowed to move along their pathlines until the assigned travel time value is reached or until a physical or plotting boundary is encountered. The terminal point of each particle is saved in two storage vector arrays. Finally, the capture zone boundary is drawn by joining the particle terminal points in sequential order.

The algorithm in MWCAP is designed to circumvent the potential problem of an overly truncated capture zone that may occur using the simpler scheme of RESSQC (Figure B.6a). Note that in the RESSQC scheme, the initial particle locations are uniformly spaced along the well boundary. Consequently, one may need to use an excessive number of pathlines (streamlines) to obtain an accurate delineation of the capture zone for a situation where the travel time is large or the shape of the capture zone is elongated.

The improved scheme used in MWCAP is shown schematically in Figure B.6b; it utilizes the control feature (the stagnation point) of the capture zone boundary. First the location of each stagnation point is identified and then two controlling pathlines that make sharp turns near the stagnation points are traced (Figure B.6b). After their sharp turn, the points on these controlling pathlines are recordecd. Coordinates of the selected points and the stagnation point are stored in the vector arrays used to store coordinates of the terminal points of the standard regularly spaced pathlines. When all the points are joined in their sequential order, an accurate delineation of the transient capture-zone is obtained.

B.3.3 Hybrid Capture Zone

A hybrid capture zone is constructed by closing the steady-state capture zone with a time-related capping boundary (Figure B.7). For a specified value of travel time, the capping boundary is drawn by locating its control points (A, B and C) and passing a quadratic curve through these control points. Control point B is located by performing reverse particle tracking along the pathline emanating from the well and proceeding in the upstream direction of ambient flow. The radial distance from the center of the well to this control point is denoted by r. This radius is then used to locate the remaining control points (A and C). The algorithm for determining the coordinates of A and C is presented in the following paragraphs.

Since both points A and C arc tentative points on the dividing streamlines, their coordinates can be readily computed. For point A, one obtains (Figure B.7):

$$x = x_i + v_{ix} \Delta t = x_i + v_{ix} \frac{\Delta s}{v_i} \tag{B.48}$$

Figure B.6

Capture Zone Boundary Truncation Error That May Occur Using RESSQC (a)
and Improved Algorithm Used by MWCAP (b)

TRUNCATED PORTION OF CAPTURE ZONE

(a)

SELECTED POINTS ON
CONTROL PATHLINE

AMBIENT FLOW

y

CONTROL PATHLINE

x

CONTROL PATHLINE

STAGNATION POINT

STREAM BOUNDARY
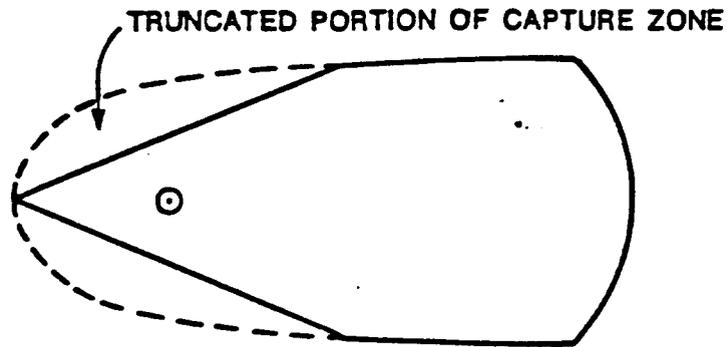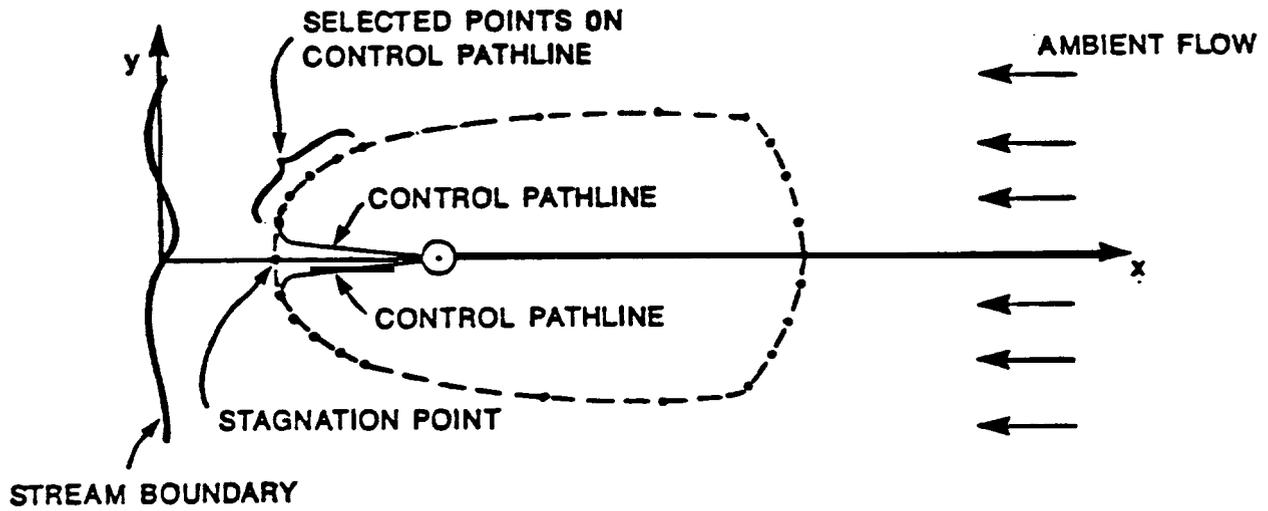
(b]

Figure B.7

Schematic Description of the Procedure Used to Locate the Capping
Boundary of a Hybrid Capture Zone
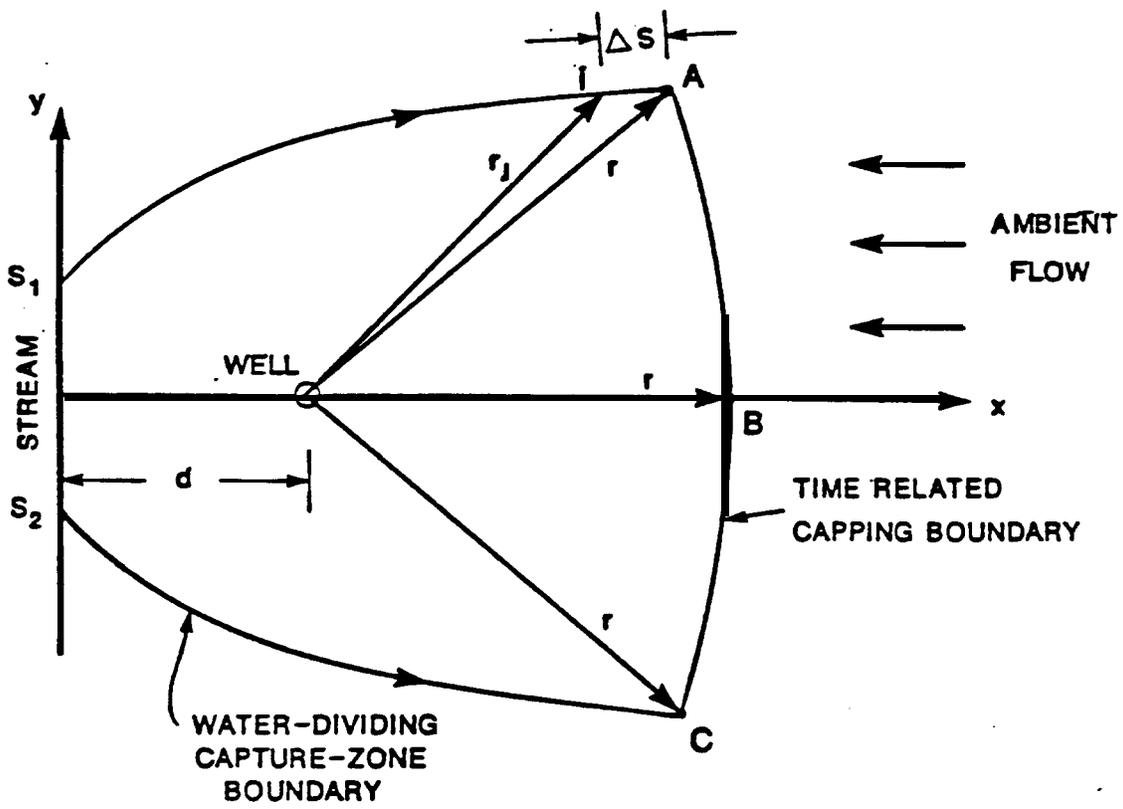
$$y = y_i + v_{iy} \Delta t = y_i + v_{iy} \frac{\Delta s}{v_i} \tag{B.49}$$

where v_{ix} and v_{iy} are seepage velocity components at point i (the previous point), v_i is the magnitude of the seepage velocity at i, and As is the incremental length along the streamline (distance between points A and i).

Let x_i^* be defined as $x_i^* = x_i - d$, where d is the distance from the stream to the pumping well. The prescribed radial distance from the well to point A may be expressed as

$$r^2 = [x_i^* + (\frac{v_{ix}}{v_i})]^2 + [y_i + (\frac{v_{iy}}{v_i}) \Delta s]^2 \tag{B.50}$$

which may be rearranged in the form

$$(\Delta s)^2 + 2\Delta x [\frac{x_i v_{ix}}{v_i} + \frac{y_i v_{iy}}{v_i}] - (r^2 - r_i^2) = 0 \tag{B. 51}$$

where

$$r_i^2 = (x_i^*)^2 + y^2 \tag{B.52}$$

Equation (B.51) can readily be solved for As. Since it is a quadratic equation, there are two roots. However, the feasible root must be a positive value. Once As is determined, the coordinates of point A can be obtained from equations (B.48) and (B.49), respectively. The coordinates of point C can be determined in a similar manner using the same calculation procedure.

B.4   Code Structure and Dimension Limits of MWCAP Module

Table B.1 is a list of program segments (subroutines) that compose the MWCAP module. A simplified flow chart for MWCAP is presented in Figure B.8. The dimension limits of MWCAP arrays are listed in Table B.2

Table B.1

Description of Subroutines That Compose The MWCAP Modlule
(Subroutines Listed In Alphabetical Order)

Subroutine Name	Description
AKTRAK	Traces steady-state capture zone boundaries using particle tracking. Particles are released from the stagnation point(s).
BKTRAK	Delineates streamlines using reverse particle tracking. Particles are released at the pumping well and are adsorbed at the stagnation point(s) or the aquifer boundary.
CHECK	Checks the accuracy of the projected particle location iteratively. If the error is too great, the time step (DT) is halved until the error is less than the tolerance (TOL) or the maximum number of iterations (NITMAX) is reached. Currently, TOL=0.05 and NITMAX=20.
CINTER	Performs quadratic finite element interpolation of coordinates of hybrid capture zone capping segment.
CZINTP	Traces bounding streamlines for time-related capture zone boundary.
MWCAP	Executes the MWCAP computational modules iteratively for I=1, NWELL where NWELL=number of wells for which capture zones are to be delineated. Initializes all problem-specific variables.
SIAQXA	Computes pumping well capture zones and swept zones using particle tracking for an areally infinite aquifer or a semi-infinite aquifer bounded by a gaining stream or a barrier boundary. Any angle of ambient flow toward the stream or barrier boundary may be specified.
STAGPT	Determines the coordinates of the stagnation points (XS,YS) and the bounding point (YA) of a stream capture zone. Applicable to aquifers with no boundary or a stream boundary only.
VSIAQ	Computes particle velocity components (VX,VY) as a function of location (X,Y) for an aquifer with no boundary, a stream boundary, or a barrier boundary. Ambient flow is at angle ALPHA measured counter-clockwise with respect to the negative x-axis.
XYTRAN	Converts any set of local coordinates to global coordinates based on the angle of rotation, ALPHA.

Figure B.8

Simplified Flow Chart MWCAP Module
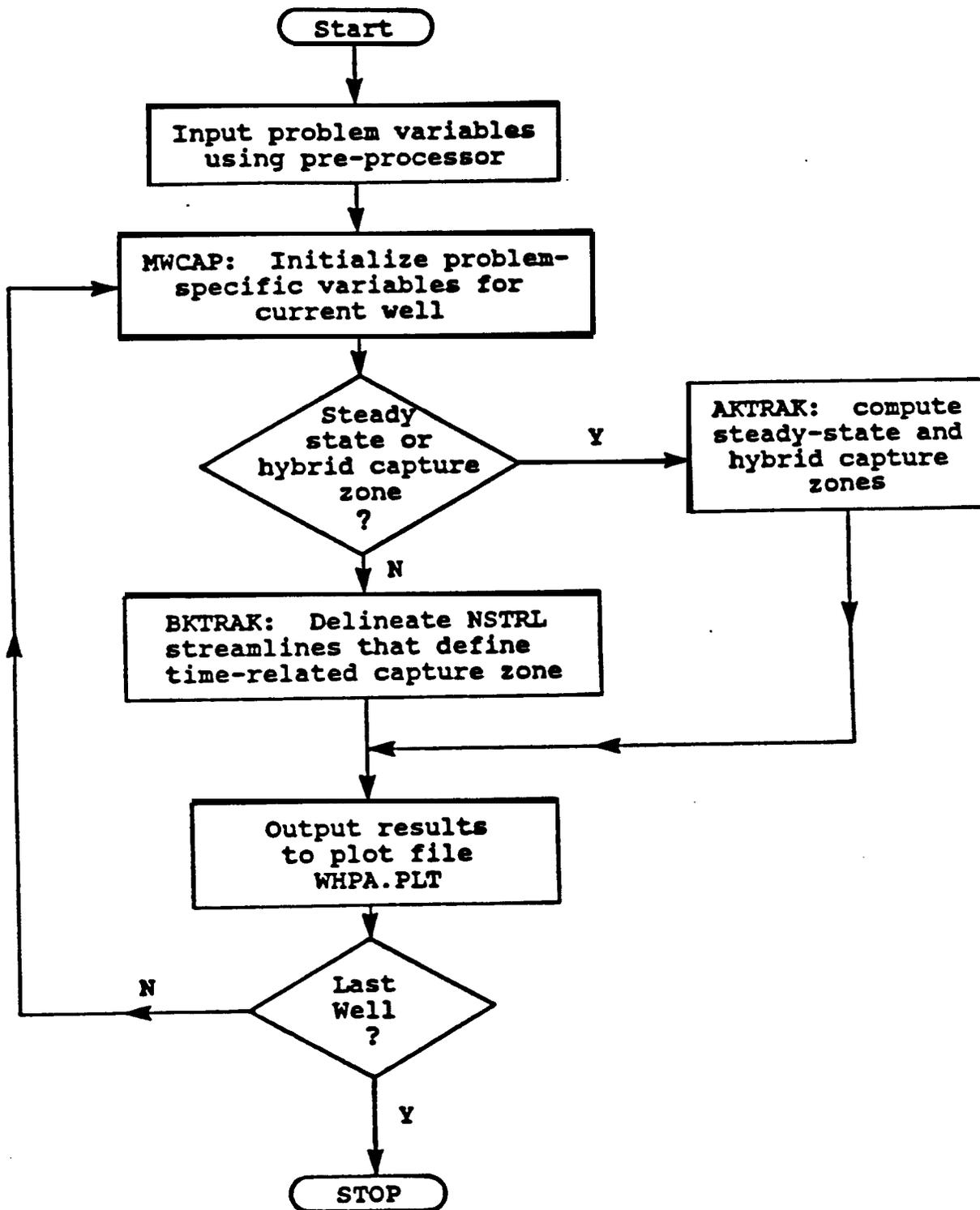
Table B.2

Dimension Limits For MWCAP Arrays

Array Name	Dimension	Description
ANGLE	50	Angle of ambient flow (0-360°)
DSW	50	Perpendicular distance from well to associated barrier or stream boundary (=0 if no boundary exists)
GRAD	50	Ambient hydraulic gradient
IBOUND	50	Array indicating the existence or non-existence of a boundary condition for a given well
ICZTYP	50	Array that specifies capture zone type (steady-state, time-related, or hybrid)
NPSTKP	4	Array to save the number of points retained for each streamline stored in the XSTLKP and YSTLKP arrays
NSTLIN	50	Number of streamlines to be delineated using reverse particle tracking
POR	50	Aquifer porosity
QAMB	50	Ambient rate of ground-water flow (equal to transmissivity * gradient)
QWELL	50	Well discharge
STRANG	500	Array of angles at which streamlines emanate from the pumping well
THETA	50	Orientation of boundary condition (0-360°)
THICK	50	Aquifer thickness

Table B.2 (continued)

Dimension Limits For MWCAP Arrays

Array Name	Dimension	Description
TMCZ	50	Time value associated with time-related capture zones
TRAN	50	Transmissivity
XCZ	(500,6)	x-coordinates for 6 possible capture zone boundary segments
XG	500	Global x-coordinates of current pathline
XL	500	Local x-coordinates of current pathline
XSTAG	2	x-coordinates of stagnation points
XSTL	500	x-coordinates of current streamline or capture zone boundary segment
XSTLKP	(500,4)	x-coordinates of special streamlines tracked close to stagnation points for time-related capture zone (maximum of 4 streamlines with 500 points per line)
XTFRNT	100	x-coordinates defining the boundary of a time-related capture zone
XTMCZ	40	x-coordinates of capping segment for hybrid capture zone
XWELL	50	x-coordinate of pumping well
YCZ	(500,6)	y-coordinates for 6 possible capture zone boundary segments
YG	500	Global y-coordinates of current pathline
YL	500	Local y-coordinates of current pathline

Table B.2 (continued)

Dimension Limits For MWCAP Arrays

Array Name	Dimension	Description
YSTAG	2	y-coordinates of stagnation points
YSTL	500	y-coordinates of current pathline or capture zone boundary segment
YSTLKP	(500,4)	y-coordinates of special pathlines tracked close to stagnation points for time-related capture zone (maximum of 4 streamlines with 500 points per line)
YTFRNT	100	y-coordinates defining the boundary of a time-related capture zone
YTMCZ	40	y-coordinates of capping segment for hybrid capture zone
YWELL	50	y-coordinate of pumping well

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Appendix C

Theoretical Development and Implementation of GPTRAC Module

C.1 Introduction

GPTRAC is a general-purpose particle tracking module designed to supplement the RESSQC and MWCAP modules. GPTRAC can handle site-specific conditions that may invalidate certain analytical assumptions mentioned in Appendices A and B. The GPTRAC module offers both semi-analytical and numerical options to perform time-related pathline and capture zone delineation. The semi-analytical option is resewed for cases involving homogeneous aquifers with relatively simple boundary conditions. It is designed to accommodate various aquifer types including confined and leaky semi-confined aquifers as well as unconfined aquifers subject to recharge or titration. Additionally, aquifers bounded on two or three sides by barrier and stream boundaries can be handled. The GPTRAC semi analytical approach also accounts for well interferences. The numerical option is intended for more complex situations involving heterogeneous and anisotropic aquifers subject to various boundary conditions. It utilizes velocity computational schemes that require knowledge of a steady-state area] distribution of hydraulic (piezometric) head in the aquifer. The required hydraulic head data can be determined using a numerical (finite element or finite difference) model to solve the governing partial differential equation of ground-water flow. Alternatively, the head data may be derived from field mapping of potentiometric or water level data.

C.2 Theoretical Background

In GPTRAC, computation of ground-water velocities is performed using two alternative approaches. The first approach is via analytical formulas derived from the potential function analytical solutions of well flow problems. This approach is used in the semi-analytical option for pathline declination. The second approach is via application of Dary's law to the hydraulic head distribution. This approach is used in the numerical option.

C.2.l Analytical Solutions Used in GPTRAC

The well flow analytical solution used in GPTRAC include those involving confined aquifers describedpreviously in Appendices A and B and three other solutions described in this section. The additional analytical velocity computation formulas correspond to the following situations:

- well flow in an unconfined aquifer with areal recharge

- well flow in a leaky semi-confined aquifer

- well flow in strip aquifers with two parallel boundaries

C.2.1.1 Unconfined Aquifer with Recharge

The analytical solutions presented in Appendices A and B are intended for nonleaky confined aquifer conditions. They may be inadequate for usc in some unconfined flow situations. An improved solution that accounts for the water-table and recharge conditions . of the unconfined system is presented in this section.

Consider a case involving a fully penetrating well pumping at a rate Q from an isotropic unconfined aquifer replenished by a constant rate of accretion N reaching the water table. The flow problem is nonlinear due to the variation of the aquifer saturated thickness. To linearize the problem, the following definition of the potential function,?, is introduced:

$$\phi = \frac{Kh^2}{2} \tag{C.l}$$

Where K is the hydraulic conductivity, and h is the hydraulic head above the base of the aquifer. By assuming that the flow in the aquifer is essentially horizontal (i.e., using the Dupuit assumptions), the governing equation for a steady-state case maybe expressed in the form:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + N = 0 \tag{C.2}$$

Equation (C.2) maybe solved for a general situation involving an areally infinite aquifer with a finite recharge applied over a circular: area bounded by $0 < r \leq R$. It is assumed that at r=R, the hydraulic head, h, and thus the saturated thickness approaches a maximum value of H. With these assumptions, the analytical solution to the problem may be expressed as:

$$\Phi = \Phi_o + \frac{Q}{2\pi} [(1 - \ln(R/r)] + \frac{N}{4}(R^2 - r^2) \qquad \textit{for } r \leq R \qquad (C.3a)$$

and

$$\Phi = \Phi_o \qquad \textit{for } r > R \qquad (C.3b)$$

where

$$r^2 = (x - x_w)^2 + (y - y_w)^2 \qquad (C.4a)$$

To ensure continuity of hydraulic gradient (i.e., zero gradient) at r=R the following condition is imposed:

$$Q = Q_{recharge}$$

thus

$$Q = \pi R^2 N$$

yielding

$$R = \left(\frac{Q}{\pi N}\right)^{1/2} \qquad (C.5)$$

The analytical solution given in (C.3a) and (C.3b) does not incorporate ambient flow. The effect of ambient flow may be taken into account in an approximate manner by superposition. This leads to the following modification of the solution:

$$\Phi = -Ub \ (x\cos\alpha + y\sin\alpha) +$$

$$\frac{Q_w}{2\pi} \ [1-\ln \ (R/r)] + \frac{N}{4} \ (R^2-r^2) \qquad for \ r \leq R \tag{C.6a}$$

$$\Phi = -Ub \ (x\cos\alpha + y\sin\alpha) + \Phi_o \qquad for \ r > R \tag{C.6b}$$

Where b is the ambient saturated thickness, assumed to correspond to H.

Once the distribution of the potential function is known the hydraulic head and Darcy velocity components can be determined from:

$$h = (2\Phi/K)^{(1/2)} \tag{C.7}$$

$$q_x = -K \ \frac{\partial h}{\partial x} = -\frac{1}{h} \left(\frac{\partial \Phi}{\partial x} \right) \tag{C.8a}$$

$$q_y = -K \ \frac{\partial h}{\partial y} = -\frac{1}{h} \left(\frac{\partial \Phi}{\partial y} \right) \tag{C.8b}$$

For the case involving a semi-infinite unconfined aquifer with a pumping well and a stream boundary, the problem can be solved by means of an imaginary recharging well. At some point (x,y) in the physical domain, the continution of the imaginary source to the potential field can be evaluated using the fundamental solution given in (C.3a) and (C.3b).

Similarly, the case involving a semi-infinite unconfined aquifer with a pumping well and a barrier boundary can also be handled using an imaginary pumping well.

C.2.1.2 Leaky Semi-Confined Aquifer

A leaky semi-confined aquifer is an aquifer that can lose or gain water through an underlying or overlying formation.When pumping takes place in such an aquifer, the resulting drawdown produces leakage into or out of the aquifer through the confining (semipervious) layers.

Consider a situation involving a uniform leaky confined aquifer with an overlying aquitard that is subject to constant head at the top boundary (Bear, 1979, p. 313). Assuming that flow in the aquifer is horizontal and leakage m the aquitard is vertical, a steady-state well flow potential solution ,Φ, for an areally infinite aquifer may be expressed as

$$\Phi_o - \Phi = \frac{Q}{2\pi b} K_o (r/\lambda) \tag{C.9}$$

where the potential function Φ is defined as $\Phi = Kh$

Φ_o is a reference potential at $r=\infty$, Q is the well pumping rate, b is the aquifer thickness, K_o is the modified Bessel function of the second kind and zero order, r is given by equation (C.4a) and λ is a leakage factor defined as

$$\lambda^2 = Kbb'/K' \tag{C.10}$$

where K is the hydraulic conductivity of the aquifer, and K' and b' are the hydraulic conductivity and thickness of the aquitard, respectively.

Equation (C.9) is a fundamental analytical solution that can be extended in the same manner as described previously (Appendices A and B) to account for ambient flow and the presence of a barrier or a stream boundary. The Darcy velocity components in the x and y directions can be obtained by differentiating equation (C.9) With respect to x and y, respectively.

C.2.1.3 Strip and Three-Sided Aquifers

A strip aquifer is defined as an aquifer bounded by two parallel sraight boundaries of infinite length. Four possible cases are of practical interest. The first and second cases correspond to an aquifier with two barrier boundarics and an aquifer with two stream boundaries. The third and fourth cases correspond to strip aquifers with a stream boundary on one side and a barrier boundary on the other side.

The analytical solution to steady-state well flow in a strip aquifer may be defined using the conformal mapping theory. For the case of strip aquifer with two barrier boundaries located at $y = O$ and $y = a$, the complex potential resulting from a well at (x_o, y_o) is given by

$$W = \frac{Q}{2\pi b} \left\{ \ln \left[\left(e^{\pi z/a} - e^{\pi z_o/a} \right) \left(e^{\pi z/a} - e^{\pi \bar{z}_o/a} \right) \right] - \frac{\pi}{a} z \right\} \tag{C.11}$$

where Q is the flow rate (> O for pumping and CO for recharge), b is the aquifer thickness and $\bar{Z}_o$ is the complex conjugate of Z_o. The velocity field can be obtained by differentiating the complex potential.

$$Re\left(\frac{\partial W}{\partial x}\right) = \frac{Q}{4ab}\left(\frac{\sinh\alpha}{\cosh\alpha - \cos\beta_-} + \frac{\sin\alpha}{\cosh\alpha - \cos\beta_+}\right) \tag{C.12}$$

and

$$Im\left(\frac{\partial W}{\partial x}\right) = -\frac{Q}{4ab}\left(\frac{\sin\beta_-}{\cosh\alpha - \cos\beta_-} + \frac{\sin\beta_+}{\cosh\alpha - \cos\beta_+}\right) \tag{C.13}$$

where

$$\alpha = \frac{\pi(x-x_o)}{a} \; ; \; \beta_- = \frac{\pi(y-y_o)}{a} \; ; \; \beta_+ = \frac{\pi(y+y_o)}{a}.$$

Similarly, a strip aquifer that is bounded by two stream boundaries at y=O and y=a can be mapped into a half plane with a stream boundary. The complex potential for this case is

$$W = \frac{Q}{2\pi b} \ln \left(\frac{e^{\pi z/a} - e^{\pi \bar{z}/a}}{e^{\pi z/a} - e^{\pi \tilde{z}/a}} \right) \tag{C.14}$$

and the gradient of the potential is

$$Re \left(\frac{\partial W}{\partial x} \right) = \frac{Q}{4ab} \left[\frac{e^{a} - \cos\beta_{-}}{\cosh a - \cos\beta_{-}} - \frac{e^{a} - \cos\beta_{+}}{\cosh a - \cos\beta_{-}} \right] \tag{C.15}$$

$$Im \left(\frac{\partial W}{\partial x} \right) = - \frac{Q}{4ab} \left[\frac{\sin\beta_{-}}{\cosh\alpha - \cos\beta_{-}} - \frac{\sin\beta_{+}}{\cosh\alpha - \cos\beta_{-}} \right] \tag{C.16}$$

where α, β_{-} and β_{+} are defied preciously.

Next, we consider a strip aquifer bounded by a barrier boundary at y=O and a stream boundary at y=a.   For this case the complex potential can be found using the theory of image wells. The complex potential is given by

$$W = \frac{Q}{2\pi b} \ln \left[\left(\frac{e^{\pi z/2a} - e^{\pi z_o/2a}}{e^{\pi z/2a} + e^{\pi z_o/2a}} \right) \left(\frac{e^{\pi z/2a} + e^{\pi \bar{z}_o/2a}}{e^{\pi z/2a} - e^{\pi \bar{z}_o/2a}} \right) \right] \tag{C.17}$$

and the gradient of the potential is

$$\frac{\partial W}{\partial x} = \frac{Q}{8ab}\left[\frac{e^\alpha - \cos\beta_-}{\cosh\alpha - \cos\beta_-} + \frac{e^\alpha + \cos\beta_+}{\cosh\alpha + \cos\beta_+}\right.$$

$$\left. - \frac{e^\alpha + \cos\beta_-}{\cosh\alpha + \cos\beta_-} + \frac{e^\alpha - \cos\beta_+}{\cosh\alpha - \cos\beta_+}\right] \tag{C.18}$$

$$\frac{\partial W}{\partial y} = -\frac{Q}{8ab}\left[\sin\beta_-\left(\frac{1}{\cosh\alpha - \cos\beta_-} + \frac{1}{\cosh\alpha + \cos\beta_-}\right)\right.$$

$$\left[-\sin\beta_+\left(\frac{1}{\cosh\alpha + \cos\beta_+} + \frac{1}{\cosh\alpha - \cos\beta_+}\right)\right] \tag{C.19}$$

where

$$\alpha = \frac{\pi(x - x_*)}{2a} \; ; \; \beta_- = \frac{\pi(y - y_*)}{2a} \; ; \; \beta_+ = \frac{\pi(y + y_*)}{2a}$$

The solution for a strip domain with a barrier at y=O and a stream at y=a can be found from the previous case using the following coordinate transformation:

$$x = x'$$
$$y = -y' + a \tag{C.20}$$

Thus, a solution at (x', y') in the z' plane can be obtained by using

$$x = x' \qquad x_o = x_o$$
$$y = -y' + a \qquad y_o = -y_o + a \tag{C.21}$$

in the solution (C.17)-(C.19). However, the sign of the y-velocity so obtained must be reversed to obtain a physically valid solution.

The analytical solutions of the four cases of strip aquifers can be readily extended to corresponding cases involving aquifers bounded on three sides by barrier boundaries, stream boundaries, or combinations of barrier and stream boundaries. The presence of a third boundary is handled in the usual manner by the use of image well theory. Treating the third boundary as a mirror, a discharging or recharging well may be introduced depending on whether the boundary is a barrier or stream boundary.

C.2.2 Darcy and Pathline Equations and Time Integration

Given an initial location (x_o, y_o) of the fluid particle, its pathline can be determined by integrating the following pair of differential equations:

$$\frac{dx}{dt} = v_x \tag{C.22}$$

$$\frac{dy}{dt} = v_y \tag{C.23}$$

where (x(t),y(t)) are coordinates of the pathline at time t.

In GPTRAC, the integration is performed using either an analytical or a numerical scheme. The appropriate scheme is selected automatically by the code. The analytical scheme, which yields an exact integration, is used wherever possible (i.e., when its limiting analytical assumptions are satisfied).

C.2.2.1 Darcy's Equations

Given a distribution of hydraulic (or piezometric) head in the aquifer, the components of Darcy velocity (specific flux) in the x and y directions may be obtained from

$$q_x = -K_{xx}\frac{\partial h}{\partial x} \tag{C.24}$$

$$q_y = -K_{yy}\frac{\partial h}{\partial y} \tag{C.25}$$

where K_{xx} and K_{yy} are the principal components of hydraulic conductivity along the x and y directions, respectively, and h is the hydraulic head The components of ground-water seepage velocity are given by

$$v_x = q_x/\theta \tag{C.26}$$

$$v_y = q_y/\theta \tag{C.27}$$

where θ is effective porosity of the aquifer.

Equations (C.26) - (C.27) are used in GPTRAC for the numerical computation of ground-water velocities. The distribution of hydraulic head is supplied to the code by a data file containing steady-state values of h at the nodal points of a rectangular grid. GPTRAC can accommodate both mesh-centered and block-centered grids. These two types of grids are illustrated in Figure Cl. The nodes are located at the intersections of grid lines for the mesh-centered grid, and at the centers of grid blocks for the block-centered grid.

C.2.2.2 Numerical Integration

The numerical integration scheme implemented into the code is an Euler predictor-corrector scheme with successive iterations to accommodate spatial variability of velocities and curvature of the flow path. This scheme is described in Appendix B.

Figure C.1

Rectangular Grids Used by GPTRAC Mesh-Centered Grid (a)
and Block-Centered Grid (b)
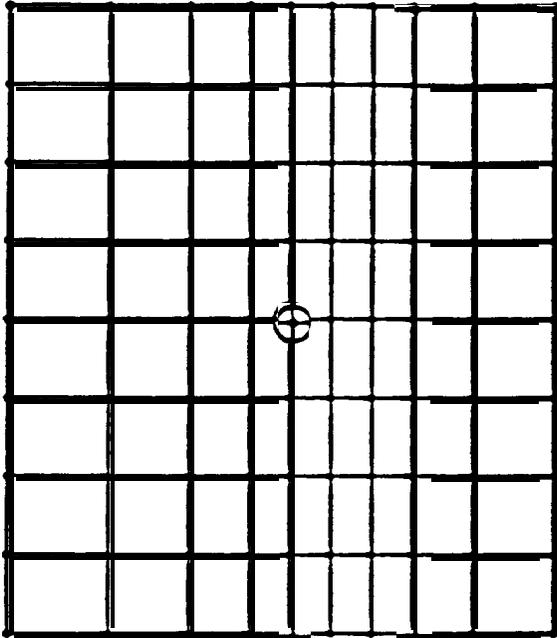
⊙ = Pumping Well

No. of nodes=90
No. of elements=72

(a)
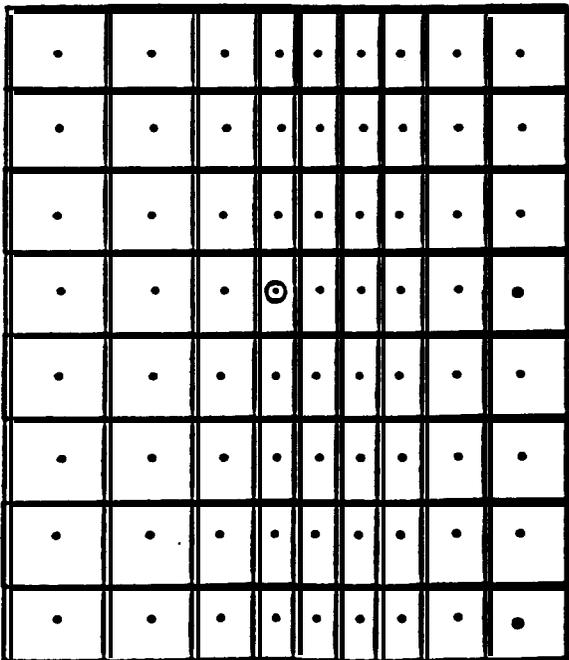
⊙ =Pumping Well

No. of nodes=72

No. of grid blocks=72

(b)

An alternative integration scheme that is applicable, but which is not used in GPTRAC is the fourth-order Runge-Kutta scheme. This scheme has been used without iterative corrections in a panicle tracking code called GWPATH (Shafer, 1987). It is based on the following Runge-Kutta formulas:

$$x(n+1) = x(n)+1/6\ [a_1+2a_2+2a_3+a_4] \tag{C.28}$$

$$x(n+1) = y(n)+1/6\ [b_1+2b_2+2b_3+b_4] \tag{C.29}$$

where (x(n),y(n)) are coordinates at the previous location of the particle, (x(n+l),y(n+l)) are coordinates at the new location, and

```
a₁ = Δt * f[x(n),y(n)]
b₁ = Δt * g[x(n),y(n)]
a₂ = Δt * f[x(n)+a₁/2,y(n)+b₁/2]
b₂ = Δt * g[x(n)+a₁/2,y(n))b₁/2]
a₃ = Δt * f[x(n)+a₂/2,y(n)+b₂/2]
b₃ = Δt * g[x(n)+a₂/2,y(n))b₂/2]
a₄ = Δt * f[x(n)+a₃,y(n)+b₃]
b₄ = Δt * g[x(n)+a₃,y(n)+b₃]
```

Equations (C.30) and (C.31) yield a higher order numerical approximation than the Euler integration formulas. However, it should be noted that the accuracy of the pathline delineation also depends on the manner in which time stepping is performed. Thus, the Euler scheme with iterative corrections and good control of time steps may be more accurate than the fourth-order Runge-Kutta scheme used without iterative corrections to control the time step size.

C.2.2.3 Analytical Integration

If a steady-state hydraulic head distribution is obtained using a numerical model, an efficient analytical integration scheme can be derived for those grid blocks (or rectangular elements) that do not contain the well nodes. Such a scheme has been successfully applied by Pollock (1988) to velocity fields obtained using the block-centered finite difference method to solve the ground-water flow equation. The scheme can also be adapted to the rectangular finite element solution of the ground-water equation. It is based on two key assumptions: (1) the x-velocity component v_x within a grid block or element is a linear

function of the x-coordinate and is independent of the y-coordinate, and (2) the y-velocity component V_y within the grid block or element is a linear function of the y-coordinate and is independent of x-coordinate. Via these assumptions, the principal velocity components inside the grid block can be expressed in the form (Figure C.2):

$$v_x = A_x(x-x_1)+v_{x1} \qquad\qquad (C.30a)$$

$$v_y = A_y(y-y_1)+v_{y1} \qquad\qquad (C.30b)$$

where A_x and A_y are constants that correspond to the components of the velocity gradient within the cell,

$$A_x = (v_{x2}-v_{x1})/\Delta x \qquad\qquad (C.31a)$$

$$A_y = (v_{y2}-v_{y1})/\Delta y \qquad\qquad (C.31b)$$

v_{x1} and v_{x2} are values of the x-velocity component at the edges of the block or element sides that are parallel to the y-direction, v_{y1} and v_{y2} are values of the y-velocity components that are parallel to the x-direction, and Δx and Δy are the dimensions of the block or element in the respective coordinate directions.

For each grid block or element, the representative (principal) values of the velocity components, v_{x1}, v_{x2}, v_{y1} and v_{y2}, are computed using a simple linear finite difference approximation for the head values at the block centers or element centroids. The centroidal values for finite element grid blocks are obtained by arithmetic averaging of head values at the comer nodes. Interlock or interelement conductivity values are obtained by harmonic averaging of individual block or element conductivities.

Linear interpolation of velocity components using equations (C.30) and (C.31) has two desirable properties. First, a continuous velocity vector field within each individual grid block (or element) that satisfies the differential equation of mass balance-everywhere within the block is produced. Second, an analytical solution of the pathline equations, (C.22) and (C.23), can be derived. The first property can be shown by substituting equations (C.30a), (C.30b), (C.31a) and (C.31b) into the following differential mass balance equation:

$$\frac{\partial}{\partial x}(bv_x) + \frac{\partial}{\partial y}(bv_y) = W \qquad\qquad (C.32)$$

Figure (C.2)

Principal Velocity Components of a Rectangular Grid Block or Element
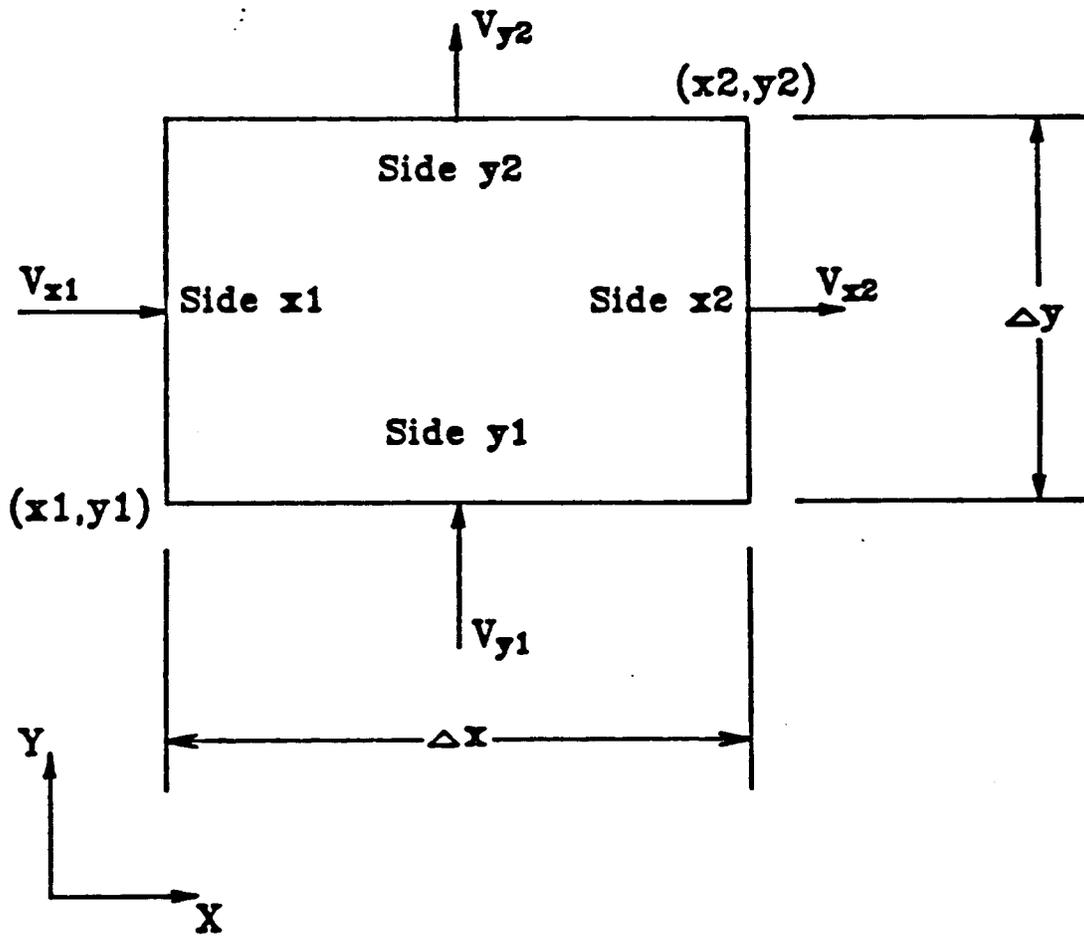
where b is the saturated thickness of aquifer, and W is the volumetric rate of recharge or discharge per unit surface area of aquifer. Assuming that b is constant over the grid block, equations (C.30a)-(C.31b) may be substituted into (C.32) to obtain

$$\frac{v_{x2}-v_{x1}}{\Delta x} + \frac{v_{y2}-v_{y1}}{\Delta y} = \frac{W}{b\Delta x\Delta y} \tag{C.33}$$

which is indeed the incremental form of the mass balance equation for a grid block or individual rectangular finite element.

Note that equation (C.33) is a good representation of (C.32) provided that any internal sources or sinks may be regarded as being uniformly distributed within the grid block or element. This is usually a valid assumption as long as the grid block does not contain a well node. For such a grid block the analytical equations describing the pathline of a given particle can be derived as described below.

Consider the situation depicted in Figure C.3, where a particle enters the block at point (x_p, y_p) and at time t_p. At a later time, \ the particle has moved along the pathline to point (x,y), which may be determined by integrating equations (C.22) and (C.23) using (C.30a) and (C.30b) to substitute for v_x and v_y as follows:

$$\int_{x_p}^{x}\frac{dx}{A_x x + B_x} = \int_{t_p}^{t}dt = t-t_p = \Delta t \tag{C.34a}$$

and

$$\int_{y_p}^{y}\frac{dy}{A_y y + B_y} = \int_{t_p}^{t}dt = \Delta t \tag{C.34b}$$

where B_x and B_y are defined as

$$B_x = v_{x1}-A_x x_1 \tag{C. 35a}$$

and

$$B_y = v_{y1}-A_y y_1 \tag{C. 35b}$$

Figure C.3
Schematic Representation of a Particle Path Through A Grid Block
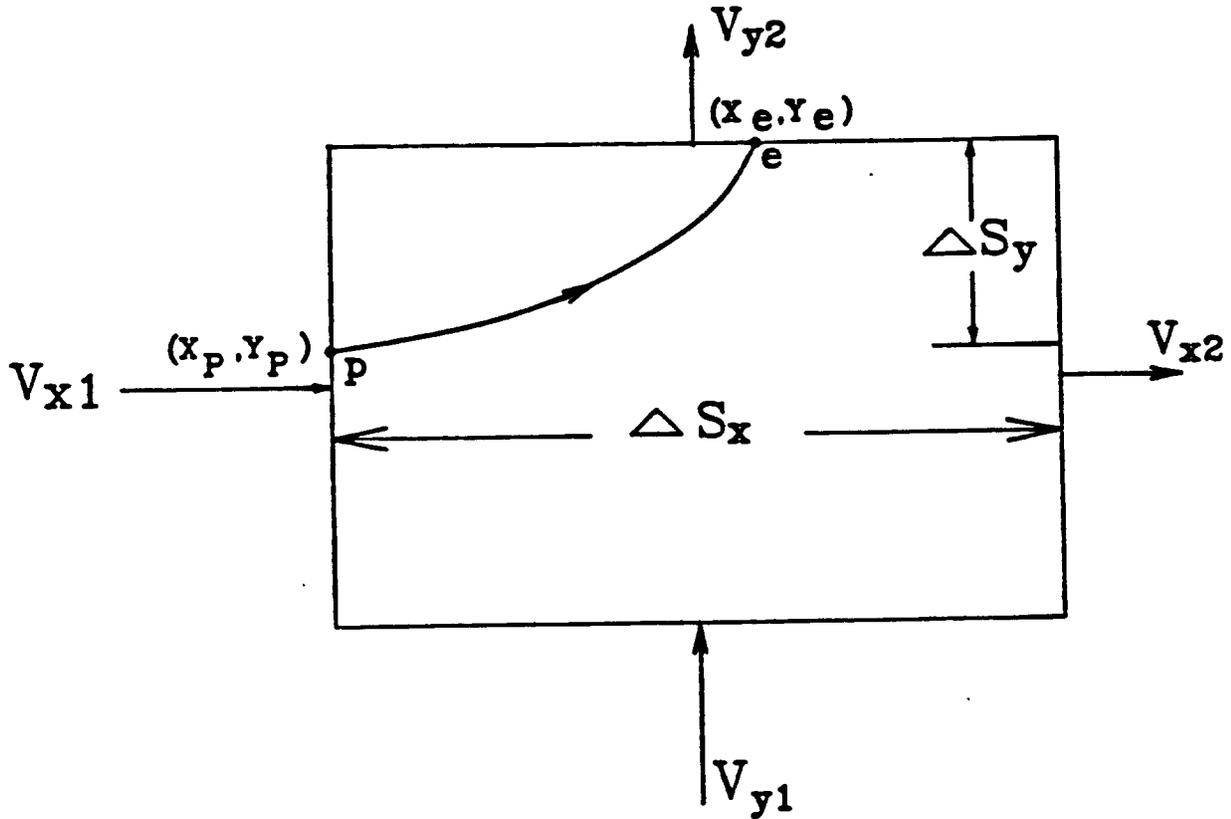
$\triangle S_x =$ X-distance travelled during time interval $\triangle t_x$

$\triangle S_y =$ Y-distance travelled during time interval $\triangle t_y$

The integrals in (C.34a) and (C.34b) can be evaluated to give

$$\ln[(A_x x + B_x)/(A_x x_p + B_x)] = A_x \Delta t \qquad \text{(C. 36a)}$$

and

$$\ln[(A_y y + B_y)/(A_y y_p + B_y)] = A_y \Delta t \qquad \text{(C.36b)}$$

which may be arranged in the form:

$$x = x_1 + \frac{1}{A_x} [v_{xp} \exp(A_x \Delta t) - v_{x1}] \qquad \text{(C.37a)}$$

$$y = y_1 + \frac{1}{A_y} [v_{yp} \exp(A_y \Delta t) - v_{y1}] \qquad \textbf{(C.37b)}$$

As shown in Figure C.3, the particle leaves the grid block at an exit point (X_e, Y_e). The coordinates of the exit point can be determined from (C.37a) and (C.37b), provided that the time increment, Δt_e, required by the particle to travel from point p to point e is known. The value of Δt_e can be determined as follows. First consider the time increment,

Δt_x, that would be required by the particle to travel from point P to side x_2 of the grid block. This is obtained using equation (C.36a), which maybe rewritten as:

$$\Delta t_x = \frac{1}{A_x} \ln[A_x x_2 + B_x)/(A_x x_p + B_x)]$$

or

$$\Delta t_x = \frac{1}{A_x} \ln[v_{x2}/v_{xp}] \qquad\qquad (C.38a)$$

Similarly, the time increment that would be required by the particle to travel from point p to side y_2 of the grid block is given by

$$\Delta t_y = \frac{1}{A_y} \ln[v_{y2}/v_{yp}] \qquad\qquad (C.\,38b)$$

If Δt_x is less than Δt_y, the particle will exit at side x_2. Conversely, if Δt_y is less than Δt_x, the particle will exit at side y_2. A third possibility is that $\Delta t_x = \Delta t_y$, in which case the particle will exit the grid block at the corner where sides x_2 and y_2 intersect. In any case, the general expression for Δt_e is given by

$$\Delta t_e = \min(\Delta t_x, \Delta t_y) \qquad\qquad (C.39)$$

where Δt_x and Δt_y are determined from (C.38a) and (C.38b) respectively.

Knowing Δt_e, the coordinates (x_e, y_e) of the exit point can be determined from

$$x_e = x_1 + \frac{1}{A_x} [v_{xp}\exp(A_x \Delta t_e) - v_{x1}] \qquad\qquad (C.\,40a)$$

$$y_e = y_1 + \frac{1}{A_y} [v_{yp}\exp(A_y \Delta t_e) - v_{y1}] \qquad\qquad (C.40b)$$

Once the exit point is known, intermediate points of the pathline within the grid block are easily determined by substituting values of Δt that are within the range $0 < \Delta t < \Delta t_e$.

The analytical procedure presented is based on the assumption that neither A_x nor A_y is zero (i.e. the velocity gradient of the grid block is non zero). In the case where $A_x = 0$, the x-velocity component is constant in the grid block and Δt_x and x_e are obtained from the simplified relations

$$\Delta t_x = (x_2 - x_p)/v_{x1} \tag{C.41a}$$

and

$$x_e = x_p + v_{x1}\Delta t_e \tag{C.41b}$$

Similarly, if $A_y = 0$, then Δt_y and y_e are given by

$$\Delta t_y = (y_2 - y_p)/v_{y1} \tag{C.42a}$$

and

$$y_e = y_p + v_{y1}\Delta t_e \tag{C.42b}$$

The preceding example focused on a specific velocity pattern where the sense of direction of all velocity components is positive. Other possible scenarios must be considered as well. For each coordinate, there are 4 possible velocity patterns. Figure C.4 illustrates the possible patterns for the x-velocity components. Pattern 2 (IPATX = 2) has been dealt with. Pattern 1 (IPATX = 1) is simply the reverse of pattern 2. In this case the particle enters the grid block at side X_2 and exits at side x_1. Pattern 3 (IPATX $=$ 3) is an interesting one. In this case, a local flow divide exists where $V_x = 0$. If a particle resides in the grid block and its V_{xp} is greater than 0, then it will exit the grid block at side x_2. On the other hand, if V_{xp} is less than zero the particle will exit at side x_1. The fourth pattern (IPATX= 4) also requires special attention. In this case the particle can not leave the grid block in the x-direction. When this condition exists, a flag is set to indicate the possibility of particle entrapment in the grid block. Particle entrapment will occur if a second flag is raised for the velocity component in the y-direction. This indicates that a strong sink (pumping well) is present within the grid block and that the particle is captured by the sink. The equivalent 4 patterns of velocity components in the y-direction are treated in the same manner as the corresponding patterns in the x-direction.

Figure C.4

Possible Patterns of the Principal Velocity Components Along the x-Direction

(a) IPATX=1

V_{X1} — V_{X2}

(b) IPATX=2

V_{X1} — V_{X2}

(c) IPATX=3, FLOW DIVIDE, $V_x = 0$

V_{X1} — V_{X2}

(d) IPATX=4

V_{X1} — V_{X2}
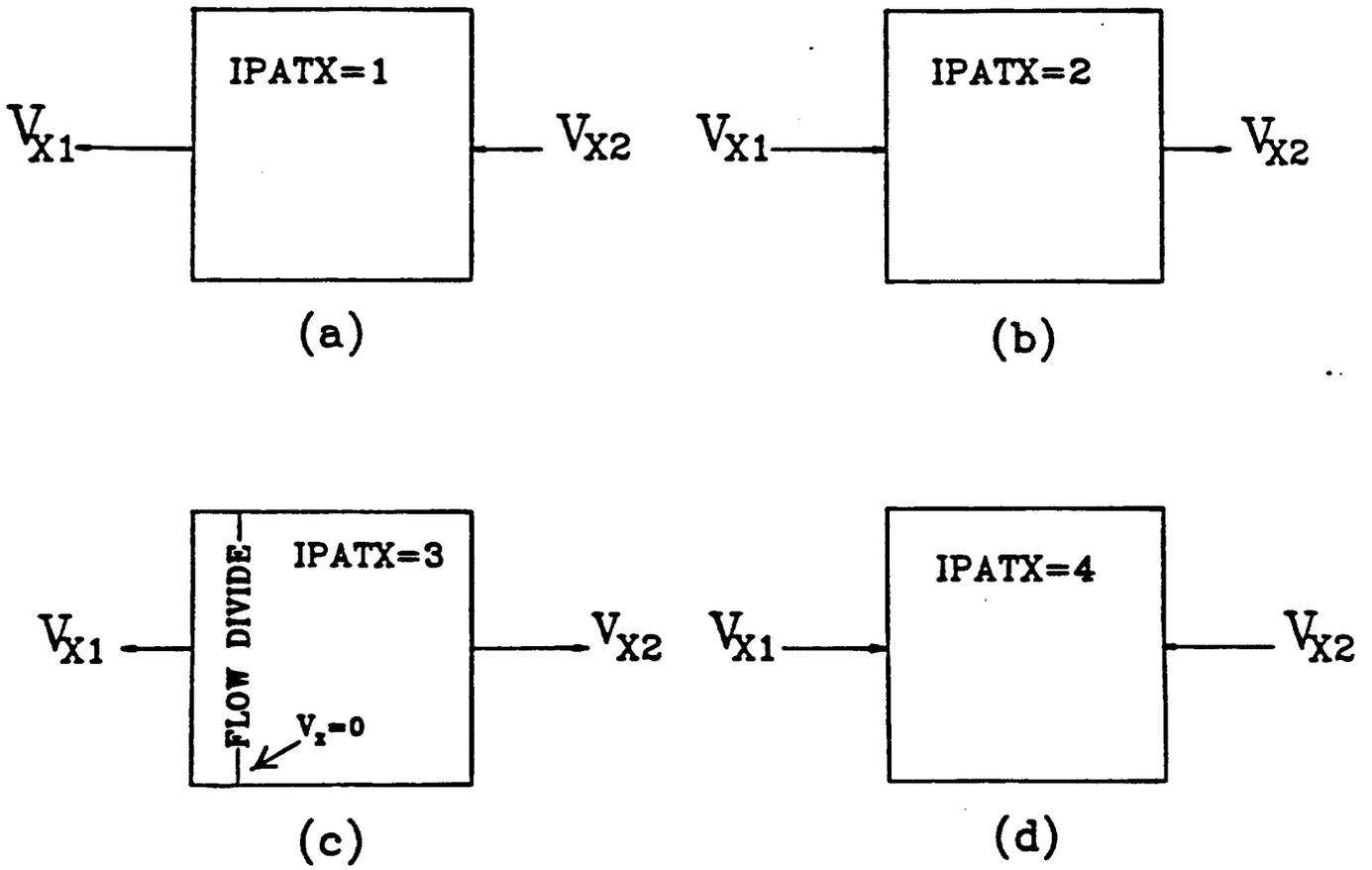
C.3 Numerical Implementation

The delineation of water-particle pathlines and well-capture zones is performed in GPTRAC using two approaches, referred to as the semi-analytical and the numerical options. The semi-analytical option uses analytical formulas to compute ground-water velocities at a series of points along each pathline. Each pathline is traced using the numerical integration procedure described in Appendix B.

In the numerical option, ground-water velocities are determined numerically from a steady-state head distribution that is supplied to the code via an input data file. The computational procedure is then applied in three major steps: (1) generation of a rectangular grid (2) computation of the principal velocity components, v_{x1}, v_{x2}, v_{y1} and v_{y2} at sides xl, x2, yl and y2 of each grid block and (3) tracking of particle pathlines using analytical integration or numerical integration when analytical integration is inappropriate. Each of these steps is described in detail in the next section.

C.3.1 Grid Generation

The generation of the rectangular grid required in the numerical option is performed automatically by GPTRAC using simple control parameters specified by the user. The two key parameters are NROWS and NCOLS, which denote the number of row grid lines parallel to the x-axis, and the number column grid lines parallel to the y-axis, respectively. Figure C.1 illustrates a sample rectangular finite element grid and a sample block-centered finite difference grid each with NROWS=9 and NCOLS=1O. Locations of discharging and recharging wells are assumed to correspond to nodal locations.

In the case of the finite element grid (Figure C.la), the nodes correspond to points of intersection of row- and column-grid lines, and each rectangular element is surrounded by 4 nodes. Thus the grid consists of 90 nodes and 72 elements, and a pumping well is represented by an internal node shared by 4 elements. In the case of the block-centered finite difference grid (Figure C.lb), the nodes are located at the centers of rectangular grid blocks. Thus the grid consists of 72 nodes and 72 grid blocks, and a pumping well is represented by a node associated with one grid block.

In addition to the above two cases, GPTRAC also admits the use of a mesh-centered finite difference grid in determining the hydraulic head distribution. This case is treated by GPTRAC in the same manner as the rectangular finite element grid.

In any case, the user must specify what type of grid has been used to determine the hydraulic head data required for velocity computation (This is done through an input control parameter, IHDATA). Head values need to be input sequentially starting from the first through the last nodes. For the sake of convenience, the code admits either a column-wise or row-wise node numbering scheme to be used for the input of head data. Grid spacings in both directions may be uniform or nonuniform. The spacings of a uniform grid are determined automatically by the code via a specification of the minimum and maximum values of the x and y coordinates. The spacings of a nonuniform grid are computed by the code once the user has input the x-coordinates of the column grid lines and the y-coordinates of the row grid lines.

The numerical option of GPTRAC can delineate pathlines in homogeneous or inhomogeneous aquifers. If the aquifer is inhomogeneous a zonal representation of the material properties is used (Figure C.5). Each zone is represented by a rectangular subdomain and assigned one set of hydraulic properties. A subdomain overlay technique (block overlay) is used to identify material zonal numbers for the individual blocks in the grid. The largest zone should always be defined first (most commonly the first zone will be the entire modeled domain), and then the smaller zones are subsequently "overlayed" upon the fist zone. Portions of the grid for which there is no zone specified will be assigned hydraulic property values used for the first zone. Each zone is identified by the coordinates of its bottom-left and top-right corners. Using this information GPTRAC identifies the material zonal numbers for each element or grid block by checking its centroidal location.

C.3.2 Velocity Computation

The semi-analytical option for pathline delineation in GPTRAC computes the ground-water seepage velocity components using analytical formulas based on the potential function analytical solution of the steady-state well flow problem. This option is limited to cases involving a homogeneous aquifer. However, the aquifer may be bounded on one or two sides by a stream and/or barrier boundary condition. The available cases include: (1) wells in an areally infinite aquifer, (2) wells in a semi-infinite aquifer with a stream boundary, and (3) wells in a semi-infinite aquifer with a barrier boundary. Each boundary is assumed to fully penetrate the aquifer. In each case, GPTRAC computes values of velocity components at a series of points along each pathline. Each pathline is traced using the numerical integration procedure described in section C.2.2.2.

Figure C.5

Zonal Representation of an Inhomogeneous Aquifer
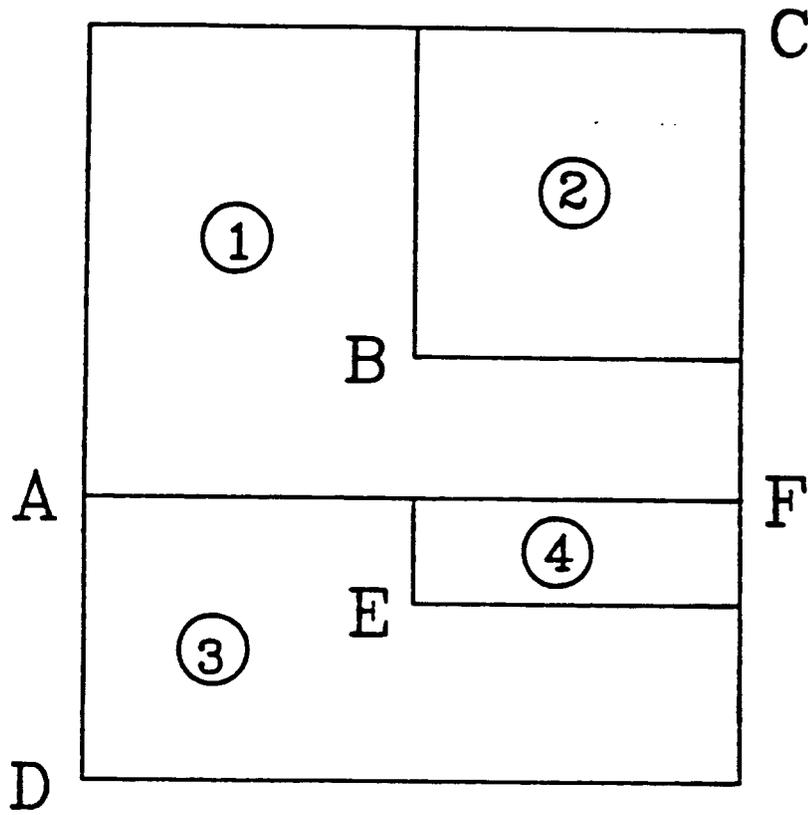
Zone	Bottom Left Corner	Top Right Corner
1	A	C
2	B	C
3	D	F
4	E	F

In the numerical option for pathline delineatio~ the velocity computation is performed using values of hydraulic head at the centers of grid blocks or the centroids of rectangular finite elements. In the latter case, the head value at the element centroid is determined by averaging the head values at the four comer nodes.

For a typical grid block or element I, the principal velocity components v_{x1}, v_{x2}, v_{y1} and v_{y2} are computed as follows (Figure C6a):

$$v_{x1} = -K_{xIW}(h_W-h_I)/\Delta x_{IW} \tag{C.43a}$$

$$v_{x2} = -K_{xIE}(h_E-h_I)/\Delta x_{IE} \tag{C.43b}$$

$$v_{y1} = -K_{yIS}(h_S-h_I)/\Delta y_{IS} \tag{C.43C}$$

$$v_{y2} = -K_{yIN}(h_N-h_I)/\Delta y_{IN} \tag{C.43d}$$

where
$$\Delta x_{IW} = x_W-x_I \ , \ \Delta x_{IE} = x_E-x_I \ ,$$
$$\Delta y_{IS} = y_S-y_I \ , \ \Delta y_{IN} = y_N-y_I \ ,$$

and K_{xIW}, K_{xIE}, K_{yIS} and K_{yIN} are harmonically averaged effective seepage conductivities between blocks in the west, east, south and north directions respectively. K_{xIW} and K_{xIE} are given by

$$K_{xIW} = \frac{K_{xI}K_{xW}(\Delta x_I+\Delta x_W)}{K_{xI}\Delta x_W+K_{xW}\Delta x_I} \tag{C. 44a}$$

$$K_{xIE} = \frac{K_{xI}K_{xE}(\Delta x_I+\Delta x_E)}{K_{xI}\Delta x_E+K_{xE}\Delta x_I} \tag{C.44b}$$

where &l, K_{xW} and K_{xE} are seepage conductives for grid blocks I, W and E, respectively. K_{yIS} and K_{yIN} are defined in a similar manner.

If the grid used corresponds to a finite element grid, velocity component values are also determined at the element centroids. The centroidal values of the velocity components are desirable for those elements that share well nodes for which pathline computation is performed using the numerical integration approach. The formulas for computing the centroidal velocity components of a typical element e (Figure C.6b) are:

Figure C.6

Notation Used In Velocity Computation For (a) Grid Block i, and (b) Element e

(a)

(b)
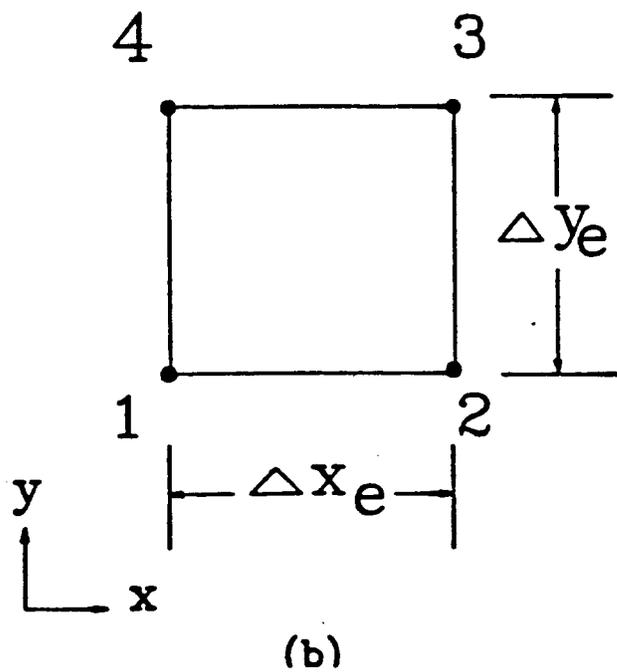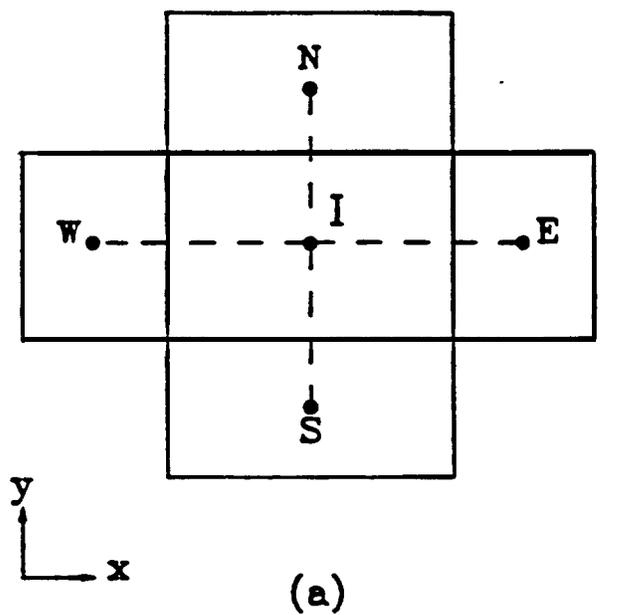
$$\bar{v}_x = -K_{xe}(h_2+h_3-h_1-h_4)/2\Delta x_e \tag{C.45a}$$

$$\bar{v}_y = -K_{ye}(h_3+h_4-h_1-h_2)/2\Delta y_e \tag{C.45b}$$

Where K_{xe} and K_{ye} are element seepage conductivities in the x and y direction respectively, and Δx_e and Δy_e are the x and y dimensions of the element.

C.3.3 Pathline and Capture Zone Delineation Procedure

GPTRAC delineates the pathline of a given particle using either the forward or reverse tracking method. Starting from the initial particle location the code uses analytical or numerical integration to determine successive locations of the particle at increasing time values. The pathline computation continues until one of several termination criteria is met. These criteria include: (1) checking to determine if the assigned value of travel time has been exceeded, (2) checking for boundaries of the flow region or plotting boundary limits, (3) checking if a stagnation point has been encountered and (4) checking for particle entrapment by a well.

When the particle enters a grid block or element having a well node, a series of checks are made to determine if the panicle will be intercepted by the well. Either pumping or injection wells are considered in the termination criterion depending upon whether forward or reverse tracking is being performed.

If a block-centered finite difference grid is used, the pattern of principal velocity components of the well-node block is first identified by checking values of IPATX and IPATY, referred to in Figure C.4 and Section C.2.2.3. If both IPATX and IPATY are equal to 4, then the particle is entrapped in the grid block and its terminal point is at the well node location.

If a rectangular finite element grid is used, the algorithm depicted in Figure C.7 provides an efficient way to determine well interception of a fluid particle. GPTRAC employs this algorithm in conjunction with a numerical integration and finite element interpolation scheme.   During any particular time step, the distance from the previous location, P_{n-1}, to the current location, P_n, is compared with the distance from the same previous location to the next location P_{n+1} (Figure C.7). If the distance from P_{n-1} to p_{n+1} is less than the distance from P_{n+1} to P_n, a flag is raised to indicate that a turning or reversal in the direction of flow of 90 degrees or more has probably occurred. Next, a

Figure C.7

**Algorithm To Determine If A Particle Has Been Intercepted
By A Nearby Well; (a) Raise Flag and (b) Continue**

$abs(p_{a-1}\ p_{a+1}) < abs(p_{a-1}\ p_a)$; raise flag

(a)
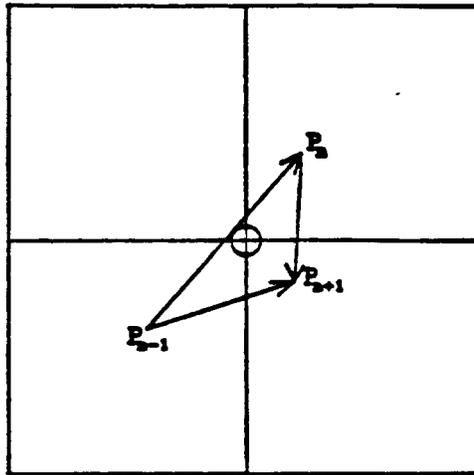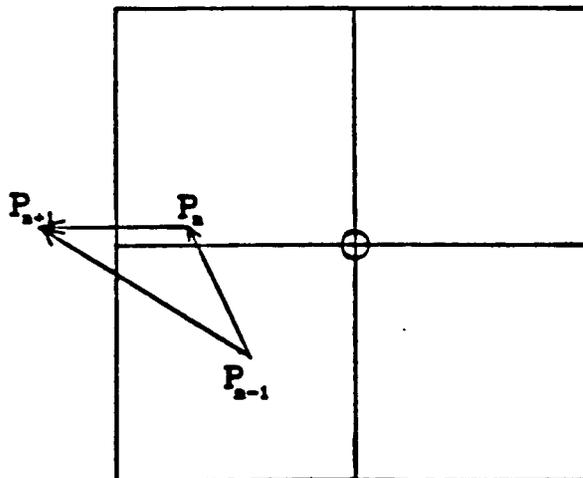
$abs(P_{a-1}\ P_{a+1}) > abs(p_{a-1}\ p_a)$; continue

(b)

second check is made to detemine if the element where the particle currently resides shares a well node with other neighboring elements.   If so, identification of the well is made to ensure that it is the correct type (pumping well for forward tracking and injection well for reverse tracking). If this check is positive, iterative projections of particle positions continue with successive reductions of time step (1/2 reduction each time) until the tentative position of the particle is sufficiently close to the well. At this point the terminal position of the particle pathline is taken to be the well location, and the pathline computation for that particle is completed.

If pumping wells exist GPTRAC allows the user to select an option to delineate the capture zone of any individual well using the reverse pathline delineation technique. First an effective radius of the well node (R_w) is estimated. If the velocity field is determined analytically, the following formula is used:

$$R_w = 0.0025*Min(XL,YL)$$ (C.46)

where XL and YL are the x and y plotting dimensions of the flow domain.

If the velocity field is determined using gridded head data the following formula is used:

$$R_w = f(A_I/\pi)^-$$ (C.47)

where A_I is the effective grid area covered by node I, assumed to be the well node, and f is a factor set equal to 1 if a block-centered finite difference grid is used and equal to 0.5 if a rectangular finite element grid is used.

Having determined the effective radius, the next step is to place a series of particles along the circular boundary of the pumping well node and perform reverse pathline tracking for each particle (Figure C.8). The number of particles released may be specified by the user - the default number is 20. The reverse pathline tracking starts at an initial time value, to, and finishes at the specified value of travel time, T. The initial time value corresponds to the time taken by the fluid particle to move from its location at the circular boundary to the well node. Assuming radial flow within the circular region, the value oft. is determined from

$$t_o = \pi R_w^2 b/Q$$ (C.48)

where Q is the pumping rate of the well, and b is the aquifer thickness.

FigureC.8

Capture Zone Delineation By Reverse Pathline Tracking
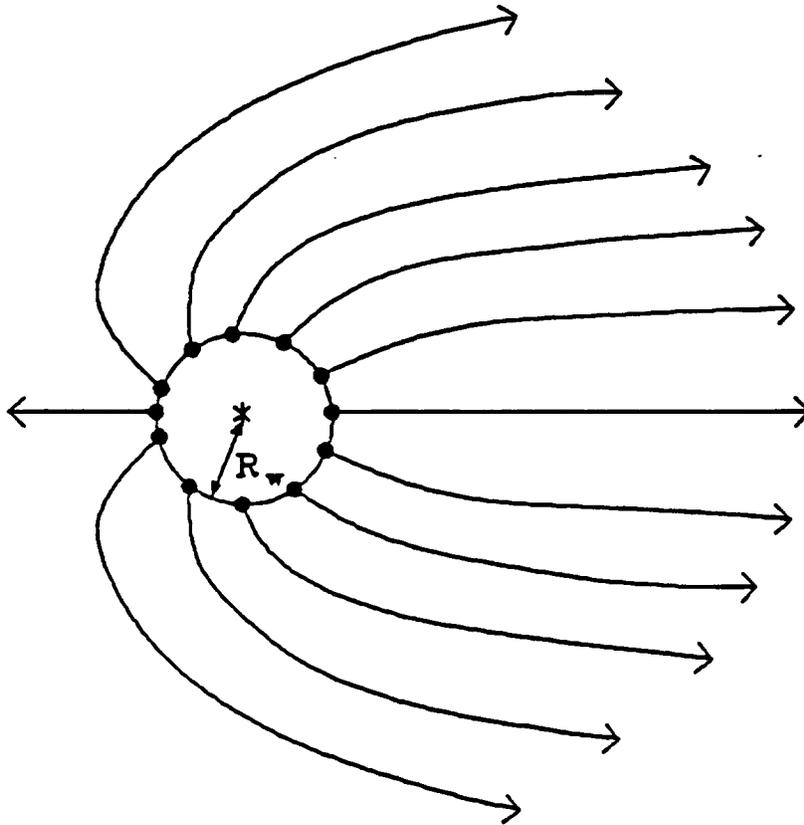
LEGEND

＊   WELL LOCATION

_____ REVERSE PATH LINE

●   INITIAL PARTICLE LOCATION

〉   TERMINAL POINT

C.3.4 Finite Element Interpolation of Velocities

When a finite element grid is used pathlines passing through elements that share a well node are computed by numerical integration. The velocity components inside such elements are determined using a simple one dimensional, quadratic interpolation scheme. The interpolation formulas for this scheme may be expressed as follows:

$$V_x = V_{x1} N_1(\xi) + V_{x2} N_2(\xi) + \bar{V}_x N_3(\xi) \tag{C.49a}$$

$$V_y = V_{y1} N_1(\eta) + V_{y2} N_2(\eta) + \bar{V}_y N_3(\eta) \tag{C.49b}$$

where V_{x1}, V_{x2}, V_{y1} and V_{y2} are the principal side velocity components of the element and $\bar{V}_x$ and $\bar{V}_y$ are the centroidal velocity components, N_1, N_2 and N_3 are one-dimensional, quadratic finite element basis functions, and ξ and η are dimensionless isoparametric coordinates defined as

$$\xi = 2(x-x_1)/(x_2-x_1)-1 \tag{C.50a}$$

$$\eta = 2(y-y_1)/(y_2-y_1)-1 \tag{C.50b}$$

The general expressions for N_1, N_2 and N_3 are given by

$$N_1(\psi) = -\psi(1-\psi)/2 \tag{C.51a}$$

$$N_2(\psi) = 1-N_1-N_2 \tag{C.51b}$$

$$N_3(\psi) = 1-\psi^2 \tag{C.51C}$$

where $\psi = \xi$ or η.

C.4 Code Structure and Dimension Limits of GPTRAC Module

Table C.1 is a list of program segments (subroutines) that compose the GPTRAC module. A simplified flow chart for GPTRAC is presented in Figure C.9. The dimension limits of the GPTRAC arrays are listed in Table C.2.

Table C.1

Description Of Key Subroutines In GPTRAC Module
(Subroutines Listed In Alphabetical Order)

Subroutine Name	Description
CPZONE	Determines time-related capture zone boundary for pumping wells.
DTCOMP	Computes the required time step for a particle to travel from its current location to an exit point at an edge of the rectangular grid block.
ECHO1	Echoes input parameters to default output file GPTRAC.OUT.
ELPROP	Identifies the material zone associated with each finite element or finite difference grid block.
FRPATH	Sets up the loop for forward or reverse pathline tracking.
GPTRAC	Execution supervisor for the grid generation, capture zone delineation, and forward and reverse particle tracking modules in GPTRAC.
GRIDGN	Generates a rectangular grid for pathline computation.
HEDCTR	Computes the nodal values of hydraulic head at the centroids of rectangular elements.
HLTCHK	Determines if pathline termination should occur due to presence of flow domain boundary or exceedence of simulation time.
PCHECK	Performs pathline computation using the Euler iterative predictor-corrector algorithm for numerical integration.
PLIDEN	Identifies the rectangular element in which the particle currently resides.
PTRACK	Performs forward or reverse pathline tracking, using analytical or numerical integration.

Table C.1 (continued)

Description Of Key Subroutines In GPTRAC Module
(Subroutines-Listed In Alphabetical Order)

Subroutine Name	Description
PTRAM	Performs pathline computation using the analytical integration algorithm.
SWITCH	Switches the node numbering of input head values from row-wise to column-wise.
VCALBL	Computes the principal velocity components of each rectangular grid block or element, and identifies the velocity pattern.
VINTQ	Computes values of velocity components at a point inside a rectangular grid block or element using quadratic interpolation.
VREVRS	Reverses the signs of velocity components for reverse pathline tracking.
WFANS	Computes the analytical steady-state flow solution in a well field subject to ambient ground-water flow.
WNIDEN	Identifies the sequential node numbers corresponding to the specified well locations.

Figure C.9

Simplified Flow Chart For GPTRAC Module
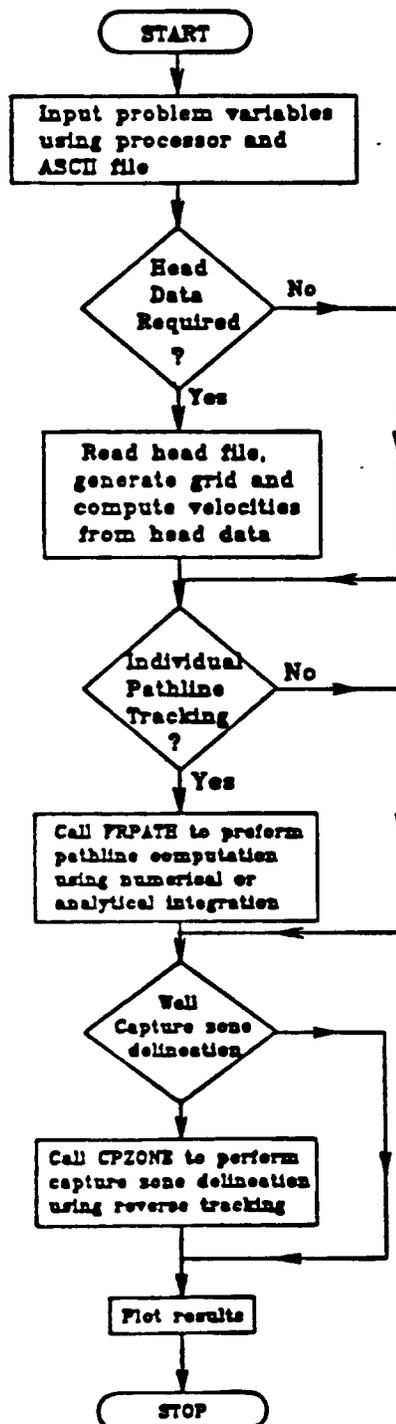
Table C.2

Dimension Limits Of Key Array Variables Used In GPTRAC

Array Name	Dimension	Description
AXKEEP	2916	Linear velocity interpolation coefficient for x-direction for each grid block
AYKEEP	2916	Linear velocity interpolation coefficient for y-direction for each grid block
BZO	200	Aquifer thickness for each zone
CONXZO	200	Hydraulic conductivity in the x-direction (K_{xx}) for each zone
CONYZO	200	Hydraulic conductivity in the y-direction (K_{yy}) for each zone
CORD	(3025,2)	x and y nodal point coordinates
ETASTO	4	Gauss-Legendre quadrature points
FSTART	(40,2)	x and y coordinates for starting location of each forward tracked pathline (maximum = 40)
HDCTR	2916	Hydraulic head values for the center of each grid block or finite element
HVAL	3025	Nodal hydraulic head values
IAXCOD	2916	Flag for each grid block indicating if flow across the block is uniform in the x-direction
IAYCOD	2916	Flag for each grid block indicating if flow across the block is uniform in the y-direction
IPATX	2916	x-direction velocity pattern for each grid block
IPATY	2916	y-direction velocity pattern for each grid block

Table C.2 (continued)

Dimension Limits Of Key Array Variables Used In GPTRAC

Array Name	Dimension	Description
IPWCZ	50	Indicates pumping wells that capture zones are to be delineated for
IRWCZ	20	Indicates recharge wells about which contaminant fronts are to be delineated (not used)
IWCHK	2916	Flag array indicating if elements contain well nodes
IZOEL	2916	Material zone number associated with each finite element or grid block
NDWELL	50	Contains node numbers that are pumping wells
NOP	(2916,4)	Rectangular finite element connectivities
NSTLIN	50	Number of pathlines to be traced for delineation of time-related capture zones
PLANG	100	Angles at which pathlines emanate from the well bore
PORZO	200	Aquifer porosity for each heterogeneous zone
QPWELL	50	Pumping well discharge rate
QRWELL	20	Recharge well injection rate
RSTART	(40,2)	x and y coordinates for starting location of each reverse tracked pathline (maximum = 40)
TZISTO	4	Gauss-Legendre quadrature points
VELX1	2916	x-velocity at block edge x_1

Table C.2 (continued)

Dimension Limits Of Key Array Variables Used In GPTRAC

Array Name	Dimension	Description
VELX2	2916	x-velocity at block edge x_2
VELY1	2916	y-velocity at block edge y_1
VELY2	2916	y-velocity at block edge y_2
VXEL	2916	x-components of velocity at element or grid block centers
VYEL	2916	y-components of velocity at element or grid block centers
XCTR	2916	x-coordinates of finite element or grid block centroids
XGRIDL	61	x-coordinates of gridline columns
XMAXZO	200	Maximum x-coordinates of heterogeneous aquifer zones
XMINZO	200	Minimum x-coordinates of heterogeneous aquifer zones
XPL	500	x-coordinates of pathline
XPLFNT	100	x-coordinates of pathline end points (not used)
XPLKP	500	
XPWELL	50	x-coordinate of pumping wells
XRWELL	20	x-coordinates of recharge wells
YCTR	2916	y-coordinates of finite element or grid block centroids

Table C.2 (continued)

Dimension Limits Of Key Array Variables Used In GPTRAC

Array Name	Dimension	Description
YGRIDL	61	y-coordinates of gridline rows
YMAXZO	200	Maximum y-coordinates for heterogeneous aquifer zones
YMINZO	200	Minimum y-coordinates for heterogeneous aquifer zones
YPL	500	y-coordinates of pathline
YPLFNT	100	y-coordinates of pathline end points (not used)
YPLKP	500	
YPWELL	50	y-coordinate of pumping wells
YRWELL	20	y-coordinate of recharge wells

Appendix D

Saving to WordPerfect

D.1 Retrieving HPGL Plotter Files Into WordPerfect 5.0

Before trying to use this feature, make sure the version of WordPerfect 5.0 you are running is dated no earlier than April 29, 1989 (your help key (F3) will indicate the version you are running in the upper right hand comer of your "Help" screen). If you are running an earlier version, call WordPerfect and ask them for the update.

With a blank screen in WordPerfect 5.0:

1. ALT F9 (Graphics Menu Screen)

    1   *Figure*
    2   *Create*
    3   *Filename:* ENTER CORRECT PATH AND FILE NAME AND HIT THE
            ENTER KEY

WordPerfect 5.0 will prompt you in the lower portion of the screen - "Please Wait - loading plotter file" message will appear. After it has loaded the plotter file, it will insert your file name in No. 1 Filename with a "(graphic)". If you get a message "Incorrect File Format", check your version of WordPerfect 5.0

You can change the figure definition by: (Graphics Menu Definition Screen):

3   *Type* (<u>Paragraph,</u> Page, or Character)

4   *Vertical Position* - offset from top of paragraph, page or character (the same selection as No. 3)

5   *Horizontal Position* - 1) Left, 2) <u>Right,</u> 3) Center, 4) Both

6   *Size*

7   *Wrap Text Around Box?* <u>Y</u> or N

To view and/or edit your plotter file (Graphics Menu Definition Screen):

8   Edit

Your file is then displayed in a graphics box with a graphics edit menu at the bottom of your screen:

1   Move   Use arrow keys to move

2   Scale   Use PgUp/Dn keys to scale

3   Rotate

4   Invert On

5   Black & White

When you are finished editing and/or viewing your graphic, press F7 to get out of the Graphics Menu: Hit the ENTER key several times, and you will see a "Fig 1" box appear. Keep hitting the enter key until you get to the end of your graphics box to see the box appear on your screen.

To save your document in WordPerfect 5.0

F7   Will prompt "Save Document? (Y/N)?" in lower left-hand comer of screen

Y   Will prompt "Document to be Saved:" Enter name of your document, ENTER

Will prompt "Exit WP: (Y/N)?" Say no.

Your document is now saved in WordPerfect 5.0.

To print your document in WordPerfect 5.0:

Shift F7   Will-then give you the print menu screen
3   "Document on Disk" menu selection

Enter name of document to be printed>

You will then be prompted ("Page(s): (ALL)" hit the ENTER key.

Your document should start printing.

D.2 Retrieving HPGL Plotter Files Into WordPerfect 5.1

With a blank screen in WordPerfect 5.1:

1.   ALT F9 (Graphics Menu Screen)

   1   *Figure*
   2   *Create*
   3   *Filename:* ENTER CORRECT PATH AND FILE NAME AND HIT THE
        ENTER KEY

WordPerfect 5.1 will prompt you in the lower potion of the screen - "Please Wait - loading plotter file" message will appear. After it has loaded the plotter file, it will insert your file name in No. 1 Filename with a "(graphic)".

You can change the figure definition by: (Graphics Menu Definition Screen):

   2   *Contents* (Displays "Empty" until you have loaded a graphic file, will then say "Graphic")
   3   *Caption* You can give your plotter file a caption name. Follow prompts on screen to enable the caption mode.
   4   *Anchor Type* (Paragraph, Page, or Character)
   5   *Vertical Position* - offset from top of paragraph page or character (the same selection as No. 4)
   6   *Horizontal Position* - 1) Left 2) Right, 3) Center, **4)** Both
   7   *Size*

8   *Wrap   Text   Around   Box?* <u>Y</u> or N

To view and/or edit your plotter file (Graphics Menu Definition Screen):

9   *Edit*

Your file is then displayed in a graphics box with a graphics edit menu at the bottom of your screen:

1	**Move**	Use arrow keys to move
2	Scale	Use PgUp/Dn keys to scale
3	Rotate	
4	Invert On	
5	Black & White	

When you are finished editing and/or viewing your graphic, press F7 to get out of the Graphics Menu. Hit the ENTER key several times, and you will see a "Fig 1" box appear. Keep hitting the enter key until you get to the end of your graphics box to see the box appear on your screen.

To save your document in WordPerfect 5.1:

F7 Will prompt "Save Document? (Y/N)?" in lower left-hand comer of screen
Y Will prompt "Document to be Saved:" Enter name of your document, ENTER

Will prompt "Exit WP: (Y/N?" **Say** no.

Your document is now saved in WordPerfect 5.1.

To **print** your document in WordPerfect 5.0:

Shift F7   Will then give you the print menu screen
3   "Document on Disk" menu selection

Enter name of document to be printed>

You will then be prompted ("Page(s): (ALL)" hit the ENTER key.

Your document should start printing.

Appendix E

**HEDCON Utility
User's Guide**

E.l Introduction and Features

The HEDCON program (CONVert HEaDs) supplied with the WHPA model is designed to create hydraulic head input files in the format required by the GPTRAC numerical option. The format required by GPTRAC is outlined in detail in Section 8.3.3. The two main options available in HEDCON are:

1. Convert a POSTMOD output file in x,y,h format into a file suitable for input into GPTRAC This option should only be used if the USGS MODFLOW code (McDonald and Harbaugh, 1988) was used to calculate a head field, and the postprocessing code POSTMOD (available from the International Ground-Water Modeling Center at Indianapolis, Indiana) was used to create a file in x,y,h format with the origin of the coordinate system at the lower left-hand corner of the grid.

2. Convert a randomly ordered file in x,y,h format into a file suitable for input into GPTRAC.

The x,y,h format referred to above simply means that there is one x-coordinate, one y-coordinate, and one hydraulic head value on each line of the file. This type of format is commonly used in commercial soft-ware packages such as SURFER (Golden Software). The x- and y-coordinates must correspond to the location of a grid node, and the head value (h) must be the head value at that node. Either a mesh-centered or a node-centered grid may be specified.

The HEDCON program input requirements are outlined in Table El. The grid parameters must be specified (either interactively or by reading a previously created file) so that HEDCON can match the nodal coordinates of the grid with the coordinates read from the input head file. HEDCON operates very similar to the WHPA model. The Escape key may be used to display an options menu, and there is full Help support throughout the program. To execute HEDCON, type HEDCON at the DOS prompt. HEDCON may not be executed from within the WHPA code.

Table E.l

Input Requirements for HEDCON Program

Program Variable	Description
XMIN: XMAX: YMIN: YMAX:	Minimum x-coordinate of grid (ft or m) Maximum x-coordinate of grid (ft or m) Minimum y-coordinate of grid (ft or m) Maximum y-coordinate of grid (ft or m)
NROWS and NCOLS, and XGRIDL(I), YGRIDL(J) for I=1, NCOLS and J=1, NROWS	Number of grid-line rows and columns, and (if non-uniform grid,) coordinates of each grid-line row and column. Note that this data may be read in using the grid file option (FILE2 below).
FILE1	Input file name that contains head values for each node of the finite element or finite difference grid. This file must be in x,y,h format.
FILE2	Input file name that contains the number of grid-line rows and columns and the x-coordinate of each grid-line column and the y-coordinate of each grid-line row (optional).

E.2 Grid File Option

HEDCON will automatically prompt the user for the number of grid-line columns and rows, and the minimum and mazimum x- and y-coordinates of the grid. If the grid is uniform (the grid-line spacings in both the x and y directions is constant), no additional information is required to generate the grid. If the grid is nonuniform, however, the x-coordinates of the grid-line columns and the y-coordinates of the grid-line rows must be supplied to HEDCON. These parameters may either be entered interactively, or they may be read from a previously created grid file the name of which may be entered into HEDCON. If the grid file option is selected, the file must be constructed prior to executing HEDCON, and it must conform to the following format:

Number of grid-line columns (NCOLS) on line 1
x-coordinate of grid-line column 1 on line 2
x-coordinate of grid-line column 2 on line 3
x-coordinate of grid-line column 3 on line 4
          .. and so on for each grid-line column

Number of grid-line rows (NROWS) on line NCOLS+l
y-coordinate of grid-line row 1 on line NCOLS+2
y-coordinate of grid-line row 2 on line NCOLS+3
y-coordinate of grid-line row 3 on line NCOLS+4
          ... and so on for each grid-line row

Refer to one of the ***.GRD files in the EXAMPL subdirector on the WHPA model diskettes for an example of a grid input file.

If you decide to enter the grid-line coordinates directly into HEDCON, the grid data will automatically be written to the file GRID.SAV. This file may then be read by GPTRAC, so the grid data does not have to be entered twice. Note that once a GPTRAC input file has been saved, the necessary grid data is retained in the saved file and the separate grid file is no longer required as input.

Appendix F

Development History of WHPA Code

WHPA Version 1.0 Released **February, 1990**

WHPA Version 2.0 Released **March, 1991**

Enhancements include:

- New analytical solutions for unconfined aquifers subject to areal recharge and leaky-confined aquifers subject to vertical leakage were implemented into GPTRAC.

- New analytical solutions for strip aquifers with two parallel stream or barrier boundaries or a stream and a barrier boundary were implemented into GPTRAC.

- The same leaky-confined aquifer analytical solution implemented into GPTRAC was implemented into MONTEC.

- The GFAF module (postprocessor) was substantially enhanced. The upgrades included the ability to obtain hard copy output from a number of commonly used devices other than the HP 7475A pen plotter; the ability to overlay up to fifteen plot files at one time; and the ability to execute the GRAF module options (e.g., map scale and overlay) prior to viewing the current plot.

- Numerous corrections, enhancements and upgrades were made to the prepro-cessor, including the ability to exit to DOS without exiting the WHPA code.

- The HEDCON utility program was revised to include menus help screens and error prompts. The ability to read in a file in x,y, head format in any order, and to subsequently reorder the file m a format suitable for the GPTRAC numerical option was also implemented.

- The restriction of a math coprocessor was eliminated: WHPA 2.0 will run on IBM compaible microcomputers with or without a math coprocessor.