ground water

Stochastic Ground Water Flow Simulation with a Fracture Zone Continuum Model

by Christian D. Langevin[1]

Abstract

A method is presented for incorporating the hydraulic effects of vertical fracture zones into two-dimensional cell-based continuum models of ground water flow and particle tracking. High hydraulic conductivity features are used in the model to represent fracture zones. For fracture zones that are not coincident with model rows or columns, an adjustment is required for the hydraulic conductivity value entered into the model cells to compensate for the longer flowpath through the model grid. A similar adjustment is also required for simulated travel times through model cells. A travel time error of less than 8% can occur for particles moving through fractures with certain orientations. The fracture zone continuum model uses stochastically generated fracture zone networks and Monte Carlo analysis to quantify uncertainties with simulated advective travel times. An approach is also presented for converting an equivalent continuum model into a fracture zone continuum model by establishing the contribution of matrix block transmissivity to the bulk transmissivity of the aquifer. The methods are used for a case study in west-central Florida to quantify advective travel times from a potential wetland rehydration site to a municipal supply wellfield. Uncertainties in advective travel times are assumed to result from the presence of vertical fracture zones, commonly observed on aerial photographs as photolineaments.

Introduction

The generalized conceptual model for a fractured bedrock aquifer consists of low-permeability matrix blocks separated by highly permeable fractures that act as preferential pathways for ground water flow. The National Research Council (NRC 1996) summarizes three approaches for simulating ground water flow in fractured aquifers. The most common approach is to represent the system with an equivalent continuum model, often referred to as an equivalent porous media (EPM) model. With this approach, equivalent continuum properties assigned to model cells represent the combined effects of individual fractures and the rock matrix. The discrete fracture model, or discrete fracture network model, is the second approach used to simulate ground water flow in fractured rocks. With this approach, flow is explicitly simulated in each fracture using, for example, solutions to the Navier-Stokes equation (Bear 1993), Kirchoff's laws for electrical circuits (Kraemer and Haitjema 1989), or hydraulically connected circular discs (Cacas et al. 1990a, 1990b). The third approach is a hybrid method that uses discrete fracture models to estimate effective properties for continuum approximations. Regardless of the approach, accurate representation of dominant fractures probably is more important than model selection (NRC 1996; Selroos et al. 2002).

The use of continuum models to directly simulate flow within individual fractures may be considered as another approach for representing fracture flow. While these continuum models are not considered true discrete fracture flow models, they can be used to explicitly simulate flow within individual fractures. Fractures and densely fractured flow zones can be represented in continuum models by adding zones of increased hydraulic conductivity in the appropriate orientation. Rayne et al. (2001) demonstrate that subhorizontal fracture zones can be represented with a continuum model by using thin, highly permeable layers that follow the depths of the mapped fracture zones. Eaton

[1]Research Hydrologist, U.S. Geological Survey, 9100 NW 36th St., Ste. 107, Miami, FL 33178; (305) 717–5817, fax (305) 717–5801; langevin@usgs.gov

Received January 2002, accepted December 2002.

et al. (2001) show that simulated head gradients are more accurate with explicitly incorporated fracture zones than with equivalent continuum properties. Svensson (2001a) shows how individual fractures can be directly incorporated into continuum models to simulate flow in a fractured aquifer in Sweden (Svensson 2001b). Selroos et al. (2002) conclude that similar estimates of travel times can be obtained with a discrete fracture model or with a continuum model that explicitly incorporates transmissive features. These are a few recent examples of what will be referred to herein as fracture zone continuum models.

This paper describes a stochastic method for developing two-dimensional fracture zone continuum models. The method is demonstrated by quantifying uncertainties in travel time estimates that result from uncertainties regarding the exact locations and orientations of vertical fracture zones. Development of the method was motivated by the common occurrence of hydraulically significant vertical fracture zones, such as those found in west-central Florida. This paper also describes a procedure for converting a calibrated steady-state EPM model into a fracture zone continuum model.

Method for Incorporating Individual Fracture Zones into Continuum Models

Ground Water Flow

Svensson (2001a) presents a method for incorporating fractures or fracture zones into continuum ground water flow models. The approach presented here is similar to Svensson (2001a) except it is intended to work with commonly used finite-difference and particle-tracking programs, such as MODFLOW (McDonald and Harbaugh 1988) and MODPATH (Pollock 1994). This paper focuses on the incorporation of fully penetrating vertical fracture zones in a two-dimensional aquifer; Svensson (2001a) shows how the method can be applied in three dimensions.

For a fracture zone at a 45º angle to the model grid (Figure 1), Svensson (2001a) shows that the exact flux, Q_e, from the center of cell (3,1) to the center of cell (2,2) is

$$Q_e = -K_f \cdot W \cdot b \frac{\Delta h}{\Delta x \sqrt{2}} \qquad (1)$$

where K_f is hydraulic conductivity of the fracture zone, W is fracture zone width, b is thickness of the aquifer, Δh is head difference, and Δx is grid spacing. In the Svensson (2001a) formulation, flow from cell (3,1) to (2,2) takes two pathways (Figure 1). One pathway leads through cell (2,1) and the other through cell (3,2). In contrast, the method used herein restricts flow through a fracture zone to a single pathway as shown by the flow vectors in Figure 1. By specifying that flow is through cell (3,2), the equation for flow from cell (3,1) to (2,2) is

$$Q_e = -K_c \cdot \Delta x \cdot b \frac{\Delta h}{2 \cdot \Delta x} \qquad (2)$$

where K_c is the cell hydraulic conductivity. By setting Equations 1 and 2 equal, K_c for a 45º angle fracture zone becomes

$$K_c = K_f \frac{W}{\Delta x}\sqrt{2} \qquad (3)$$

The general equation for K_c, determined by evaluating various fracture zone orientations, is

$$K_c = K_f \frac{W}{\Delta x}[\sin(\theta) + \cos(\theta)] \qquad (4)$$

where θ is the angle measured from the x or y axis, whichever is less.

Flow between matrix blocks and a fracture zone, as calculated with the methods presented here, may be slightly affected by fracture zone orientation. For fracture zones in a permeable matrix, small flow errors may result because MODFLOW uses K_c (an adjusted value only valid for fracture zone flow) and harmonic averaging to calculate internodal conductance values with the four adjacent cells. Future applications of this method would benefit from a fracture zone conductance package for MODFLOW that uses the adjusted K_c value to calculate conductances only between fracture zone cells. Harmonic averaging would use K_f, instead of K_c, to calculate internodal conductances between fracture zone cells and matrix cells.

The spatial extent of a fracture zone is only one cell wide in the model grid, but use of Equation 4 allows the true width of fracture zones to be specified. Therefore, the hydraulic effect of fracture zone width is indirectly included in the ground water flow calculations through adjustment of cell hydraulic conductivity. This approach limits detailed evaluation of particle traces in and directly adjacent to fracture zones, because true widths and spatial extents of fracture zones are not explicitly included in the model grid. In the example presented in this paper, widths of fracture zones are assumed equal to cell spacing.

Adjustment for Particle Tracking

With this method for incorporating fracture zones, an adjustment is also required for particle-tracking routines, such as MODPATH (Pollock 1994). MODPATH's semi-analytical particle-tracking method approximates velocities at particle locations using a piecewise linear interpolation scheme. For fracture zones that align with rows or columns, MODPATH will calculate accurate travel paths and travel times. For fracture zones at an angle to the model grid, however, particle paths and travel times calculated by standard MODPATH would not be accurate unless an adjustment is made. Figure 2a shows the travel paths for three particles within a transmissive fracture zone surrounded by impermeable rock matrix. None of the paths in Figure 2a are straight because of the velocity interpolation scheme. Thus, for certain fracture zones, standard MODPATH calculates travel times that are too long. Moreover, travel times through the fracture zone are not uniform; each path

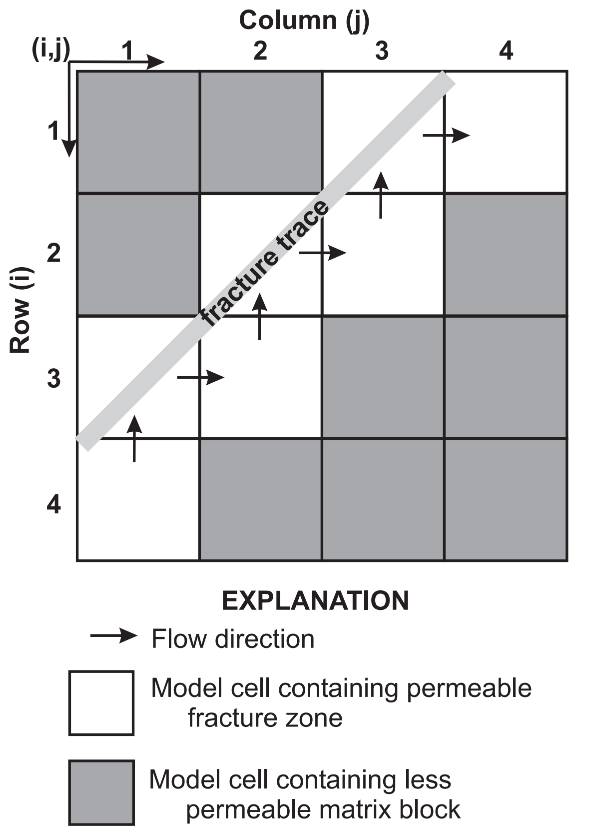

Figure 1. Model grid showing cells selected to represent permeable vertical fracture zone.

should be straight and particles should travel at the same velocity.

A simple solution to this problem can be obtained by noting that particle paths calculated by standard MODPATH intersect cell boundaries at the correct locations, although the path within the model cell is inaccurate (Figure 2a). The correct path is a straight line from where the particle enters the cell to where the particle exits the cell. The true travel time through the cell can be calculated by dividing the travel distance by the average of the flow velocities at the two cell boundaries. Figure 2b shows straight travel paths and uniform travel times for the same three particles after this adjustment was implemented in MODPATH. Each particle moves at the same velocity (the actual velocity in the fracture zone) and arrives at the same time.

There are two cases where this adjustment for particle velocity is not required. The first case is where the fracture zone is not significantly more permeable than the surrounding rock matrix. The second case is where fracture zones intersect. At a fracture zone intersection, it may not be appropriate to assume a straight travel path through the model cell. Accordingly, the adjustment for particle velocity and travel path is only made if most of the flow is through one face in the *x* direction and through one face in the *y* direction. In the problems evaluated thus far, the particle path adjustment is made if the *x* velocity for one cell face is 10 times greater than the *x* velocity for the other cell face, and same for the *y* direction. The factor of 10 was selected based on the hydraulic conductivity ratio between fracture zones and rock matrix.

For fracture zones with orientations other than 0º, 45º, and 90º with the model grid, a travel time error, as much as 8%, may result because the travel paths are not straight lines (Figure 2c). The largest error will occur for fracture zones with angles of 22.5º and 67.5º.

Method for Stochastic Analysis with Fracture Zone Continuum Model

Stochastic methods are powerful tools for quantifying uncertainty in model predictions that result from the inability to completely describe the physical system. In most studies of ground water flow (particularly those where measurements of the physical system are sparse, difficult to obtain, and costly), stochastic methods can be used to quantify predictive uncertainties (Peck et al. 1988; Freeze et al. 1990; Chiles and de Marsily 1993; Gelhar 1993). Monte Carlo analysis is one such stochastic method that is commonly used to quantify predictive uncertainties because the method is conceptually straightforward and works well with numerical models (Freeze et al. 1990).

Monte Carlo analysis with a numerical model is a multistep process. The first step is to statistically characterize uncertainty in one or more of the model input parameters by formulating a probability density function (PDF) for each uncertain parameter. The next step is to randomly generate many statistically reasonable sets of input parameters from the PDFs and use a numerical model to simulate each one. Each individual model is called a realization. Finally, the uncertainty of a selected model result is quantified by performing statistics on the ensemble.

Statistical Characterization of Fracture Zone Properties

The success of the stochastic method applied in this paper relies on the ability to generate realizations of fracture zone networks that are statistically similar to those in the field. To generate stochastic realizations of fracture zone networks, statistical descriptions in the form of PDFs are required for one or more of the properties that describe fracture zones. In this paper, the pattern of the overall fracture zone network is characterized by density, and the individual fracture zones are characterized by length, orientation, and transmissivity.

Sophisticated strategies exist for reproducing complex fracture patterns. For example, McKoy and Sams (1997) summarize increasing levels of complexity that can be used to describe fracture networks. With the most complex level, fractures form in “swarms” or clusters. In this paper, the Poisson process is used to generate randomly located fracture zones, although more sophisticated cluster strategies could be used if necessary. With the Poisson process, a negative exponential function describes the distribution of distances between fracture zones.

Representing fracture length and orientation with a PDF is relatively straightforward (Chiles and de Marsily 1993). One method for determining lengths and orientations of fracture zones is to perform photolineament analysis using aerial photographs (Mabee et al. 1994). A PDF can then be developed by matching the appropriate func-

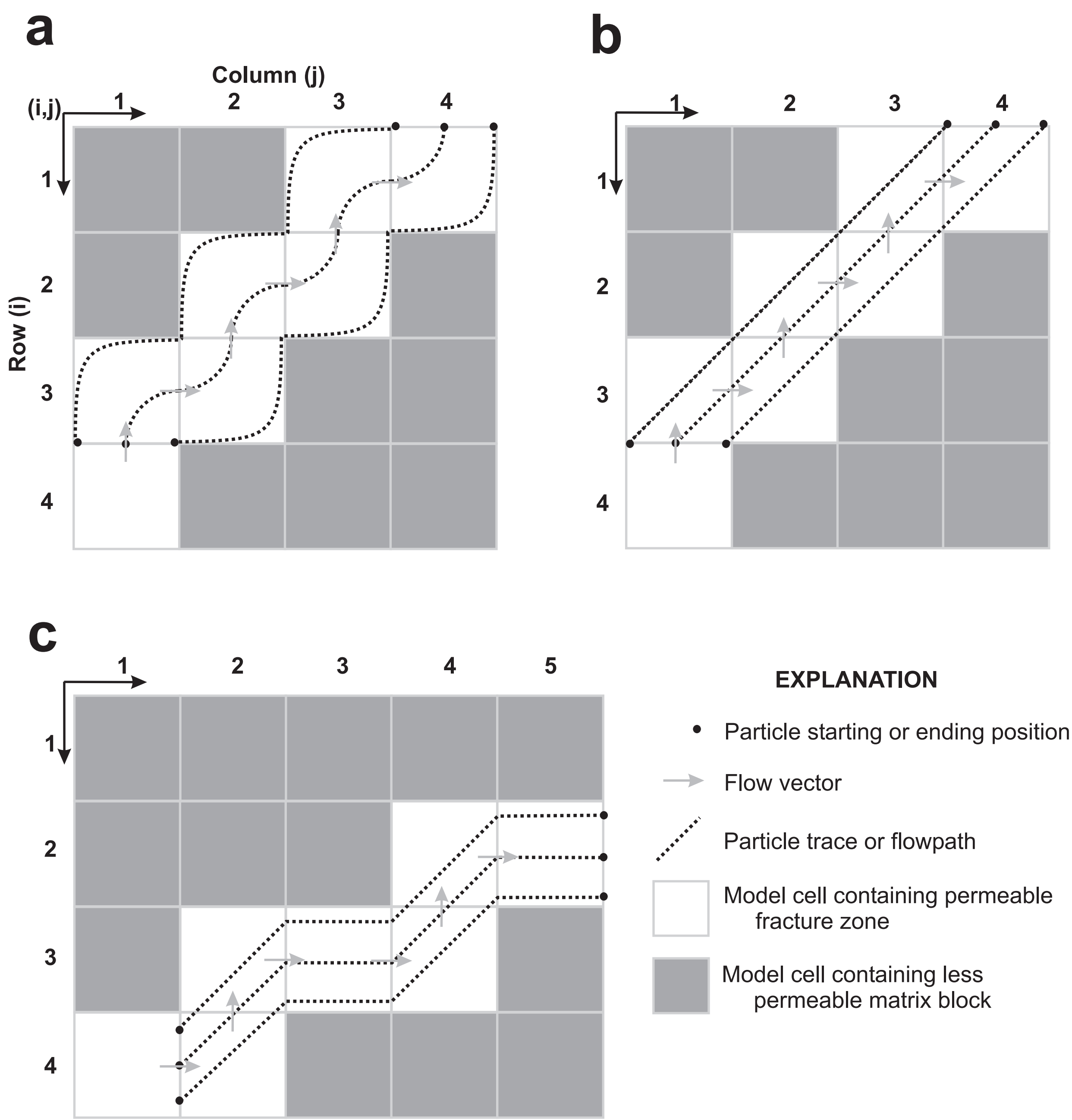

Figure 2. Simulated particle traces through permeable fracture zones: (a) standard MODPATH without modifications, (b) MODPATH modified to represent particle traces in permeable fracture zones, and (c) modified version of MODPATH for a fracture zone with a 22.5° orientation.

tion to a histogram of the observed lengths. A similar approach also can be used for developing a PDF for fracture zone orientation.

One of the more challenging aspects of fracture studies is quantifying fracture zone transmissivity, defined here for a two-dimensional aquifer as the fracture zone hydraulic conductivity multiplied by the vertical height of the fracture zone within the aquifer. The NRC (1996) recommends further research on fracture zones because there are few reported estimates of fracture zone transmissivity. Matrix block transmissivity is the hydraulic conductivity of the block multiplied by the vertical height of the block in the aquifer. Conceptually, a ratio is a straightforward way to represent the relation between fracture zone and matrix block transmissivity. Although a deterministic ratio is used for the example in this paper, the ratio or actual value of transmissivity may be statistically described with a PDF.

The hydraulic significance of a fracture network is controlled primarily by connectivity (Kraemer and Haitjema 1989; Cacas et al. 1989) because fractures that are connected have a much larger influence on ground water flow than unconnected fractures. If the PDFs describing the fracture zones adequately represent field conditions, many randomly generated sets of fracture zones, on average, will have connectivity similar to that observed in the field.

The fracture zone statistics are used to generate statistically reasonable networks of fracture zones. Each network realization is constructed by using random numbers to select fracture zone properties from the PDFs. For example, one might start by randomly selecting, from a uniform distribution, an *x* and *y* location within the area of interest. This location would correspond to an endpoint of the fracture zone. Values for length, orientation, and transmissivity also are randomly selected from the respective PDFs. The result is a line within the area of interest that can be considered to represent a statistically reasonable fracture zone. Along this line, the hydraulic conductivity, or transmissivity, in the intersected cells is adjusted according to Equation 4. This Poisson procedure for generating fracture zones is repeated until the simulated density of fracture zones is equal to the density of fracture zones observed in the field (or the density selected from a density PDF). Using this approach, any number of fracture zone properties can be treated stochastically. For the Monte Carlo analysis described later, many thousands of fracture zone networks are generated using this approach. Each network realization is then used as input to a numerical model of ground water flow, and statistics performed on the ensemble provide the probability of a particular model prediction.

Development of an Equivalent Porous Media Model

The EPM assumption is commonly used when simulating flow and transport in many aquifers, even those subjected to fracturing and dissolution. Prior to incorporating individual fracture zones into the continuum model, an EPM model is first developed for the domain of interest. In many cases, it may be appropriate to use an existing model with little or no modification.

Calibration of the EPM model should focus on assigning equivalent transmissivity values. Equivalent transmissivity is defined here as the homogeneous transmissivity value used in an EPM model to yield the same flow as the heterogeneous domain with explicitly incorporated fracture zones. In an aquifer system dominated by permeable fracture zones, the equivalent transmissivity value may be similar to the transmissivity of fracture zones. If, however, there are few fracture zones, or the hydraulic significance of the fracture zones is minimal, the equivalent transmissivity value may closely match the transmissivity of the less permeable matrix blocks. The appropriate equivalent transmissivity value assigned to the EPM model should be within the range defined by matrix block and fracture zone transmissivity.

Establishing Relation Between Matrix Block and Bulk Transmissivity

When referring to a fractured aquifer or a model that explicitly includes individual fracture zones, bulk transmissivity is used here to describe the overall aquifer transmissivity, which includes the combined effects of fracture zones and the rock matrix. Ideally, the equivalent transmissivity of a well-calibrated EPM model should approximate bulk transmissivity of the aquifer. The EPM model can be converted into a fracture zone continuum model if the equivalent transmissivity can be separated into fracture zone and matrix block transmissivities. The method used in this paper to establish the transmissivity relation is to run a model with different fracture zone and matrix block properties and evaluate the resulting bulk transmissivity. Other analytical approaches can also be used to bracket the expected relation. For a fracture network that is highly connected with infinitely long fracture zones, Snow (1965) sums the directional permeability components for each fracture to calculate an equivalent permeability tensor. For two-dimensional steady uniform flow in a heterogeneous medium with lognormally distributed hydraulic conductivity, the effective hydraulic conductivity is the geometric mean of the conductivity values (Gelhar 1993). The Snow (1965) method results in high estimates for bulk transmissivity because the fractures are assumed to be infinite and fully connected (NRC 1996). Conversely, the geometric mean will give low estimates for bulk hydraulic properties because that solution for the effective conductivity does not account for long, domain-spanning features and bimodal transmissivity distributions. However, these two methods bracket a reasonable range and may provide insight into the expected relation between bulk and matrix block properties.

A preliminary Monte Carlo analysis with the fracture zone continuum model can be used to determine the relation between bulk transmissivity and matrix block transmissivity for a given description of fracture properties. Along two opposite sides of a simple box model, specified heads are used to impose a hydraulic gradient across the model domain. No-flow boundaries are used for the two remaining boundaries. A fracture zone network is generated and incorporated into the grid using the procedures that were described. The box model is run using the basic Monte Carlo approach. Separate Monte Carlo analyses are performed with different block transmissivity values. For each simulation with the flow model, bulk transmissivity is calculated by summing the total flux into or out of the specified head cells on one side of the box model and dividing the total flux by model width and imposed hydraulic gradient. Median values of bulk transmissivity are then plotted against the specified values of block transmissivity. This relation is used to select the appropriate block transmissivity such that the model with explicitly included fracture zones yields the same flow as the EPM model.

Procedure for Monte Carlo Analysis

After the fracture zone realizations have been generated, the Monte Carlo analysis is relatively straightforward in theory, but can be difficult to perform unless a program is written to automate the process. Depending on the number of stochastic variables, thousands of model runs may be required to adequately characterize the statistics of all possible outcomes. The appropriate number of model runs can be determined by plotting the mean and standard deviation of a particular output of interest as a function of number of model runs. The mean and standard deviation will converge on single values as the appropriate number of model runs is reached.

A program was written to implement the methods described. The objective of the implementation stage was to develop a program that could be used with most grid-based models of ground water flow and particle tracking. The program was specifically developed for MODFLOW (McDonald and Harbaugh 1988) and MODPATH (Pollock 1994), but could be modified to work with most flow and particle-tracking models. First, the program reads input variables such as those that describe fracture statistics. Then the program starts a loop in which a fracture network is randomly generated and incorporated into the model, the flow simulation and particle tracking is performed, and selected output is stored in a single file. Outside of the program, statistics performed on the ensemble are used to evaluate the probability of a particular occurrence.

Application to West-Central Florida

The North Lakes wetland is a possible candidate for rehydration with reclaimed water. The main concern with wetland rehydration at North Lakes is that the residence time of reclaimed water in the aquifer may be too short for sufficient renovation. Located ~1.4 km from the wetland, the Section 21 wellfield is permitted to withdraw ground water at an average annual rate of 40,000 m^3/day (Figure 3). The Section 21 wellfield is operated by the City of St. Petersburg and supplies potable water to the residents of Hillsborough County. Environmental managers at the Southwest Florida Water Management District have suggested that reclaimed water added to the wetland should reside in the underlying Floridan Aquifer for at least two years prior to being withdrawn by a municipal supply well.

Uncertainties in travel time from the wetland to the wellfield are assumed to result from the presence of solution-enhanced vertical fracture zones. These vertical fracture zones commonly occur in west-central Florida (Vernon 1951; Ritchie 1983) and are often hydraulically significant (Moore 1981; Williams 1985). Morrison (1995) used a fracture zone continuum model to show how the results from an ambiguous aquifer test at the Section 21 wellfield can be explained by the presence of permeable fracture zones. The intersection of a vertical fracture zone with land surface can be identified on aerial photographs as linear patterns of tonal differences, referred to as photolineaments. A well located within a photolineament has a greater chance of being completed in a permeable fracture or fracture zone and producing more water (Lattman and Nickelson 1958; Lattman and Parizek 1964; Parizek 1976; Siddiqui and Parizek 1977; Moore 1981). This application of the fracture zone continuum model is based on the

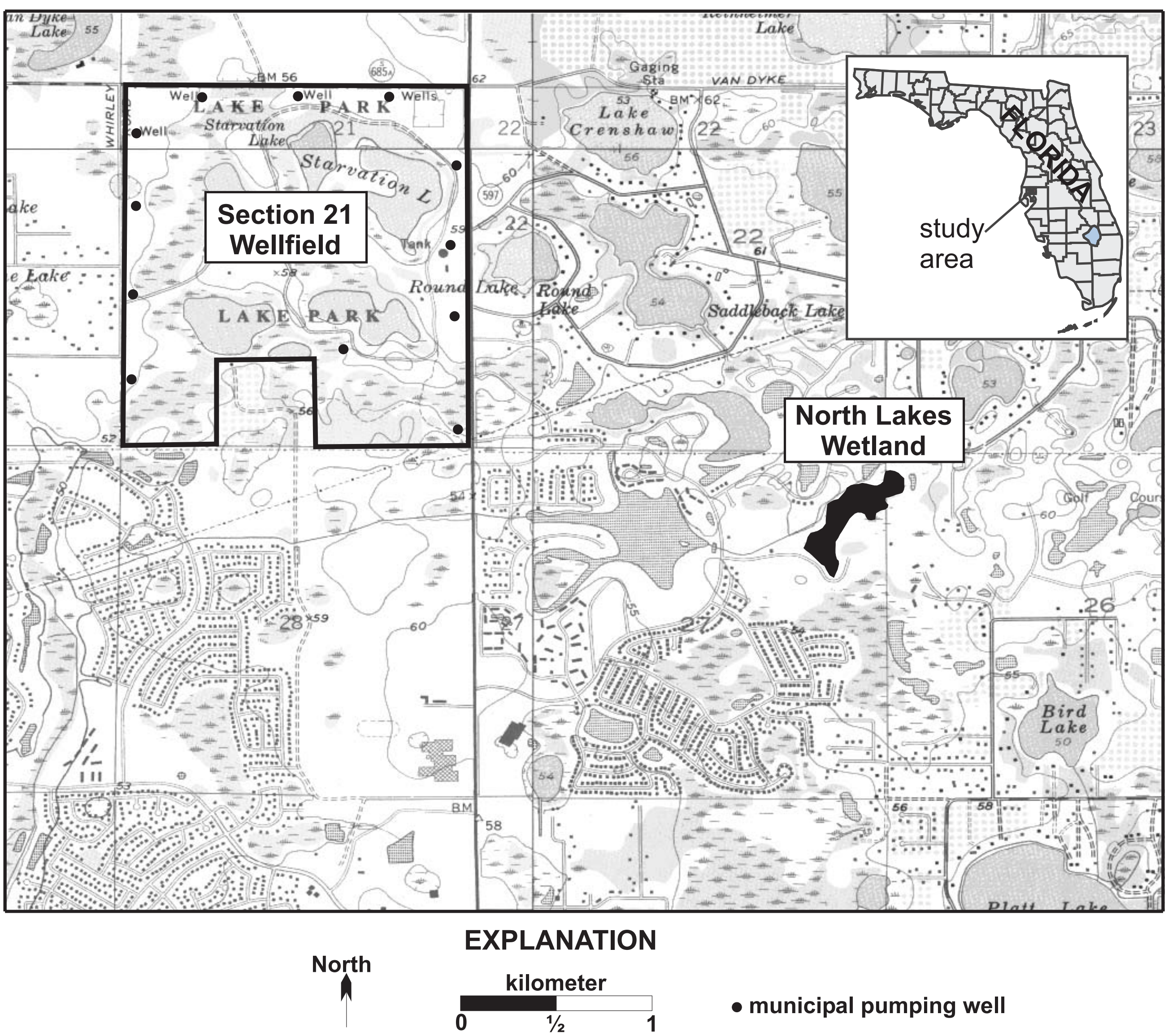

Figure 3. Location of the North Lakes wetland and Section 21 wellfield, west-central Florida.

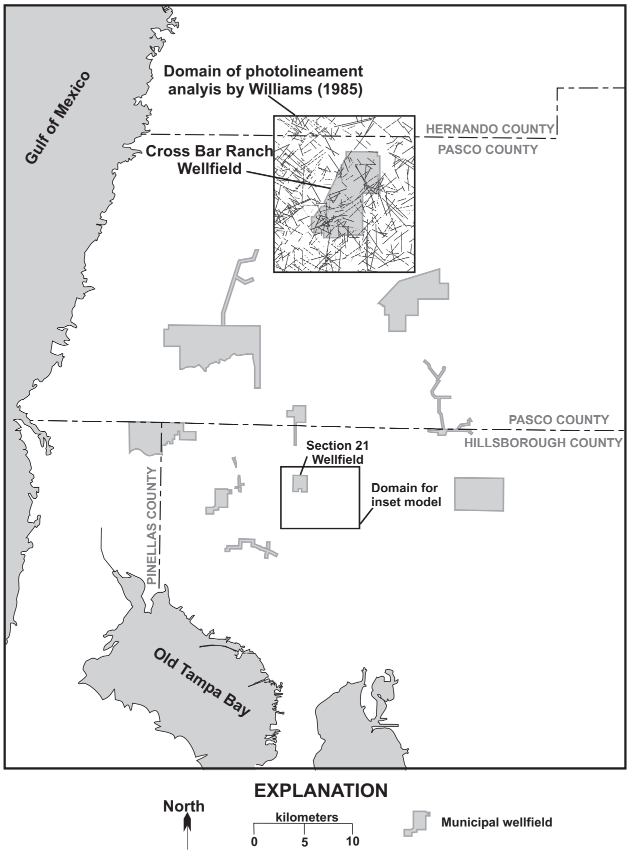

Figure 4. Map of west-central Florida showing photolineaments at the Cross Bar Ranch wellfield (modified from Williams 1985), the Section 21 wellfield, and the domain of the inset local-scale model.

premise that long vertical fracture zones, observed as photolineaments, act as preferential pathways for horizontal ground water flow. This analysis considers advective travel only; dispersive transport is not considered. Uncertainties in travel times that result from other model input parameters, such as recharge and boundary conditions, are not examined in this evaluation.

Fracture Zone Statistics

Williams (1985) conducted a detailed study of the photolineaments at the Cross Bar Ranch wellfield in west-central Florida and included histograms of fracture length and orientation. It is assumed herein that the statistical properties of the photolineaments mapped by Williams (1985) are stationary and representative of the length and orientation of the fracture zones in the North Lakes study area. The study area for the Cross Bar Ranch wellfield is relatively close to North Lakes (~20 km), and the Williams (1985) analysis is supported by other studies in Florida of photolineament length and orientation (Vernon 1951; Ritchie 1983). Criteria used by Williams (1985) to define the lineaments included differences in soil tone, occurrence of sinkholes, sinkhole elongation and alignment, tree alignment, vegetation patterns, elongation and alignment, and linear stream segments. The 618 photolineaments that were identified in the Cross Bar Ranch study area are presented in Figure 4.

Photolineaments range in length from 0.2 to 10 km. Photolineaments shorter than 0.2 km presumably were unable to be detected on the aerial photographs or were not present. A normalized frequency histogram suggests that fracture length may be lognormally distributed (Figure 5a) with a mean and standard deviation of 0.14 and 0.64, respectively, of the natural log transformed dataset. Lognormal distributions are presented in Figure 5 to illustrate the match between the PDF and the observed data.

Fracture zone orientation is defined on the north half of a compass by an azimuth ranging between 270º and 90º. Note that this definition of fracture zone orientation is different from the θ angle described in an earlier section. A frequency histogram of azimuth suggests that fracture zone orientation is bimodal, with most values occurring at 310º and 50º, or possibly trimodal, with another mode at 355º (Figure 6). Bootstrap resampling was used as a nonparametric statistical method to randomly generate values for fracture zone orientation, thus avoiding problems associated with fitting a PDF to azimuthal data.

The sum of all photolineament lengths is 876 km. The study area for the Cross Bar Ranch wellfield is 13.3 km $\times$ 14.9 km. The fracture density, therefore, is 4 km/km^2. For the North Lakes application, the density of fracture zones is treated as a deterministic parameter. In addition to identifying the lengths and locations of photolineaments, Williams (1985) also assigned each photolineament a qualitative ranking that ranges from definite to possible. According to her analysis, about half of the photolineaments are definite, whereas the rest are ranked as possible to probable. Only the definite photolineaments are included in this analysis. Therefore, a fracture density of 2 km/km^2 is used rather than the mapped value of 4 km/km^2.

Statistical characterization of fracture zone transmissivity is particularly difficult because hydraulic testing has not been performed in the limestone aquifers of west-central Florida to quantify the hydraulic significance of fracture zones. A single deterministic ratio is used in this example to calculate fracture zone transmissivity from block transmissivity. This ratio is based on the transmissivity of a highly permeable limestone aquifer that has been subjected to fracturing and dissolution. The Biscayne Aquifer is one of the most permeable limestone aquifers in the world and has hydraulic conductivity values exceeding 3000 m/day (Fish and Stewart 1991). Hydraulic conductivity (6 to 50 m/day) of the limestone aquifer at the North Lakes wetland (Langevin 1998; Langevin et al. 1998) is about two orders of magnitude less than the hydraulic conductivity of the Biscayne Aquifer. Based on this comparison, fracture zones are assumed to be 100 times more permeable than the surrounding limestone aquifer. This ratio probably results in fracture zone transmissivity values that are too high, providing conservative estimates for advective travel times to the wellfield that are shorter than what might be observed.

Equivalent Porous Media Model

To develop a ground water flow model that incorporates both the Section 21 wellfield and the North Lakes wetland, a telescopic mesh refinement (TMR) approach was used to generate a local-scale inset model (Figure 4) from a larger regional-scale model. The regional-scale,

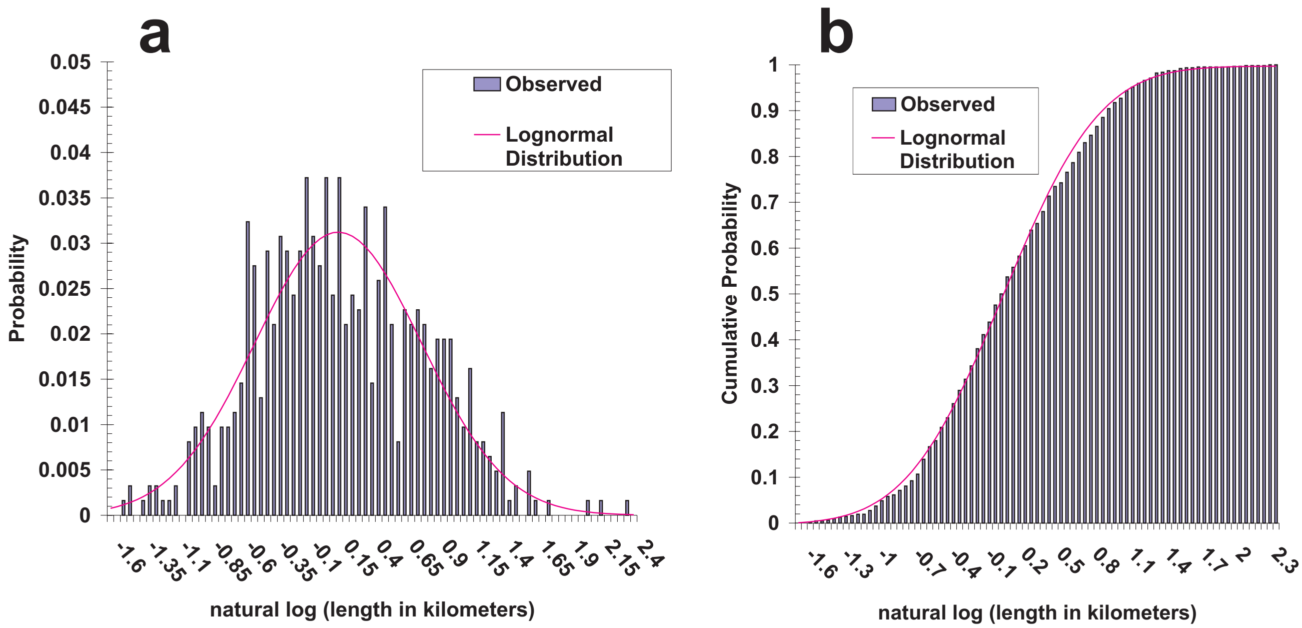

Figure 5. Frequency histograms for fracture length of the photolineaments mapped by Williams (1985).

quasi-three-dimensional MODFLOW model, which extends beyond the domain of Figure 4, was developed and calibrated by SDI Environmental (1994) to simulate ground water flow in west-central Florida between 1971 and 1993. The regional-scale model contains two layers: the upper layer represents the surficial aquifer and the lower layer represents the Upper Floridan aquifer. The model is quasi-three-dimensional in the sense that the semi-confining unit, located between the surficial and Upper Floridan aquifers, is simulated with a vertical resistance term. Within the vicinity of the Section 21 wellfield and North Lakes wetland, the cell size for the regional model is ~400 m in both the east-west and north-south directions.

A commercially available software package was used to generate a local-scale model from the regional-scale model. The local-scale model includes the Section 21 wellfield and the North Lakes wetland. The local model grid has 2 layers, 160 rows, and 192 columns with a uniform cell size of 25.15×25.15 m^2. There are 256 cells in the local-scale model for each cell in the regional-scale model. The TMR software assigns specified head-boundary conditions around the local-scale model with head values interpolated from the regional-scale model. The local-scale model was simulated with steady-state conditions using average annual hydrologic conditions for 1993.

Two parameter zones within the North Lakes and Section 21 area define equivalent transmissivity for the Upper

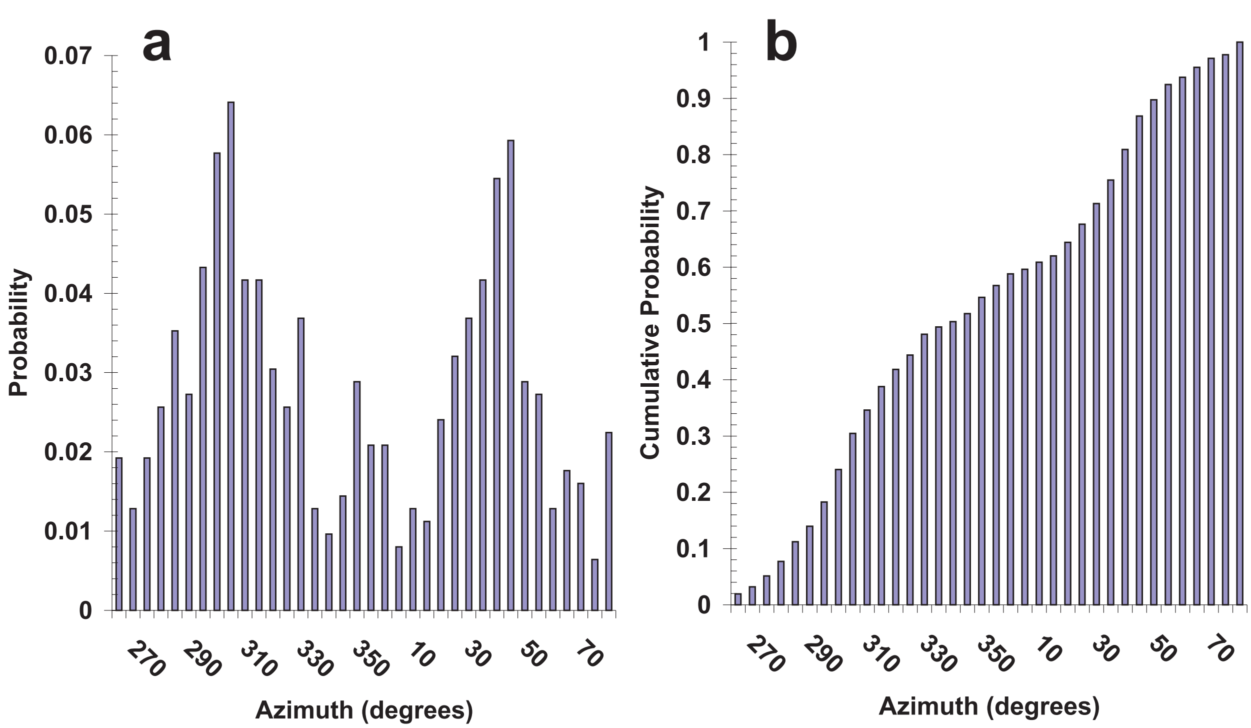

Figure 6. Frequency histograms for photolineament azimuth as mapped by Williams (1985).

Floridan aquifer (Figure 7). The equivalent transmissivity zones in the regional-scale model also are included in the local-scale model. The western half of the local-scale model has an equivalent transmissivity value of 5570 m^2/day. The eastern half of the model has an equivalent transmissivity value of 1860 m^2/day. Initially, the local-scale MODFLOW model was run as an EPM model.

MODPATH was used to perform forward-in-time particle tracking using results from the local-scale MODFLOW model. The purpose of the particle tracking was to determine if ground water at the North Lakes wetland travels to the Section 21 wellfield and if so, to provide an estimate of the advective travel time. This was achieved by inserting a single particle in the Upper Floridan aquifer (layer 2) directly beneath the North Lakes wetland. Initial placement of the particle in the Upper Floridan aquifer slightly reduces the total simulated travel time, because downward flow through the surficial aquifer is neglected, but measured travel times through the surficial aquifer are less than 100 days (Langevin et al. 1998). To perform the particle-tracking analysis, a deterministic value of 3% was specified for effective porosity. This porosity value for the Upper Floridan aquifer was estimated from a forced-gradient tracer test conducted at the North Lakes wetland (Langevin 1998; Langevin et al. 1998). Treating effective porosity as a deterministic parameter creates additional uncertainty in the Monte Carlo results; however, this rela-

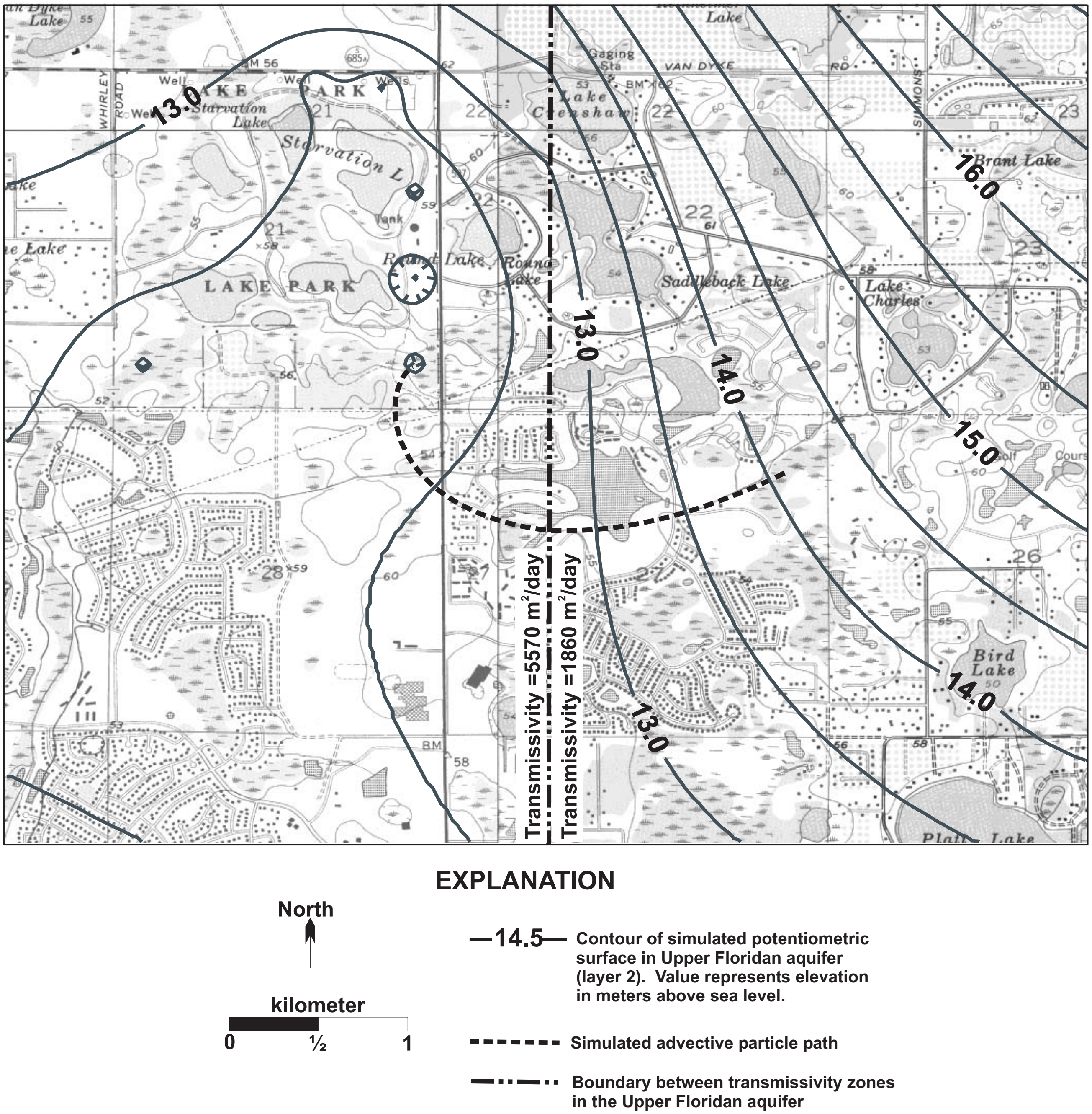

Figure 7. Simulated heads and advective particle path from the equivalent porous media model.

tively low porosity value is thought to provide conservative estimates of travel time to the wellfield.

Results from the flow model and particle tracking suggest that ground water beneath the North Lakes wetland is eventually withdrawn by a supply well at the Section 21 wellfield (Figure 7). Using the 1993 average hydrologic conditions, the simulated travel time to the Section 21 wellfield is approximately 24 years, much longer than the two-year minimum travel time established by the Southwest Florida Water Management District. Based on this EPM simulation, application of reclaimed water to the North Lakes wetland would be acceptable in terms of the minimum travel time requirement.

Relation Between Matrix Block and Bulk Transmissivity

A simple, two-dimensional MODFLOW box model was used to ascertain the effect that fracture zones have on the bulk transmissivity of the aquifer. The model domain used for the analysis was 4753 m × 4753 m. Specified heads were assigned to the eastern and western boundaries, and no-flow boundaries were assigned along the northern and southern edges of the model. Each model cell was 25.15 m × 25.15 m, resulting in a grid that consists of 189 rows and 189 columns. Values for the specified head cells were selected in such a way that the resulting hydraulic gradient is 1×10^{-3} and flow is from east to west.

Seven Monte Carlo analyses were conducted in which fracture length and orientation were treated as stochastic parameters using the statistical descriptions of Williams (1985). A different value was specified for the block transmissivity in each Monte Carlo analysis. The ratio between block transmissivity and fracture transmissivity, however, was held constant at 100. The seven values used for block transmissivity were 1000, 2000, 3000, 4000, 5000, 6000, and 7000 m^2/day. The resulting values of bulk transmissivity plot as a straight line against values of block transmissivity (Figure 8). Error bars represent one standard deviation. This linear relation is used later to determine block transmissivity values for the two transmissivity zones in the North Lakes local-scale model.

Also included in Figure 8 are transmissivity relations calculated using the projection method (Snow 1965) and geometric mean (Gelhar 1993). Both of these relations were calculated for fracture zones that are 100 times more transmissive than the surrounding matrix blocks, and thus are comparable with the numerically established relation. The projection method results in bulk transmissivity values that are higher than those calculated from the Monte Carlo analysis, because the projection method assumes that fracture zones are infinite in length. Using the geometric mean results in bulk transmissivity values that are less than those calculated with the Monte Carlo analysis. The substantial differences between the three relations suggest the transmissivity relation must be numerically established with a Monte Carlo analysis.

A model that explicitly represents fracture networks may be used to estimate large-scale hydraulic properties for continuum, or EPM, models. In a separate analysis, the box model was run with the hydraulic gradient imposed at different angles to the fracture zones in order to calculate a transmissivity ellipse. For each rotation angle, a Monte

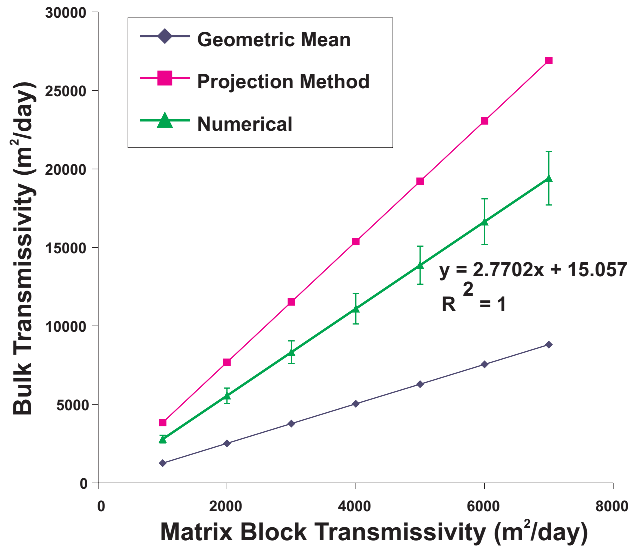

Figure 8. Relation between bulk transmissivity and matrix block transmissivity. Error bars represent one standard deviation.

Carlo analysis was performed using a block transmissivity value of 5700 m^2/day and a fracture zone transmissivity ratio of 100. Rather than plotting as an ellipse, the square root of bulk transmissivity plots almost as a perfect circle. The largest deviations from the median bulk transmissivity are <10% and occur for azimuths of 310º and 50º, which correspond to the most frequently observed orientations Figure 6). This analysis suggests that an isotropic assumption may be used for most large-scale EPM models in west-central Florida, provided the fracture zone properties used in the analysis accurately describe the fracture zones in the Upper Floridan aquifer.

An important assumption in this application is the specification of the deterministic ratio between fracture zone and matrix block transmissivity. If this ratio or fracture zone transmissivity value were treated stochastically, there may not be a distinct relation between the bulk and matrix block transmissivities. Parameter estimation techniques (Hill 1998) could be used in this circumstance to estimate matrix block transmissivity for each simulation within the Monte Carlo analysis. Matrix block transmissivity could be estimated by using field data as observations, or by using the equivalent transmissivity from the EPM model as an observation. This step would ensure that bulk transmissivity for each simulation in the Monte Carlo analysis would match the equivalent transmissivity from the EPM model, or that the model would remain calibrated to field data. Incorporating parameter estimation techniques into the Monte Carlo loop is a logical next step with this method.

Monte Carlo Analysis

In the previous series of simulations, a simple box model was used to derive a relation for converting an EPM model into a stochastic continuum model that explicitly includes fracture zone networks. In the following analysis, the EPM model developed for the North Lakes study area is converted into a stochastic fracture zone model to quantify the uncertainty in estimating travel times between the North Lakes wetland to the Section 21 wellfield. Fracture zones are incorporated into the North Lakes model using the derived relation between bulk and block transmissivity (Figure 8). To maintain the appropriate values for bulk transmissivity in the fracture zone model, the transmissivity values from the original model were adjusted according to the equation in Figure 8. Using bulk transmissivity values of 5570 and 1860 m^2/day (from the EPM model), calculated values of block transmissivity are 2000 and 670 m^2/day, respectively. This adjustment will ensure that the Upper Floridan aquifer in the fracture zone model will have a bulk transmissivity value similar to the equivalent transmissivity value assigned to the Upper Floridan aquifer in the EPM model.

The North Lakes stochastic model was run 50,000 times with MODFLOW and MODPATH to evaluate the range of possible ground water flowpaths. To ensure stability of the Monte Carlo analysis, mean travel times were calculated for progressively larger sample sizes. The Monte Carlo analysis converged to a median travel time of 20.3 years and a standard deviation of 23.9 years after about 35,000 simulations. A single particle placed within the Upper Floridan aquifer (layer 2) beneath the North Lakes wetland was used for each particle-tracking simulation. The results from one realization, which include both flow and particle-tracking simulations, are presented in Figure 9. This figure shows the effect that fracture zones have on ground water flowpaths. The particle tends to travel within the highly permeable fracture zone except where the

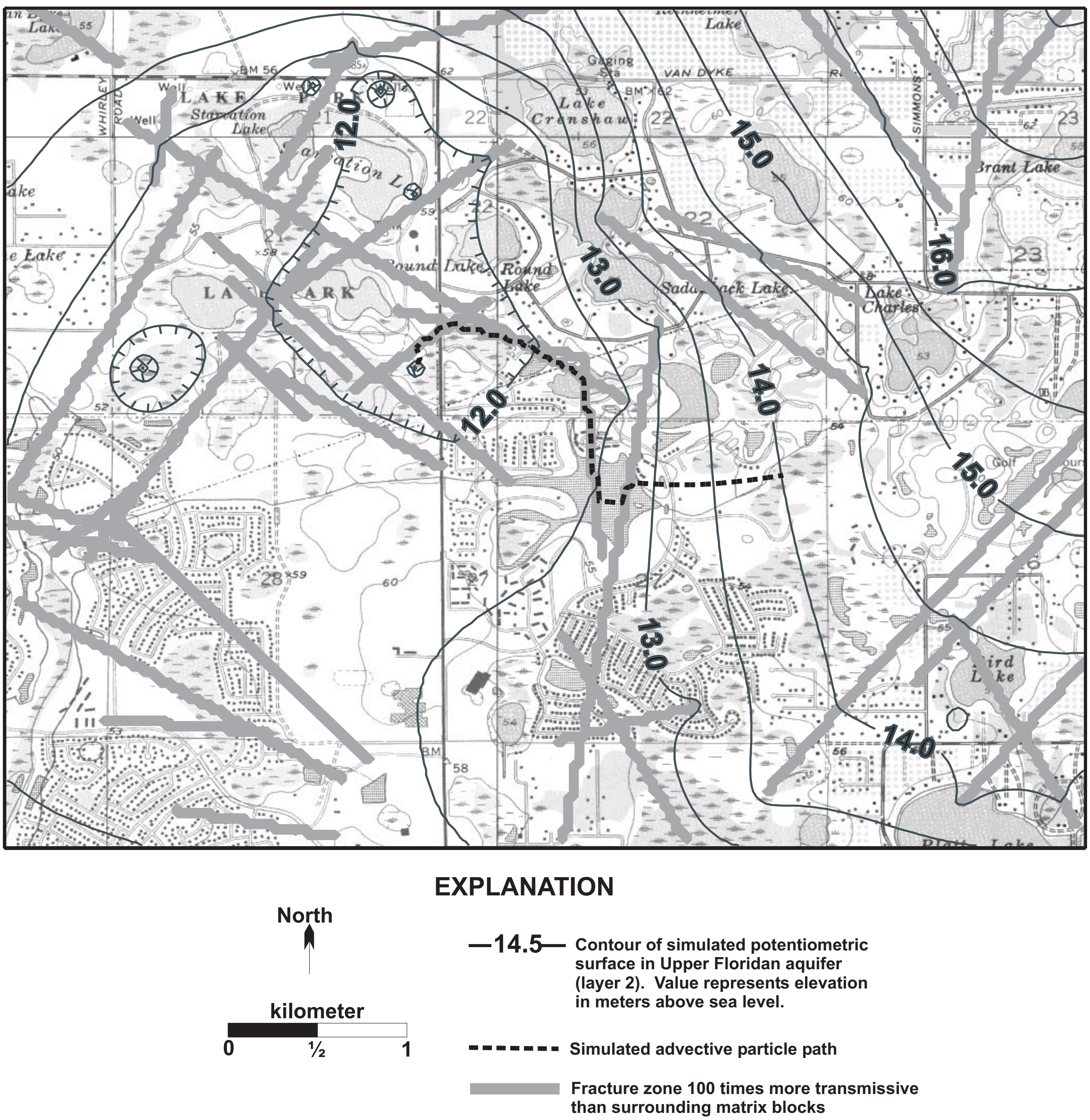

Figure 9. Simulated heads and advective particle path for a single realization of a fracture zone network.

hydraulic gradient forces the particle into a lower permeability matrix block.

Most of the simulated flowpaths lead from the North Lakes wetland to the Section 21 wellfield (79% of the particles are captured by the Section 21 wellfield). Figure 10 shows the travel paths for the first 100 simulations and illustrates the variability of the simulated travel paths, which are clearly affected by the fracture zones. Figure 11 presents a histogram of travel times for the captured particles; the left axis represents the percentage of particles that were captured during a particular year. Most of the particles (2.8%) were captured during year 12, but some particles take as long as 147 years for capture by a municipal supply well. The minimum particle capture time is 0.5 year. The cumulative probability (right axis) suggests there is about a 10% chance that the travel time will be less than seven years, and a 1.3% chance that the advective travel time from the North Lakes wetland to the Section 21 wellfield will be less than two years. This is new and valuable information beyond the reach of the original EPM model.

Summary and Conclusions

This paper describes a method for simulating the effect of large-scale vertical fracture zones on steady state ground water flow and advective transport. Fracture zones are discretely incorporated into a continuum model of ground water flow by adding high hydraulic conductivity features to the model grid. Two adjustments are required if the orientation of the fracture zone is not coincident with model rows or columns. First, the hydraulic conductivity used in the model must be set greater than the actual fracture zone hydraulic conductivity to account for the longer flowpath through the model grid (Equation 4). Second, travel time

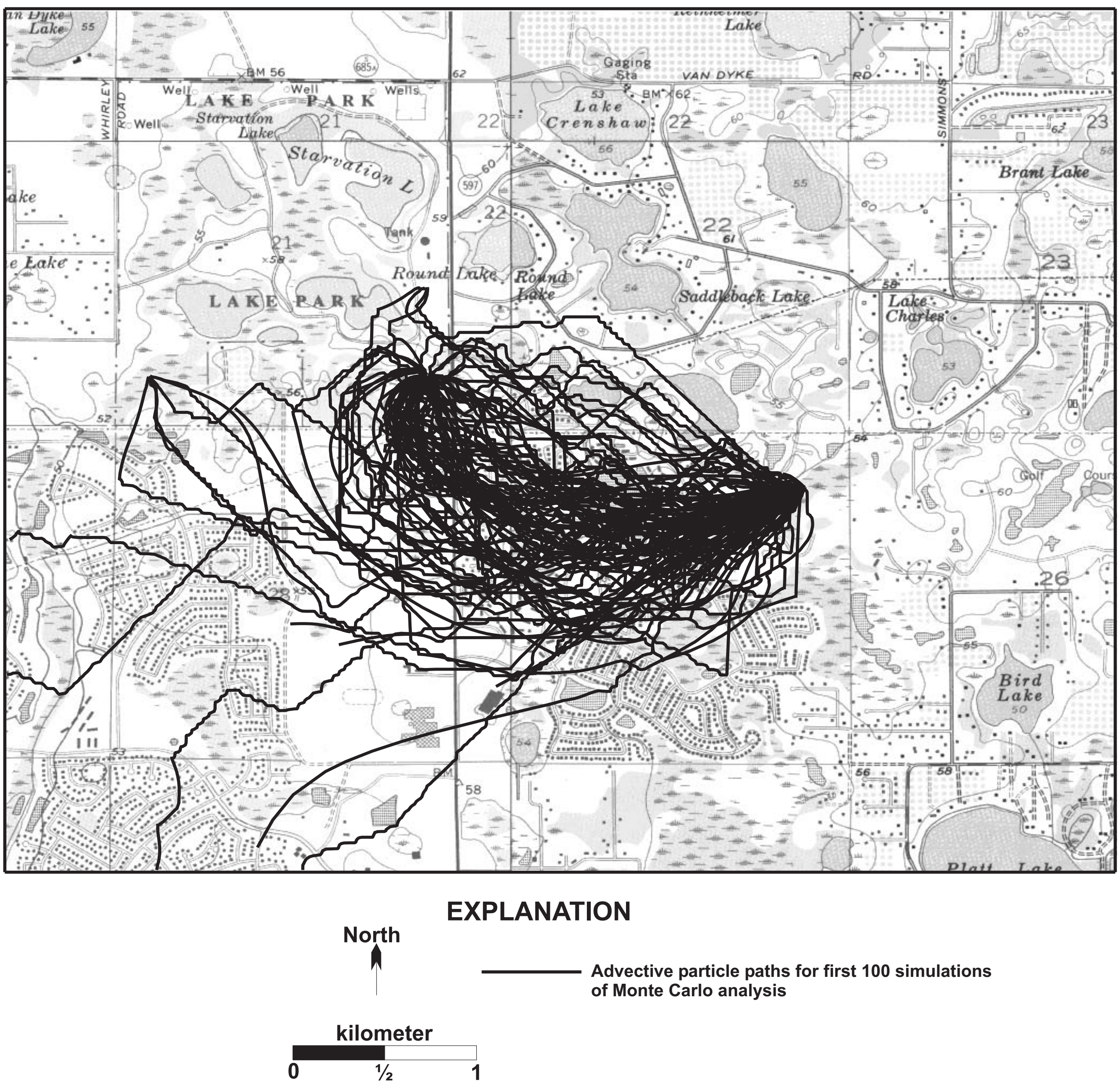

Figure 10. Advective particle paths for 100 realizations of fracture zone networks.

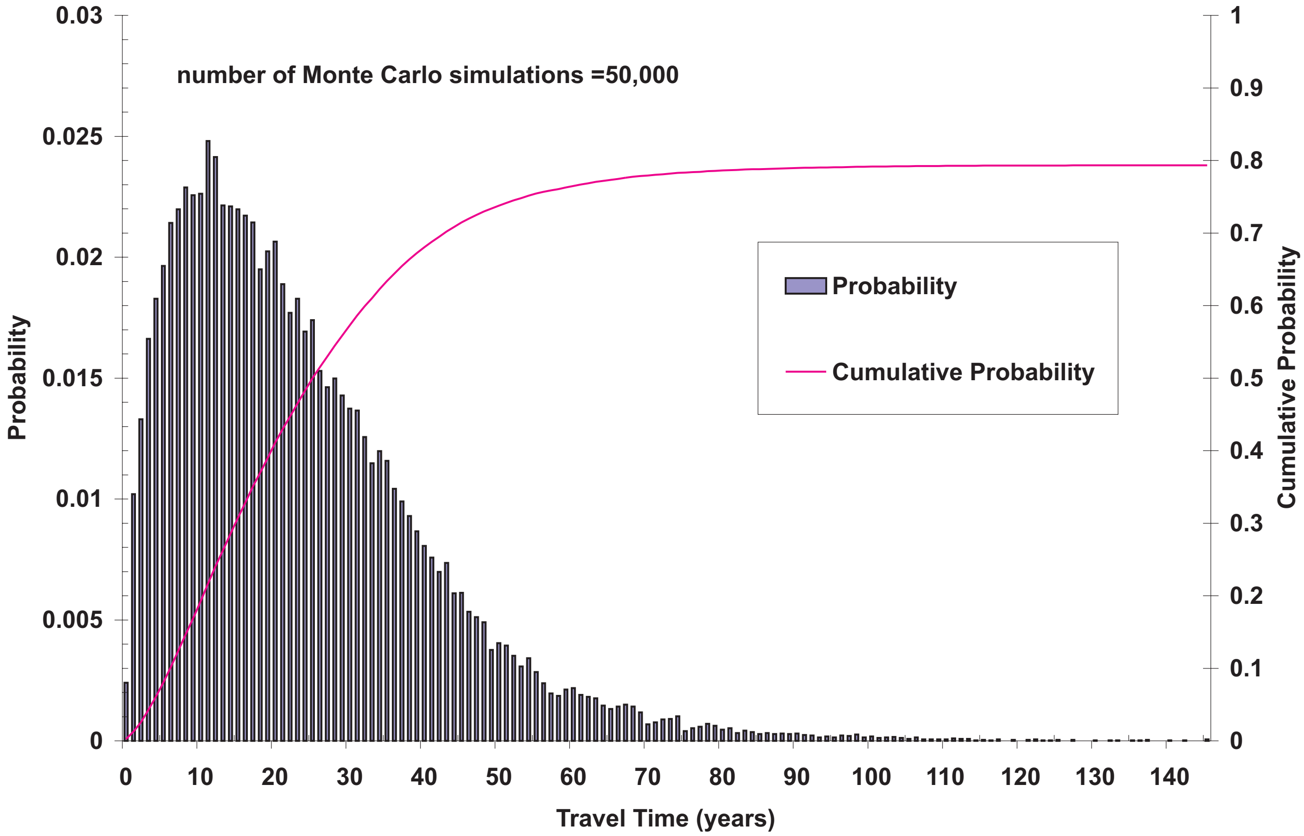

Figure 11. Plot of probability and cumulative probability for the simulated advective travel time between the North Lakes wetland and the Section 21 wellfield.

corrections are required during periods when a particle is traveling through the highly conductive fracture zone. By making these corrections, the hydraulic effects of fracture zones can be directly represented with cell-based models of ground water flow. Simulated travel times through some fracture zones may contain an error of up to 8%.

Monte Carlo analysis is used with the fracture zone continuum model to quantify uncertainties in one or more of the model results that arise from a limited understanding of fracture zone locations and properties. Based on field observations, fracture zone properties are statistically characterized using PDFs. The PDFs are then randomly sampled to generate many realizations of statistically reasonable fracture zone networks. Each fracture zone network is explicitly incorporated into a flow model formerly calibrated with the EPM assumption. To incorporate the network, matrix block transmissivity is adjusted so that the bulk transmissivity of the fracture zone model is similar to the equivalent transmissivity of the EPM model. The adjustment is based on a relation established with simple box models of different matrix block transmissivities. Uncertainties in simulated travel times are characterized by performing numerous simulations with the different network realizations. Future applications with this method could use parameter estimation techniques directly within the Monte Carlo analysis, rather than the transmissivity relation, to ensure that realizations accurately represent field data.

The methods developed in this paper are applied to a hydrologic investigation in west-central Florida that aims to quantify uncertainty in estimates of simulated ground water travel times from a wetland to a municipal supply wellfield. Results from an EPM flow and particle-tracking model suggest that the advective travel time from the wetland to the wellfield is 24 years. The problem with using the deterministic EPM model, however, is that there is no way to quantitatively estimate the confidence of the predicted travel time. This limitation poses a problem because potential health risks are associated with advective travel times of less than two years. The travel time estimate of 24 years is misleading considering that fracture zones may act as highly permeable pathways for ground water flow. One must conclude that the estimate of 24 years contains a large degree of uncertainty; however, the routine application of a deterministic model does not directly provide the uncertainty of the results. Sensitivity analyses can be performed using the numerical model, but these analyses provide only a qualitative feel for the uncertainty that may be present in the model.

By incorporating fracture zones into the numerical model, correcting for bulk transmissivity, and performing a Monte Carlo analysis, the uncertainty in simulated estimates of advective travel time is quantified. Results from the Monte Carlo analysis suggest that there is a 10% chance that the travel time will be less than seven years, and a 1.3% chance that the travel time will be less than two years. This type of information, which cannot be obtained by using the original EPM model, provides resource managers with a better understanding of the uncertainty associated with simulated estimates of advective travel times.

Acknowledgments

The author appreciates the encouragement and suggestions from his dissertation advisor, Mark Stewart, and others from the University of South Florida, including H. Len Vacher, Mark Ross, Thomas Juster, and Carl Steefel. Colleagues from the U.S. Geological Survey—Robert Renken, Dan Yobbi, Mike Deacon, Rhonda Howard, and Sandra Cooper—provided helpful comments on substance and presentation. Valuable discussions with Carl Albury initiated this research. The author would also like to thank Mary Anderson, two anonymous reviewers, and especially Douglas Walker for providing suggestions that significantly improved the quality of this paper. Appreciation also is extended to current and former staff of the Southwest Florida Water Management District, including Don Thompson, Kathleen Coates, Gregg Jones, Ron Basso, and Dave Moore, for funding and participating in the North Lakes wetland feasibility study.

References

Bear, J. 1993. Modeling flow and contaminant transport in fractured rocks. In *Flow and Contaminant Transport in Fractured Rock,* ed. J. Bear, C.F. Tsang, and G. de Marsily, 1–10. San Diego, California: Academic Press.

Cacas, M.C., E. Ledoux, G. de Marsily, and B. Tillie. 1989. The use of stochastic concepts in modeling fracture flow. In *Groundwater Contamination: Use of Models in Decision-Making,* ed. G. Jousma et al., 467–476. Dordrecht, The Netherlands: Kluwer Academic Publishers.

Cacas, M.C., E. Ledoux, G. de Marsily, B. Tillie, A. Barbreau, E. Durand, B. Feuga, and P. Peaudecerf. 1990a. Modeling fracture flow with a stochastic discrete fracture network: Calibration and validation, 1: The flow model. *Water Resources Research* 26, no. 3: 491–500.

Cacas, M.C., E. Ledoux, G. de Marsily, A. Barbreau, P. Calmels, B. Gaillard, and R. Margritta. 1990b. Modeling fracture flow with a stochastic discrete fracture network: Calibration and validation, 2: The transport model. *Water Resources Research* 26, no. 3: 479–489.

Chiles, J.P., and G. de Marsily. 1993. Stochastic models of fracture systems and their use in flow and transport modeling. In *Flow and Contaminant Transport in Fractured Rock,* ed. J. Bear, C.F. Tsang, and G. de Marsily, 169–236. San Diego, California: Academic Press.

Eaton, T., M.P. Anderson, and K.R. Bradbury. 2001. Heterogeneity in groundwater flow modeling; simulating fractures in a regional aquitard. *Abstracts with Programs–Geological Society of America* 33, no. 6: 169.

Fish, J.E., and M. Stewart. 1991. Hydrogeology of the surficial aquifer system, Dade County, Florida. U.S. Geological Survey Open-File Report 90–4108.

Freeze, R.A., J. Massmann, L. Smith, T. Sperling, and B. James. 1990. Hydrogeological decision analysis, 1: A framework. *Ground Water* 28, no. 5: 738–766.

Gelhar, L.W. 1993. *Stochastic Subsurface Hydrology.* Englewood Cliffs, New Jersey: Prentice Hall.

Hill, M.C. 1998. Methods and guidelines for effective model calibration. U.S. Geological Survey Water-Resources Investigations Report 98–4005.

Kraemer, S.R., and H.M. Haitjema. 1989. Regional modeling of fractured rock aquifers. In *Groundwater Contamination: Use of Models in Decision-Making,* ed. G. Jousma et al., 467–476. Dordrecht, The Netherlands: Kluwer Academic Publishers.

Langevin, C.D. 1998. Stochastic methods for evaluating the potential for wetland rehydration in covered-karst terranes. Ph.D. dissertation, Geology Department, University of South Florida-Tampa.

Langevin, C.D., D. Thompson, J. Laroche, C. Albury, W.B. Shoemaker, and M.T. Stewart. 1998. Development of a conceptual hydrogeologic model from field and laboratory data. Phase II results. North Lakes Wetland Project, Hillsborough County, Florida. A report prepared for the Southwest Florida Water Management District. Tampa, Florida.

Lattman, L.H., and R.P. Nickelson. 1958. Photographic fracture mapping in the Appalachian Plateau. *American Association of Petroleum Geologists Bulletin* 2, 2238–2245.

Lattman, L.H., and R.R. Parizek. 1964. Relationship between fracture traces and the occurrence of groundwater in carbonate rocks. *Journal of Hydrology* 2, 73–91.

Mabee, S.B., K.C. Hardcastle, and D.U. Wise. 1994. A method of collecting and analyzing lineaments for regional-scale fractured-bedrock aquifer studies. *Ground Water* 32, no. 6: 884–894.

McDonald, M.G., and A.W. Harbaugh. 1988. A modular three-dimensional finite-difference ground-water flow model. U.S. Geological Survey Techniques of Water-Resources Investigations, Book 6, Chapter A1.

McKoy, M.L., and W.N. Sams. 1997. Tight gas reservoir simulation: Modeling discrete irregular strata-bound fracture networks and network flow, including dynamic recharge from the matrix. In *Proceedings of the Natural Gas Conference Emerging Technologies for the Natural Gas Industry.* Washington, D.C.: U.S. Department of Energy's Federal Energy Technology Center Publication.

Moore, D. 1981. Geophysical signatures to photolinears at the Cross-Bar Wellfield, Pasco County, Florida. M.S. thesis, Geology Department, University of South Florida-Tampa.

Morrison, K.E. 1995. A numerical model of a fractured aquifer with dual porosity. M.S. thesis, Geology Department, University of South Florida-Tampa.

National Research Council. 1996. *Rock Fractures and Fluid Flow: Contemporary Understanding and Applications.* Washington, D.C.: National Academy Press.

Parizek, R.R. 1976. On the significance of fracture traces and lineaments in carbonate and other terrains. In *Karst Hydrology and Water Resources: Proceedings of the U.S. Yugoslavian Symposium,* volume 1, 47–108. Fort Collins, Colorado: Water Resource Publications.

Peck, A., S. Gorelick, G. de Marsily, S. Foster, and V. Kovalevsky. 1988. Consequences of spatial variability in aquifer properties and data limitations for groundwater modeling practice. IAHS Publication 175.

Pollock, D.W. 1994. User's guide for MODPATH/MODPATH-PLOT, version 3: A particle tracking post-processing package for MODFLOW. U.S. Geological Survey Open-File Report 94–0464.

Rayne, T.W., K.R. Bradbury, and M.A. Muldoon. 2001. Delineation of capture zones for municipal wells in fractured dolomite, Sturgeon Bay, Wisconsin, USA. *Hydrogeology* 9, 432–450.

Ritchie, A.W. 1983. Fracturing in carbonate rocks in central Florida. In *Proceedings of the 32nd Annual Meeting, Southeastern Section, Geologic Society of America,* Tallahassee, Florida, March 16–18, 1983. Boulder, Colorado: GSA.

SDI Environmental. 1994. An integrated surface and groundwater flow model. A report prepared for the West Coast Regional Water Supply Authority. Tampa, Florida: SDI Environmental.

Selroos, J.O., D.D. Walker, A. Strom, B. Gylling, and S. Follin. 2002. Comparison of alternative modeling approaches for groundwater flow in fractured rock. *Journal of Hydrology* 257, 174–188

Siddiqui, S.H., and R.R. Parizek. 1977. Hydrogeologic factors influencing well yields in folded and faulted carbonate rocks, central Pennsylvania. *Water Resources Research* 7, 1295–1312.

Snow, D. 1965. A parallel plate model of fractured permeable media. Ph.D. dissertation, University of California-Berkeley.

Svensson, U. 2001a. A continuum representation of fracture networks, Part I: Method and basic test cases. *Journal of Hydrology* 250, 170–186.

Svensson, U. 2001b. A continuum representation of fracture networks, Part II: Application to the Aspo Hard Rock laboratory. *Journal of Hydrology* 250, 187–205.

Vernon, R.O. 1951. Geology of Citrus and Levy Counties, Florida. Florida Bureau of Geology Bulletin 53.

Williams, S.R. 1985. Relationship of ground water chemistry to photolineaments in a karst aquifer. M.S. thesis, Geology Department, University of South Florida-Tampa.