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# **HYDROGEOLOGY**

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## **ASSESSMENT OF GROUNDWATER CONTAMINATION FROM AN INDUSTRIAL RIVER BY TIME SERIES-, FLOW MODELING- AND PARTICLE TRACKING METHODS**

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### **ABSTRACT**

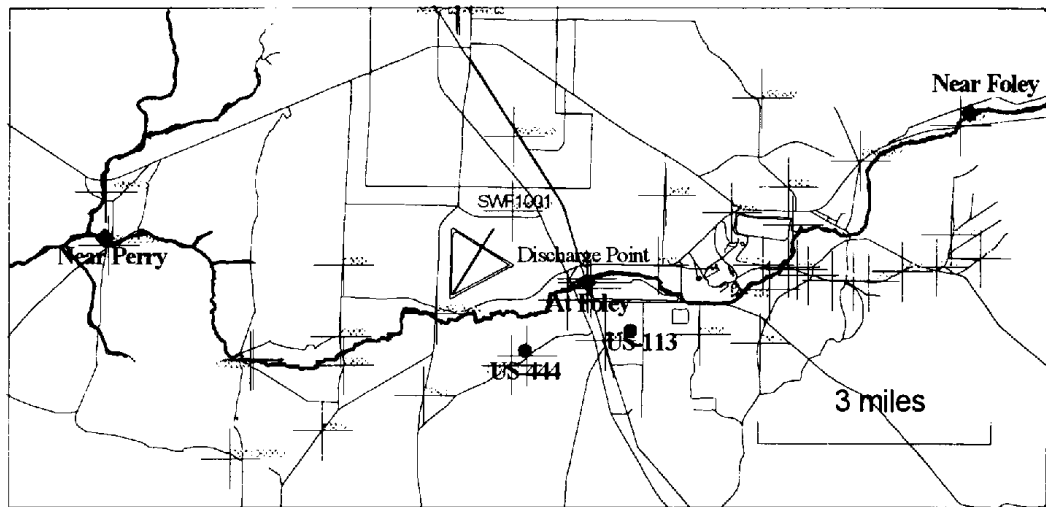
The interaction of an industrial river and the groundwater aquifer in Florida are modeled by time series-, flow modeling- and particle tracking methods. The major purpose of the modeling effort is to delineate the possible contamination corridor in the aquifer as may be caused by the infiltration of polluted water from the industrial river. The interrelations of precipitation, river discharge and groundwater data series are first analyzed by methods of structural time series, in order to quantify the interdependence of the groundwater table and river gauge heights, and thus to statistically examine the hydraulic possibility of aquifer contamination. The interaction of the stream and the groundwater is simulated by the USGS MODFLOW model. For the calibration, simulated water tables are compared with the historical records of monitoring wells in the adjacent aquifer. Lateral 'stagnant' points of the water flow based on the transient simulation are connected to delineate the maximal contamination corridor along both sides of the stream. In addition, particle tracking simulations with varying water sources and forcing conditions are conducted to compute the dynamic movements of water particles out and along the river banks. The modeling results show that lateral migration of contaminants close to the industrial discharge point might be up to several thousands feet in cross-river direction during times when the normally gaining (effluent) stream becomes sectionally a losing (influent) stream. The last situation occurs especially during multiyear-long time spans with less-than-normal precipitation which, for Florida, happens during times between major El Niño occurrences; i.e. during La Niña years.

### **1. HYDROLOGICAL BACKGROUND AND GOAL OF THE STUDY**

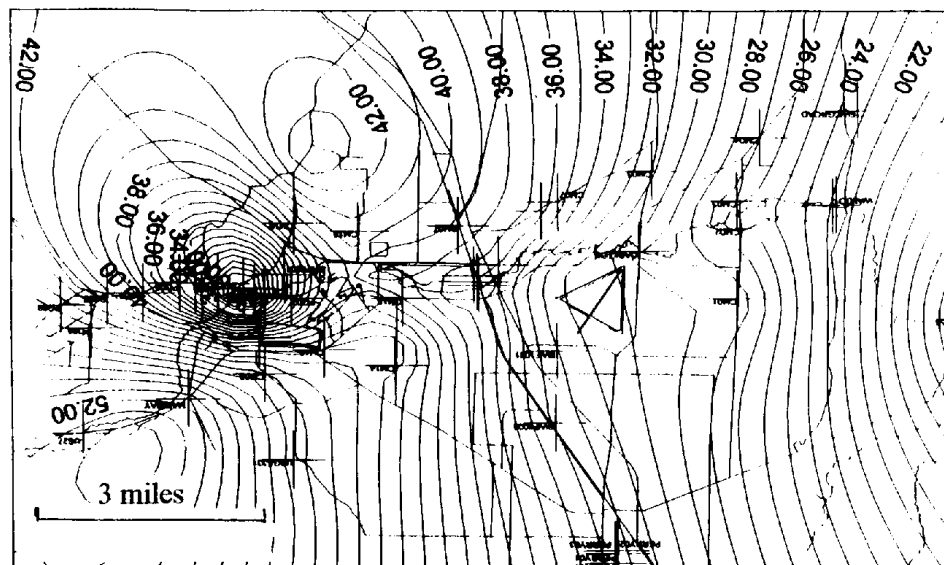
The small industrial river studied here is the Fenholloway river and is located in Taylor County in northwest Florida (Fig. 1). The stream has an average flow discharge of 132 ft<sup>3</sup>/s as has been measured at the USGS river gage station 'At Foley' near the US 19 bridge over the last 40 years (USGS, 1992), though with strong

seasonal variations. A few hundred feet upstream of this gage station, a paper mill factory has been discharging constantly about 70.5 ft<sup>3</sup>/s of wastewater into the river since the beginning of its operation in 1954. In fact, the Fenholloway presents a 'present-day anomaly' in the sense that it is the only river left in Florida that is still classified as a 'category-five' river which, by Florida law, is a stream whose only purpose is to serve as an open wastewater channel. The amount discharged by the paper mill is approximately equal to the quantity of water pumped by the factory from the underground by means of 7 to 8 production wells (Fig. 1). Although some additional water entering the hydrological system is produced from the timber decomposition process, it appears to be essentially lost through evaporation. The discharge water from the paper mill factory contains various organic constituents (Watts and Riotte, 1991), that are formed during the cellulose manufacturing process. The organic constituents isolated from the lignin residue of Fenholloway river samples (the 'Fenextract') can be classified into purgeable, extractable and NPTOX (Non-Purgeable Total Organic Halogen) organic compounds.

As most of the rivers in Florida, the Fenholloway river is generally an effluent or gaining stream, which means that the groundwater is recharging the river along its course. However, because of the paper mill's 70.5 ft<sup>3</sup>/s of contaminated water discharge into the river, a water-mound of about 1-2 feet is created close to the effluent point which may cause a reverse of the natural hydraulic gradient in its vicinity. The severity of this reverse gradient might increase during long dry seasons when the water table in the surrounding aquifer can become very low, while a high stream gage elevation is still maintained by the paper mill's huge effluent. Then the river may become influent in the section close to the discharge point, i.e., it may lose water to the surrounding aquifer and the potential of groundwater contamination by the polluted river water can arise. Also, because the paper mill pumps an average of 70 ft<sup>3</sup>/s of water from the underground, a wide drawdown depression cone of about 4 miles in diameter is formed around the pumping well gallery (Fig.2). This depression cone lowers the regional groundwater table even further during dry seasons, thus further increasing the lateral inverse hydraulic gradient. It is to be expected that the mounding effect in the vicinity of the paper mill's discharge point is less prevalent during a wet season, when the natural river discharge is already high. We call the above hydraulic situation in the present paper also the 'dry-season' scenario for aquifer contamination from sections of a normally effluent stream that have become influent. Since most of the residents along the Fenholloway river get their drinking water from their own private backyard wells, and given the above mentioned potential for groundwater pollution, it has been proposed by Florida public health authorities to connect the residents within the 'risk-corridor' along the river to public water supply lines. For this reason it is necessary to define the extreme boundaries (or water-lines) of this possibly polluted corridor along the Fenholloway river. This is the major objective of the present study and it will be achieved by



**Figure 1.** Study region with Fenholloway river and locations of wells (crosses) and streamgages (diamonds). Also depicted is the discharge point of the paper mill's wastewater effluent.



**Figure 2.** Water table contour map (ft) for 5/11/1994, generated with the SURFER plot package.

means of time series-, flow modeling- and particle tracking methods. Various conceptual models of this system that may lead to hydraulic conditions prone to aquifer contamination from polluted river water are tested by using hydrological and meteorological data from both historical records and obtained from a five-month-long groundwater and stream survey of the study region. Ultimately, 'worst-case' estimates of the possible spatial extensions of a contaminant plume emanating from the river over the short and the long term will be established by these models.

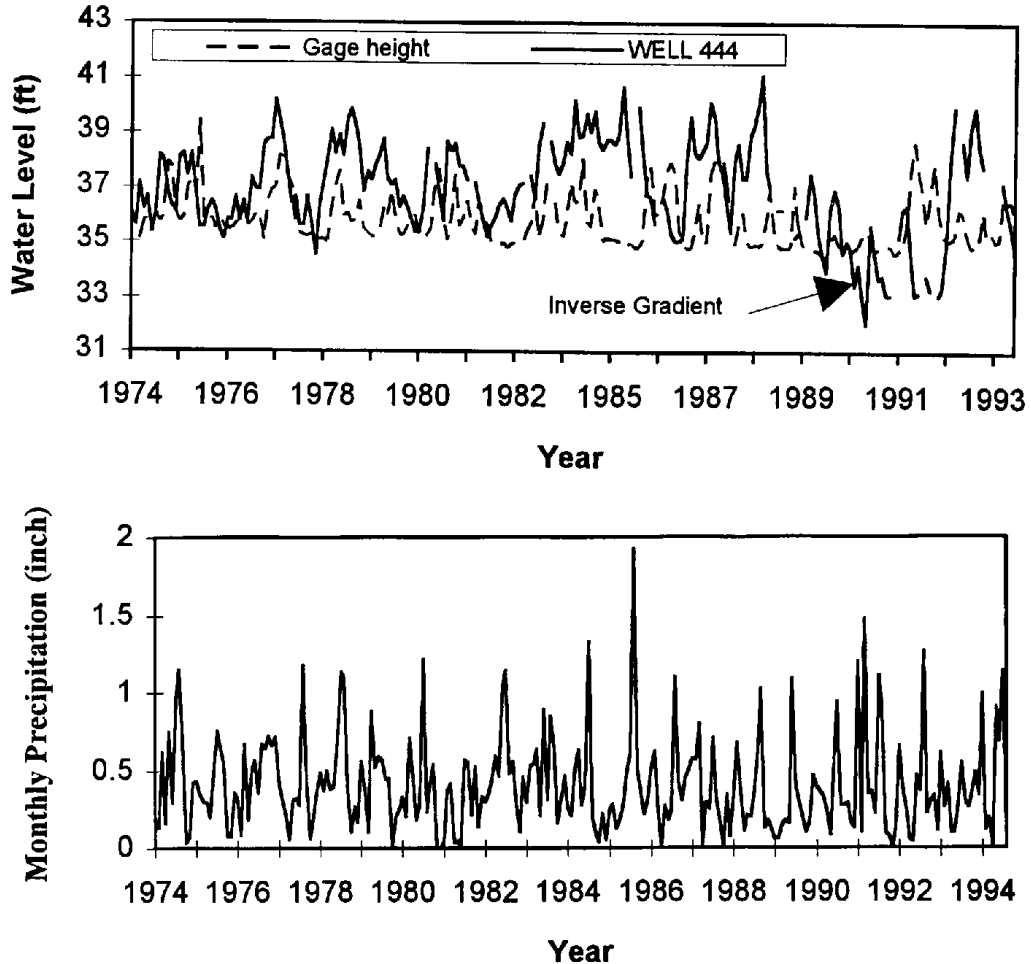
It should be noted, however, that the present study will only consider a hydraulic or advective flow approach to establish conservative water-lines beyond which no groundwater contamination from in-flowing river water is to be expected. Therefore, the classical solute transport mechanisms of hydrodynamic dispersion, adsorption and other chemical and biological decay reactions will not be included in the model. The implications of these limitations on the calculated estimates of the water-lines are discussed in detail in Koch et al. (1995). For example, neglecting adsorption will discard the process of retardation which, depending on the nature of the contaminants, can slow down its migration by factors ranging between 1-3 (Bear, 1979; Maidment, 1993). This means that the water-lines established in the present study by means of an advective travel-path analysis will represent the most extreme (worst-case) bounds. In other words, the proposed corridor of residential wells along the river that is to be connected to the public water supply has an inherent safety factor built in.

## **2. HYDROLOGICAL TIME-SERIES MODELING AND SYSTEM FEEDBACK STUDY**

Time series analysis helps to statistically define the characteristics of the data series involved and helps to quantify interrelations and possible correlations between different data series. The data series investigated here are the stream gages and -flow and the groundwater table elevations and precipitation records.

The gage-height data series analyzed consists of the monthly average records measured by the USGS over the last 20 years at the station ATFOLEY downstream of the paper mill's effluent point. The water table elevation series over that time period is taken from the USGS well #444 which is located about 1000m south of the river and 1500m west of US19. Note that other well-data was also available and could be tested using the same techniques, however this well was chosen because it is located outside the drawdown cone of depression and, therefore, its groundwater table elevations are not significantly affected by possible variations of the pumping rate of the plant. Fig. 3 depicts the time-series plots for both the stream gage elevations and the water table heights. Note in particular the inverse hydraulic gradient between the stream and ambient aquifer during the long drought period of 1988-1992 with anomalously low precipitation. The latter is also shown in Fig. 3 and has been gathered from the Florida Climate Data Center.

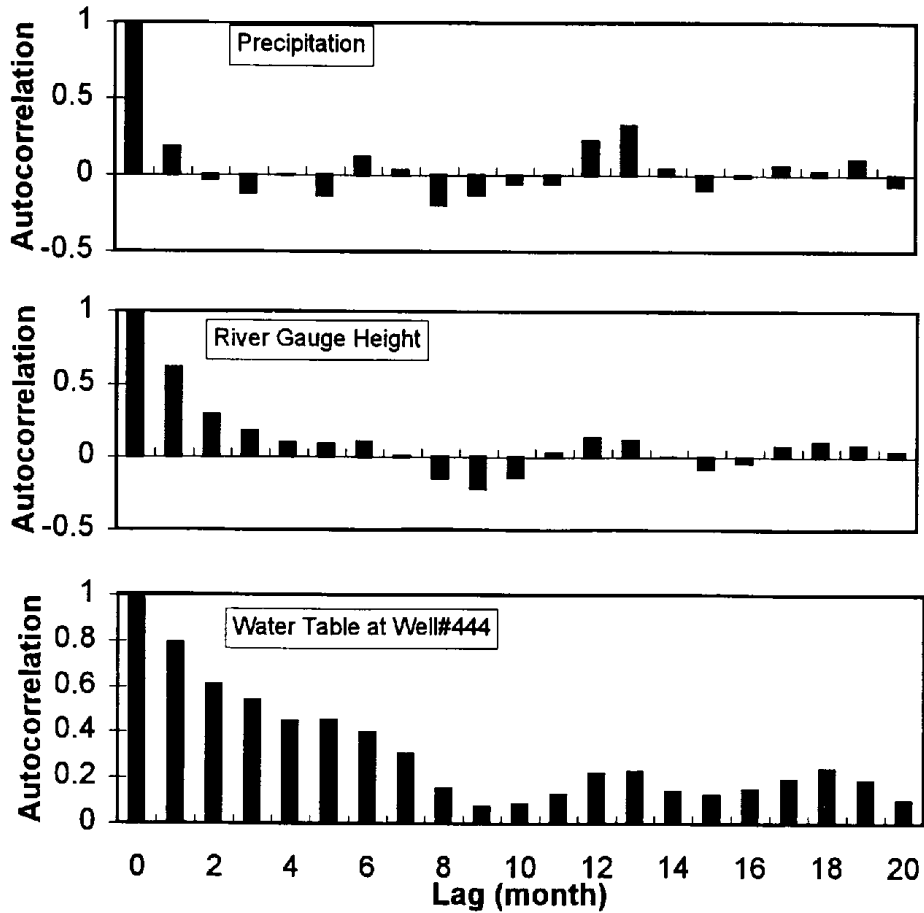
Using the Box-Jenkins methodology (Box and Jenkins, 1976; Pankratz, 1991) seasonal autoregressive integrated moving average (ARIMA) univariate models are established for groundwater table elevations, stream gage heights and precipitation levels. For a detailed discussion of the steps involved in the set-up of an ARIMA model, see Sun and Koch (1996) and Sun et al. (1997a).



**Figure 3.** River gage heights and water table elevations at well #444 (top panel) and precipitation in the area (bottom panel) for the last 20 years.

The three autocorrelation plots in Fig. 4 give some insight into the physical phenomena that govern the three processes of precipitation, water table elevations and river gage heights, respectively. For example, the computed autocorrelations for the precipitation are significant only for very short lag-periods of one to two months which shows that rainfall variations are rather short-term processes. Moreover, the autocorrelations exhibit to some extent the seasonality of the rainfall.

The autocorrelations for the stream gage heights look somewhat different from what is usually observed for a natural stream (Maidment, 1992), in the sense that correlations are significant over a long period of time. This is the direct consequence of the large permanent industrial discharge into the river. Finally, the autocorrelation for the groundwater table elevations demonstrates illustratively the long-term (low



**Figure 4.** Autocorrelations of precipitation (top panel), river gage height (middle panel) and water table elevations at well #444 (bottom panel).

frequency) processes that govern the recharge of an aquifer. One notices significant autocorrelations over longer lag-periods and the water table changes exhibit less seasonal trend than the precipitation.

As an example we provide in Eq. (1) the ARIMA model for the water table elevation ( $h_t$ ) of USGS well #444, as computed by means of the SAS statistical package (SAS Inc., 1993):

$$(1+0.2445B^2) \nabla h_t = (1-0.23B^2-0.217B^{10}) a_t \tag{1}$$

Here  $B$  is the backward shift operator with  $B X_t = X_{t-1}$ ,  $\nabla$  is the differencing operator with

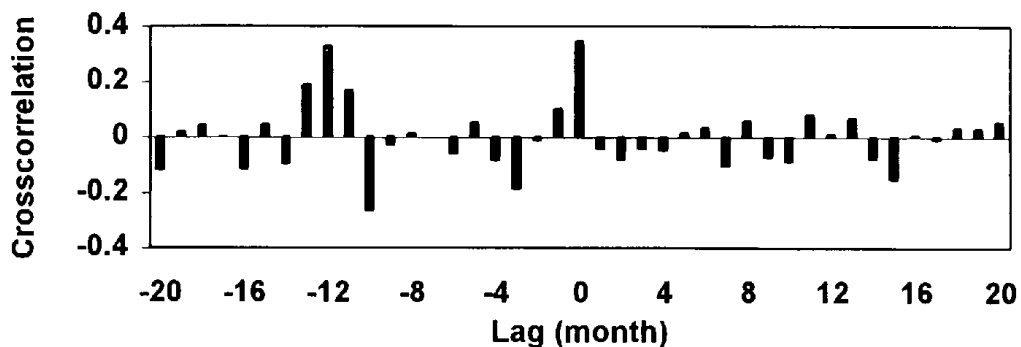


$\nabla=(1-B)$  which is used to make the time series stationary, and  $a_t$  is the random shock component. The form of the left side of Eq. (1) with the term  $B^2$  illustrates that the water table elevations have a 'memory' of up to two months.

Under a natural condition, the groundwater flow of the effluent river is a one-way process; i.e., water moves from the ambient aquifer into the river and the stream gage elevations depend on the groundwater level. This would imply, when setting up a so-called dynamic regression or linear transfer model (cf. Pankratz, 1991; and Sun and Koch, 1996), that the groundwater table elevation is the input signal and the river gage height the output signal of the model.

On the other hand, with 45 million gallons/day of wastewater discharged into the Fenholloway river, the question arises whether this interaction process in the vicinity of the effluent point is still one-way; i.e., whether the water is still only flowing in one direction from the aquifer towards the stream. If the answer is no, then the question arises about the possibility of reverse lateral migration of river water into the adjacent aquifer. In a time-series analysis, river gage heights (which over rating curves are related to the discharge rates of the river itself) will no longer only be a passive output signal. There is a 'system feedback' from the output to the input signals. The system feedback relates to the interaction (or the interrelationship) of the groundwater table and stream gage levels.

In order to examine this interrelation of the "input and output" data series, both river gage height- and ground water table data series are prewhitened by the above ARIMA model (1). Their residual series are then crosscorrelated. As shown in Fig. 5, significant correlations exist at both positive and negative lags after this prewhitening process. Whereas the significant positive crosscorrelations for positive lag-times imply that the river gage heights are related with the groundwater table



**Figure 5.** Crosscorrelations between river gage heights at ATFOLEY and water table elevations at Well #444.

elevations, the significant crosscorrelations at negative lags state that feedback from river gage elevations to groundwater table elevations exist as well. Thus, the water table elevations of well #444 and the river gauge heights at gage ATFOLEY at a given time are not independent from each other, leading to the possibility of hydraulic infiltration of polluted river water into the aquifer during certain periods of the analyzed 20 year-long data series.

### 3. FLOW MODELING OF THE STUDY SITE

To quantify the extent of the previously stated possible lateral migration of stream particles into the surrounding aquifer, the USGS finite difference groundwater flow model MODFLOW (McDonald and Harbaugh, 1984) will be used in the present section.

#### 3.1 Governing equations of the flow system

The groundwater flow equation solved by MODFLOW is the classical groundwater flow equation which, for the purpose of the present 2D (horizontal) application, is written here as (Bear, 1979; McDonald and Harbaugh, 1984):

$$\frac{\partial}{\partial x} \left( k_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_{yy} \frac{\partial h}{\partial y} \right) - N = S_s \frac{\partial h}{\partial t} \quad (2)$$

where  $k_{xx}$  [ $LT^{-1}$ ] and  $k_{yy}$  [ $LT^{-1}$ ] are the local hydraulic conductivities along the axes  $x$  and  $y$  (which are taken as isotropic though in the present case; i.e.,  $k_{xx} = k_{yy}$ );  $h$  [ $L$ ] is the hydraulic head;  $N$  [ $T^{-1}$ ] is the volumetric flow per unit volume of water sources and/or sinks; and  $S_s$  [ $L^{-1}$ ] is the specific storage.

Within the study area, the superposition of three major factors will essentially control the piezometric head distribution and, therefore, the overall groundwater flow pattern: (1) The regional groundwater flow (which is mainly driven by the topography of the area and will be generated in the model by means of appropriate boundary condition, as will be discussed further down), (2) the stress of the pumping well field of the paper mill, and (3) the interaction of the Fenholloway river with the ambient aquifer, the understanding of which is, of course, the eventual goal of this part of the study.

Regarding the simulation of the stream-aquifer interaction, the equations which need to be specifically mentioned here are the leakage equations as used in the river package of MODFLOW. The river package allows, on one side, water to flow from

the aquifer to the sink reservoir, thereby removing water from the model by seepage into particular reaches of the stream. On the other side, it also permits water to flow out of the stream into the aquifer. The river package uses the streambed conductance ( $C_{riv}$ ) ( $L^2T^{-1}$ ) to account for the length ( $L$ ) and width ( $W$ ) of the river channel in the cell, the thickness of the river bed sediments ( $M$ ), and their vertical hydraulic conductivity ( $K_r$ ) where

$$C_{riv} = \frac{K_r L W}{M} \quad (3)$$

The rate of leakage ( $Q_{riv}$ ) ( $L^3T^{-1}$ ) between the river and the aquifer in the case when the riverbed is fully saturated is calculated from

$$Q_{riv} = C_{riv}(H_{riv} - h) \quad h > R_{bot} \quad (4)$$

where  $H_{riv}$  is the head in the river (the gage elevation) and  $h$  is the head in the ambient aquifer. Depending on whether  $H_{riv} - h$  is negative or positive, the river will become a gaining (effluent) or losing (influent) stream, respectively. However, when the water table in the aquifer falls below the bottom of the streambed ( $R_{bot}$ ), leakage stabilizes and  $Q_{riv}$  is calculated from

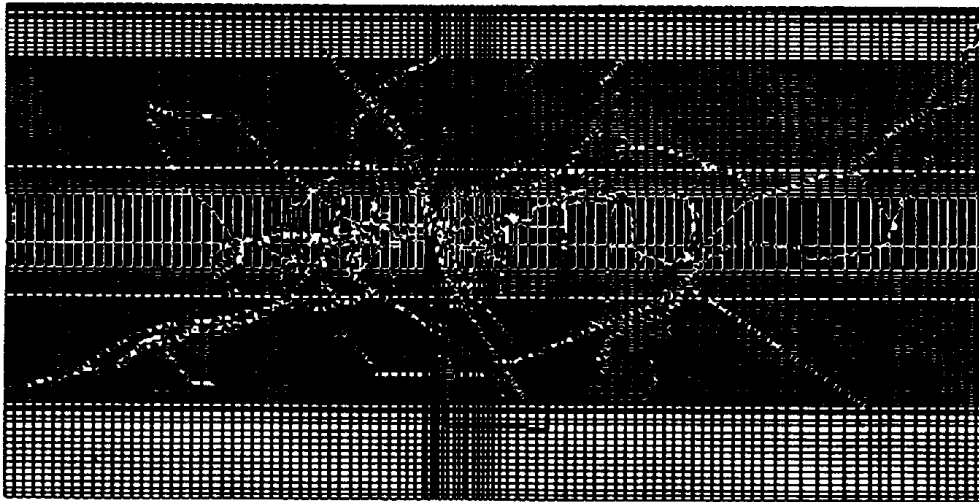
$$Q_{riv} = C_{riv}(H_{riv} - R_{bot}) \quad h \leq R_{bot} \quad (5)$$

## 3.2 Calibrated steady state models

### 3.2.1 Finite difference grid and general set-up of the models

The finite difference grid of the study area is shown in Fig. 6. The area of the model has a size of about 40 x 20 km and is centered in E-W direction close to US 19. The model area covers the paper mill's pumping well field and the ponds, and extends westward close to the gulf coast. The mesh is telescopic with finer grid-sizes in the center of the model domain in the vicinity of the paper mill's discharge point along the river; i.e., the area which is naturally of interest here. The gridding of the mesh results in a resolution of 50 to 100 m in NS direction on both sides of the Fenholloway river and of about 100 m in EW direction in the vicinity of the effluent point.

The primary purpose of the steady-state calibration is to determine optimal values for



**Figure 6.** Finite difference grid used in the MODFLOW models .

the hydraulic conductivity of the aquifer and possibly lateral variations of the latter, as might be indicated by the surficial geological formations in the region. For this reason the model-layer is divided in up to four zones; each of which is a different hydraulic conductivity assigned to, which are refined during the calibration process. The classification of these zones is somewhat arbitrary and is based essentially on the observed pattern of the gradient of the flow and the topography.

As discussed by Anderson and Woessner (1992), selection of appropriate model boundaries and boundary conditions in a numerical model is one of the most crucial, but also difficult tasks. With the location and size of the model grid as shown in Fig. 6, direct natural boundaries of the Fenholloway groundwater flow system are not matched, particularly not for the northern and the southern boundaries of the model. The situation is slightly more favorable for the eastern and western boundaries, although in the east these do not extend fully to the watershed boundary that divides the Fenholloway from the Suwannee river watershed, whereas in the west only the southwest corner of the model reaches the Gulf of Mexico.

### **3.2.2 Boundary conditions and enforcement of stream gauges**

For the steady-state models all four boundaries of the model are set up as constant head (Dirichlet) boundaries, with the head-values extracted approximately from the krigged isoline contour maps of the measured water table elevations of the January-June, 1994, field survey (see Fig. 2). Because of the rather large distance of the

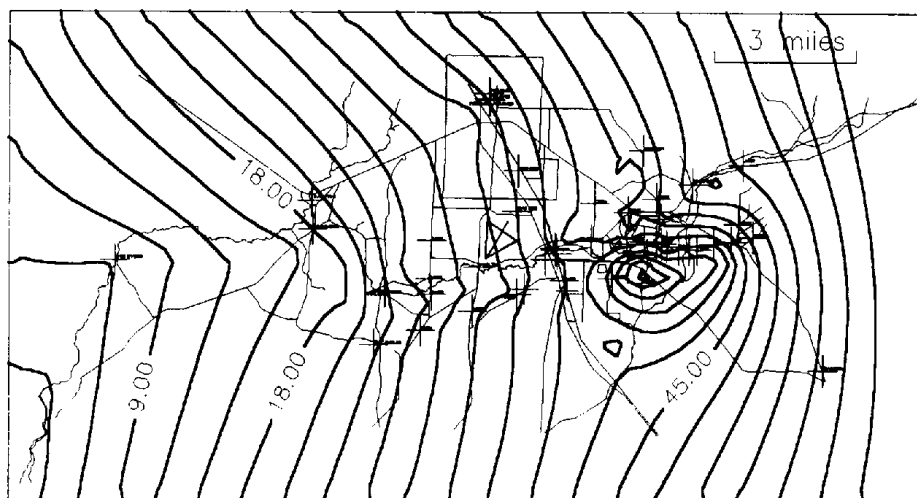
boundaries from the central model region of interest, the exact specification of the boundary head values is not too crucial, and the model is mostly constrained by the interior nodal values for the head which are taken from the real observations.

The Fenholloway river is implemented by means of the river and drain packages. The drain package works in much the same way as the river package, discussed earlier, except that leakage from the drain to the aquifer is not allowed and that discharge to the drain is zero whenever heads in the cells adjacent to the drain are equal to or less than the assigned bottom elevation of the drain. Because of this, drains can only be used for the simulation of a permanently gaining (effluent) river, unlike river-nodes, which can mimic both an effluent and an influent stream.

With these considerations, the Fenholloway river is modeled in the region of interest, which extends from about 1000 m east of the paper mill's discharge point over a length of about 7 km to the west, where the river turns toward the north, by river nodes to allow for influent and effluent conditions. Further downstream toward the Gulf of Mexico the river is treated as a set of drains, because it can be assumed that the Fenholloway is an exclusively gaining stream in this section. The river bottom elevations are read from topographical maps, and the river gage heights are calculated through linear interpolation from the values measured at the USGS stream gage station 'AT FOLEY', close to the discharge point, and the station 'NEAR PERRY', about 5 miles further downstream (Fig. 1), and using the average topographic slope of the Fenholloway river.

### 3.2.3 Model calibrations and hydrological implications

The steady-state model is calibrated based on water table elevation data of the January-June, 1994, field survey. Because of only moderate variations of the precipitation during that time period, no major differences of the piezometric heads are inferred for the different sampling days in this period. Therefore, as the reference data set for the calibration, we have used the elevation data sampled on 5/11/1994 which is rather complete (Fig. 2). In addition to this visual check of the calibration results and optical comparison of the modeled with the measured piezometric contour map, the residuals between measured and modeled watertable elevations are calculated at the locations of the monitor wells. Initial conductivity ranges were obtained from Bush and Johnston's (1988) discussion of the regional hydrogeology and some aquifer pump test data. Numerous calibration simulations were performed, with values for the hydraulic conductivities  $k$  ranging between 50 and 400 ft/day (whereby in one model the  $k$  values within the four assigned conductivity zones increase slightly toward the west) and river conductances (taken as constant along the river course) ranging between 20000 ft<sup>2</sup>/day and 70000 ft<sup>2</sup>/day. An average aquifer thickness of 1500 ft has been assumed in the calculations.



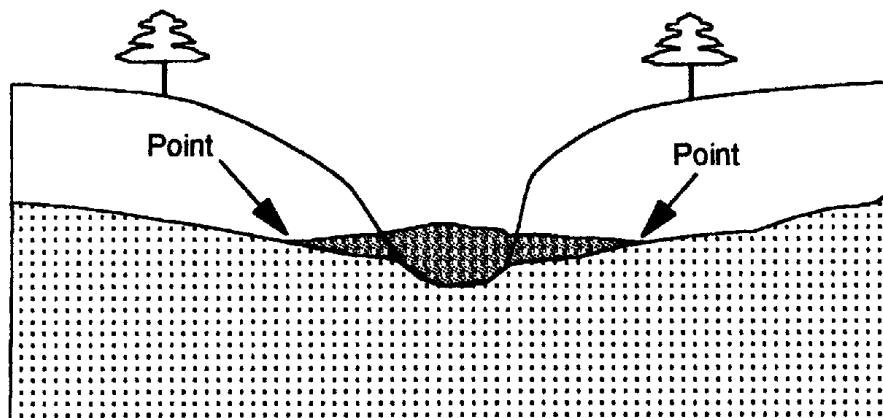
**Figure 7.** Calibrated steady-state model for elevation data (ft) of 5/11/94.

Results of steady-state four-zone MODFLOW calibration model are depicted in Fig. 7. In addition to providing calibrated conductivities and river conductance values, this steady-state model generates also the initial head condition for the transient simulations to be carried out in the next section.

### 3.3 'Static' transient model line and the delineation of water lines

#### 3.3.1 Objective and formulation of the conceptual model

The objective of these 'static' transient MODFLOW models is to simulate a pre-specified lowering of the groundwater table due to a recharge deficit and drainage during an extended dry season, as it has been observed at some of the wells in the vicinity of the river during the long drought period of 1988-1991 (Fig. 3). Therefore, the 'static' model attempts to mimic hydraulic conditions that are prone to infiltration of river water into the surrounding aquifer. It should be clear that it is the variation of the natural recharge of the aquifer through rainfall that is the physical trigger mechanism for the groundwater table fluctuations. A deficit of precipitation and increased evaporation during a long dry season is responsible for a groundwater table drop. However, these effects are not included in the present static model, since we are interested here only in the hydraulic implications of a lowering of the water table beneath the sustained stream gage elevation (see below) on the head distribution in the ambient aquifer. Fig. 8 shows a cross-sectional view of the conceptual model



**Figure 8.** Conceptual cross-sectional model for the delineation of static water lines

which is the basis of the delineation of the static water lines. The lowered groundwater table results in a positive hydraulic gradient from the river bed into the aquifer so that, by virtue of Darcy's law, a river particle will be driven toward the aquifer.

This conceptual model is based on the assumption that the minimum river gauge is sustained during the time span of the simulated drought and during the groundwater table drop. This, of course, is not the case for a natural stream which is in equilibrium with the surrounding aquifer and where the stream-bed might be drying out completely during an extreme drought as is often the case for the section of the Fenholloway river upstream of the paper mill's discharge point. On the other hand, because the industrious plant is constantly recharging the Fenholloway river with approximately 45 million gallons per day, there will be a minimal river gauge height downstream of the discharge point, which should always be sustained. This is supported by the records of the USGS river gauge station "AT FOLEY", which reveal an absolute stage height minimum of 34.56 ft measured during the dry season of 1989-1990 (as compared with a monthly average of about 36 ft over the last 30 years (Fig. 3)). This is the value being used in the MODFLOW river package and it is kept constant throughout the transient static simulation.

### 3.3.2 Boundary and initial conditions

The boundary conditions used in the transient models are different from those in the steady-state models earlier and are also more intricate to implement into the MODFLOW model. Since the piezometric heads at the boundaries are also changing in time and are not known *a priori*, they cannot be used in the transient simulations.

Instead, flux boundary conditions are employed which are selected to first order in such a way as to sustain approximately the average observed steady-state regional flow. This means in particular that the above combination of flux boundaries was chosen such as to generate an average regional groundwater flow in the southwestern direction, as observed from the piezometric contour lines, deduced from the historical well-data records and from the January-to-June, 1994, field survey (Fig. 2). With this we have for the boundary and initial conditions:

***Eastern and northern boundaries:*** Inflow flux boundaries to simulate horizontal recharge of the aquifer due to the topographic gradient. It is implemented by means of the well-package of the MODFLOW model, whereby 100 injection wells in the north and 149 wells in the east are placed at the nodal points along both boundaries. The amount of the injected water for each well is calculated based on the total incoming recharge at average steady-state conditions and using Darcy's law  $q = kA \nabla h$ , where  $q$  = flow rate,  $k$  = conductivity,  $h$  = pressure head,  $A$  = area, and  $\nabla$  = gradient operator. In the present situation  $\nabla h$  is equal to  $dh/dx$ , the regional flow gradient, and is estimated from the observed and previously modeled piezometric head contour lines of the January-to-June, 1994, survey and  $A$  is the product of the cell length and the effective saturated aquifer depth  $b$ .

***Western and southern boundaries:*** Drain boundaries. The exact specification for the drain depths at the western and southern boundaries is not too important for the purpose of the present static transient simulation of a 'worst-case' scenario of a water-table drop during a long dry season. Therefore, the drain depths have been chosen after various trial-and-error runs in such a way, as to make sure that the groundwater table can drop in the eastern section of the model by about 5 ft and in the area north of the Fenholloway by about 3 feet. Again, the conceptual idea of the transient simulation is to simulate a 'worst-case' scenario of a long dry season during which the groundwater table in the vicinity of the paper mill's discharge point may drop by about 3 or 4 feet.

***Initial conditions:*** The initial conditions for the transient simulations are created from the previous steady-state simulations. As such they would be representative of the piezometric head distribution of 5/11/1994. However, this particular condition is not of importance for the purpose of the present static model which simulates only what could happen hereafter, if the groundwater table were to drop due to a long dry season. Therefore, although the simulations presented start from the 5/11/94 initial head distribution, they simulate a realistic scenario that might have happened in the past, as indicated by the historical records for the water table elevations, or that may occur in the future.

### 3.3.3 Calibration of the static transient model



The criteria for the calibration of the transient model are: (1) piezometric heads agree satisfactorily with the limited measured historical head data available; (2) the depression cone created by the paper mill's pumping well is adequately represented; (3) the overall mass balance budget of the model is in reasonable compliance with the hydrological constraints of the Fenholloway stream/aquifer system.

The main hydraulic parameters to be adjusted in the calibration process and which directly affect one or more of the above factors are: (1) the hydraulic conductivity  $k$ ; (2) the storativity factor  $S$ ; (3) the river and drain conductance  $k_r$ ; and (4) the effective aquifer thickness  $b$ .

The present MODFLOW models show the highest sensitivity to the variation of the hydraulic conductivity  $k$ . With increasing  $k$  the regional flow might 'wash away' the depression cone that is created by the pumping well field, whereas with decreasing  $k$  the latter becomes deeper. The aquifer thickness  $b$  needs also to be adjusted in this one-layer unconfined-aquifer flow model which, following the Dupuit-assumption, assumes that the flow in the vertical direction is negligible (Bear, 1979).

In addition to the hydraulic parameters, some numerical parameters that might affect the reliability of the MODFLOW solution are to be adjusted as well. These are the length of the stress period and of the time step increments within one stress period. Although by nature of the numerical implementation (implicit time-integration), the MODFLOW program is unconditionally stable, regardless of the time-step used, time steps too large may cause problems with the convergence during the iterative solution process. Changes of the aquifer thickness  $b$  greatly affect the budget analysis. Within the transient calibration, through changes of  $b$ , of the enforced boundary conditions, such as the injection wells and the drains (see previous section), and of the storativity  $S$ , the amount of drained water can be calibrated.

The mass-balance calculation provided within MODFLOW provides a clue of what are the important in- and outflow components of the aquifer/stream system. The calibration models show that the storage factor has a strong impact on the budget balance. Whereas with relatively small storativities ( $S = 0.1$ ) the mass budget is fairly balanced, for values of  $S$  too large (e.g.  $S=0.4$ ), unbalanced budgets may be produced. On the other hand, larger  $S$  facilitate the convergence of the solution process, since large  $S$  imply that the unconfined aquifer can yield enough water from the pore-storage without a large drop  $\Delta h$  of the water table.

### 3.3.4 Model results: Delineation of static water lines

Numerous calibration simulations were executed, during which the hydraulic conductivities, the river conductance and the storativity are varied in the model over

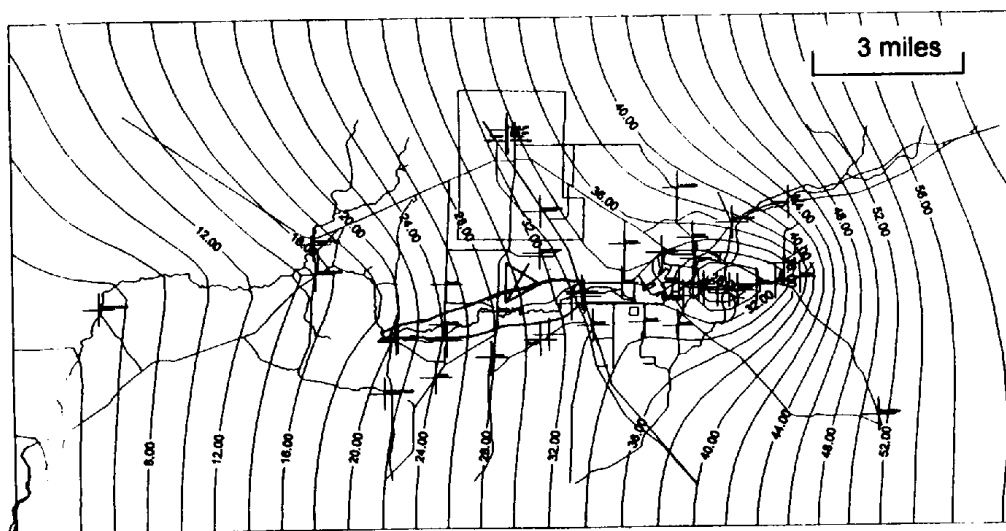
a reasonable range of values. Among these model cases we show the results of three particular simulation models, with the most important hydraulic parameters as indicated:

**Model case #1:** Hydraulic conductivity  $k=90-120$  ft/day, river conductance  $k_r=20000$  ft<sup>2</sup>/day, thickness of the aquifer  $b=1000$  ft, storativity  $S=0.1$ ;

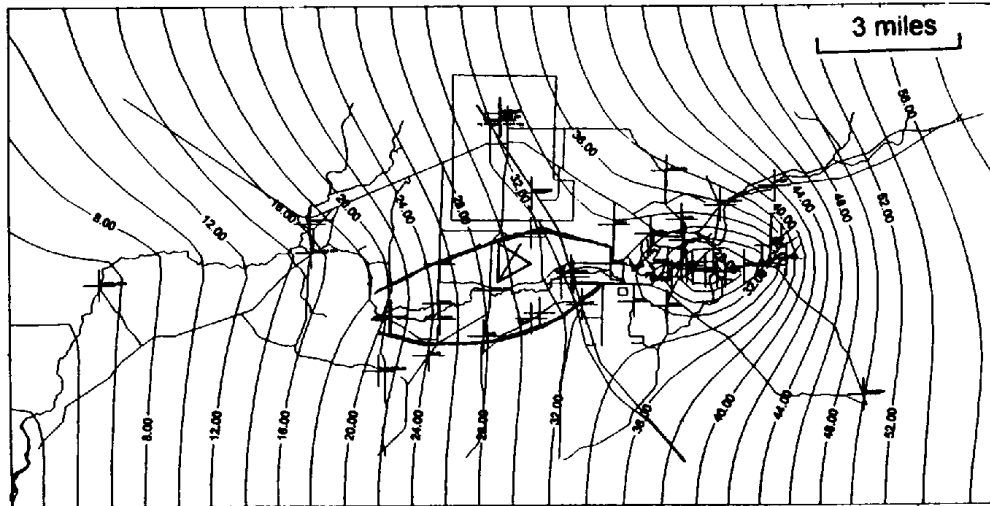
**Model case #2:** Hydraulic conductivity  $k=150-180$  ft/day, river conductance  $k_r=20000$  ft<sup>2</sup>/day, thickness of the aquifer  $b=1000$  ft, storativity  $S=0.1$ ;

**Model case #3:** Hydraulic conductivity  $k=90-120$  ft/day, river conductance  $k_r=20000$  ft<sup>2</sup>/day, thickness of the aquifer  $b=1000$  feet, storativity  $S=0.15$ .

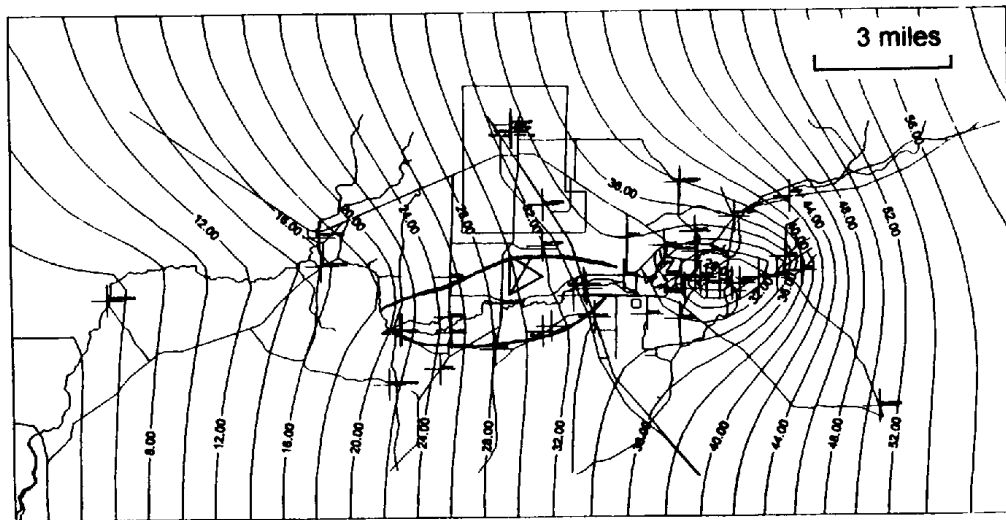
The Figs. 9, 10 and 11 show that, as the dry season goes on, the groundwater table elevation drops slowly because of the water drainage out of the aquifer. This behavior is visualized best by following one particular isoline and watch it moving upstream (in eastern direction) as time increases. However, up to about simulation day 200, the curvature of these isolines in the vicinity of the Fenholloway river is such, that lines orthogonal to the piezometric isolines (which by Darcy's law are the groundwater flow lines) are directed downstream (westward) and toward the river, i.e., the latter is still a gaining stream. From simulation day 240 on, the piezometric isolines close to the river change direction and perpendicular lines will point away from the river, i.e., it becomes a losing stream. Therefore, lateral migration of river contaminants into the aquifer becomes now possible.



**Figure 9.** Transient static simulation of water table drop (ft): Model case #1, after 240 days. Solid lines on both sides of the river are the static water lines.



**Figure 10.** Transient static simulation of water drop (ft): Model case #2, after 448 days.



**Figure 11.** Transient static simulation of water drop (ft): Model case #3, after 448 days.

An envelope for the outgoing flowlines on each side of the river can be constructed by connecting those points on a head isoline where it curves toward the river again. These two envelopes define the hydraulic boundaries which river pollutants would not be able to penetrate under any circumstances if they were to migrate out to these

points. They are called here the *static water-lines* and define the most extreme corridors of possible Fenholloway river/aquifer pollution. However, they move further outward, away from the river, as the water table continues to drop with increasing length of the dry season. After 448 days, when the groundwater table in the vicinity of the paper mill's discharge point has dropped by approximately 3 feet, these water lines have extended to about 1.5 to 2 miles in northern and southern direction from the river and reach about 2.5 miles after 800 days of dry-season simulation. To illustrate the effects of the different hydraulic conductivities and storativities, snapshots for model cases #2 and #3 are shown in Figs. 10 and 11, respectively. After 450 days of dry-season simulation, for model case #2 with a conductivity  $k$  of 150-180 ft/day the inferred water lines are very similar to those of model case #1, though the depression-cone of the paper mill's pumping well field becomes shallower (see Figs. 10 and 11). This tendency is in agreement with those of the previous steady-state MODFLOW models. The 450-days snapshot for model case #3 (Fig. 11), with a storativity of  $S=0.15$ , exhibits a slightly narrower water-line corridor than that obtained for the model case #1 (storativity  $S=0.1$ ). This is due to the fact that the aquifer can now sustain more drainage out of pores without the need of a major groundwater table drop.

### 3.3.5 Discussion and implications of the static flow models

**Table 1.** Simulated transient water table drops (ft) in several wells to be used for the selection of the appropriate water lines.

| Wells\Days |                          | 240                  | 330  | 448  | 601(days) |
|------------|--------------------------|----------------------|------|------|-----------|
| Wells      | WaterLevel<br>in 5/11/94 | Water Table Drop(ft) |      |      |           |
| US#444     | 36.50                    | 5.20                 | 5.50 | 6.00 | 6.30      |
| US#113     | 37.72                    | 4.72                 | 5.22 | 6.22 | 6.70      |
| MW#13      | 36.18                    | 2.68                 | 3.18 | 4.18 | 5.10      |
| MW#09      | 33.28                    | 0.88                 | 1.08 | 1.58 | 2.78      |
| MW#02      | 32.03                    | 0.90                 | 1.02 | 1.90 | 2.03      |
| SWF1001    | 34.00                    | 2.00                 | 2.20 | 2.70 | 3.79      |

The piezometric head contour plot for 5/11/94 (Fig. 2) represents the initial heads for the transient model. The mass balance taken from the MODFLOW output pointed out that the river could be both losing water to and gaining water from the surrounding aquifer along its course. Figs. 9 to 11 of the results for the transient model give an idea of what the possible piezometric head configuration might be, if the water table close to the discharge point dropped by 3 to 4 feet.

Do the real groundwater table elevations ever drop by such an amount below the levels of the 5/11/94 initial water table? The historical records shown certainly indicate this. In fact, as illustrated in Fig. 3, it occurred several times in some of the wells north and south of the paper mill's discharge point since 1960 during the long drought periods. Consequently, Fig. 9 to 11 may represent a realistic historical dry season scenario. Table 1 summarizes the simulated transient groundwater table drops of the Figs. 9 to 11 for several monitor wells with respect to the initial groundwater table. These values indicate that after 450 days of simulation time the water table in the wells listed has decreased more than what has been probably observed in reality in the Fenholloway region over the past 30 years. Therefore, the static water lines shown in Figs. 9 to 11 would represent the outer bounds of a possibly polluted aquifer corridor along the Fenholloway river that are in realistic compliance with the historical observations. The maximum static distance that may be reached by a contaminated river particle might extend to about 1.5 miles north of the river to the Perry airport (large triangle in the maps). From there on, further downstream, the water line begins to slowly converge back toward the Fenholloway river. A similar situation holds for the maximum reach of the static water lines south of the river.

#### **4. DYNAMIC PARTICLE TRACKING OF STREAM/AQUIFER INFILTRATION**

##### **4.1 Motivation**

The *static water-lines* established in the previous sections by means of the transient MODFLOW simulations are the outer hydraulic flow barriers of horizontally infiltrating stream water; i.e. the latter cannot move beyond these water lines. However, since these barriers were calculated assuming a final groundwater table drop during a certain drought period, they do not account for the actual total movement of a river particle that begins to migrate outwards into the aquifer, as soon as the groundwater table elevation falls beneath the stream gage height and the stream becomes influent. In fact, the same particle might be swept back again towards the river, when during a normal season the latter becomes an effluent stream again. This behavior can only be mimicked by means of a dynamic particle tracking technique that allows the computation of advective travel-paths of conservative tracers emanating from the river under appropriate transient hydrological conditions. For this purpose a semianalytical particle tracking method was developed in Koch et al. (1994) and Koch and Cekirge (1996) and it will be used in the following sections to define, what we now call *dynamic water-lines*.

## 4.2 Methodology

We only summarize here the most relevant features of the conceptual model underlying the dynamics of the river-to-aquifer particle movement and the final particle tracking technique (see Koch et al. 1994; and Koch and Cekirge, 1996, for details). A 1-D cross-section of this conceptual model is shown in Fig. 8. Assuming a downward hydraulic gradient from the river to the aquifer at a certain time at the beginning of the dry season, a river particle will be advected downgradient into the aquifer. At this stage a *Green's function method* (cf. Tikhonov and Samarskii, 1963) is used for the solution of the one-dimensional (1D) version of the transient groundwater flow equation (2) for the head  $h(y,t)$  and applied in the semi-infinite, cross-sectional direction  $y$ , that extends from the middle of the stream into the aquifer to the right (see Fig. 8). One of the appealing features of the Green's function method is that it naturally includes (1) time-varying Dirichlet boundary conditions  $h(y=0,t) = h_B(t)$  at the left boundary ( $y=0$ ) of the domain (the river) and which are set equal to the measured stream gage heights; (2) a time- and spatially dependent source/sink term  $N(x,t)$  that are related to the effective recharge of the groundwater aquifer (=infiltration due to the difference between precipitation and evaporation); and (3) initial conditions for hydraulic heads  $h(y,t=0) = h_i(y)$  that are specified from assumed or measured groundwater table elevations fitted by a functional relationship which is based on Dupuit's theory for the groundwater table change towards the river bed (Bear, 1979).

As the particle moves out of the stream into the aquifer, it will also be dragged downstream by the regional groundwater flow; I.e., the particle moves effectively in a two-dimensional (2D), transient potential field  $h(x,y,t)$  that is the superposition of the 1D head-distribution  $h_G(y,t)$  computed above by means of the Green's function, and the regional hydraulic gradient field  $h_R(x,y,t)$ . The local flow velocity of the particle at a particular point in the 2D regional area can then be computed by applying Darcy's law  $\mathbf{v} = -k \nabla h$ , to the total head field  $h(x,y,t)$  at that point. The new position  $(x_1, y_1)$  of a particle after a small time increment  $\Delta t$  can then be calculated from the previous position  $(x_0, y_0)$  by

$$\begin{aligned} x_1 &= x_0 + u \Delta t \\ y_1 &= y_0 + v \Delta t \end{aligned} \tag{6}$$

where  $u$  and  $v$  are the components of the flow velocity  $\mathbf{v}$ . The final position of a particle is then obtained by integration of Eq. (6) over the total time. This is nothing else than classical particle tracking.

Note that the whole process is fully dynamic, because as the particle propagates into the aquifer at the beginning of a drought, it will sense different piezometric heads which themselves are changing over time, due to the seasonal variations of the rainfall and, ergo, changes in the effective aquifer recharge. In fact, as the drought ceases and the groundwater table rises again because of positive precipitation recharge, the hydraulic gradient will reverse itself and the river particle may partly move back towards the river bed. However, by then it has already irreversibly contaminated a corridor along the river. What we call the *dynamic water-lines* are then the envelopes of the extreme endpoints of all particle tracers on each side of the river. They define the boundaries of this maximal corridor of possible aquifer pollution by the industrial river.

#### 4.3 Setup of the particle tracking model and selection of model parameters.

The coding, numerical implementation and setup of the Green's function particle tracking model is described in detail in Koch et al. (1994) and Koch and Cekirge (1996). The simulations start at time zero when the river is still effluent. An initial groundwater table  $h_i(y)$  is assumed and the boundary condition  $h_B(t)$  is set equal to the river gage elevation above the average water table at the bottom of the stream bed. A time-dependent source function  $N(x,t) = N(t)$  is applied in the model that mimics the net recharge of the aquifer. The time variation of the source function is one of the most instrumental parameter in the simulation, since it is the form of  $N(t)$  that simulates the absolute magnitude and the period of possible cyclic change from a wet to a dry season and vice versa. The form of  $N(t)$  used here is

$$N(t) = N_o \sin \left( \frac{2\pi t}{T_o} \right) \quad (7)$$

where  $N_o$  is the maximal source/sink rate of the net recharge process and is a parameter to be adjusted in both the calibration and the sensitivity study.  $T_o$  is the period of the wet/dry season cycle and, as will be discussed further down, its choice is of ultimate importance for the simulation of 'worst-case' stream/aquifer pollution scenarios.

It should be clear that only cycles with long periods  $T_o$  for the wet/dry interchange will lead to a significant lateral penetration of river particles into the surrounding aquifer, as soon as the groundwater table drops beneath the river gage level. If the drought interval of the cycle is too short, the particles barely have time to move into the aquifer, before they are driven back by the reversed gradient that builds up again when the consecutive wet-season interval of the cycle begins.

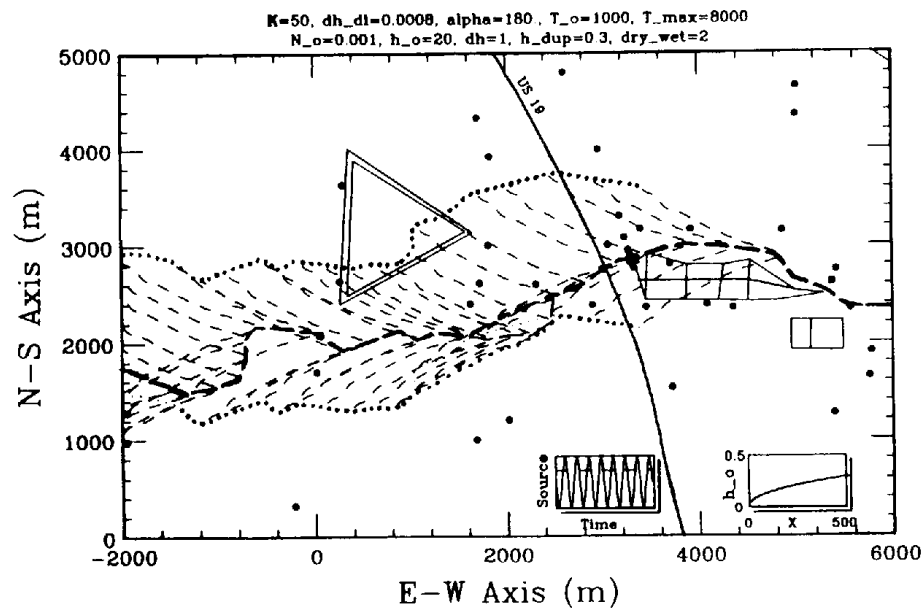
The visual inspection of the time series of precipitation, river gage heights and groundwater table elevations in Fig. 3 illustrates that these variables have, in addition to the normal seasonal cycle (with a period of about six months), longer cycles with multiyear periods of changes from highs to lows and vice versa. As the more detailed analysis of Koch et al. (1994) and Koch and Cekirge (1996) shows, these long-term variations are related to the El Niño/Southern Oscillation (ENSO), which has been shown to have a profound effect on the global hydrometeorological cycles, and those of the continental US, in particular (Kahya and Darcup, 1993). ENSO results from anomalous cyclic variations of the sea surface temperature as measured in the southeastern Pacific Ocean. In particular, an El Niño event occurs when the ocean surface temperature is above normal. Historical records show that El Niños have a recurrence rate of about 4 to 6 years. Normal times in between two El Niño events are also called a La Niña.

The effects of El Niño and La Niña events on long-term precipitation on a global scale varies with the region. For example, severe droughts might occur in Australia during an El Niño year, whereas high floods might be prevalent in south America during that time (Ropelewski and Halpert, 1987). For Florida, precipitation above and below the long-term average of up to 40% can be expected in an El Niño and a La Niña year, respectively (Sun, 1996; Sun et al., 1997b). This response of precipitation to the ENSO cycle implies that in a La Niña year, a lower groundwater table can be anticipated within the study region. Since the stream gage elevations for the Fenholloway river remain relatively constant, due to the large industrial discharge (see Fig. 3), a reverse hydraulic gradient from the stream towards the aquifer; i.e., an influent stream, can be created over a relatively long time period. Therefore, a wider corridor of aquifer contamination along the river may be expected in a La Niña year.

#### 4. 4 Application to the delineation of dynamic water lines

Fig. 12 shows a typical result of the application of the dynamic particle tracking to the delineation of dynamic water lines. A recurrence period  $T_o$  of 1000 days for the wet/dry season cycle, which mimics approximately the length of the long-term El Niño/La Niña cycle discussed above and, therefore, represents a kind of 'worst-case' scenario, has been used in this calculation. The movements of the river particles have been tracked over a total time of 22 years which comes close to the total time of operation of the paper mill. A hydraulic conductivity of  $k=50$  m/day which, from the previous steady-state MODFLOW calibrations, was found as the most appropriate for the aquifer region under study, is used. The amplitude  $N_o$  of the effective recharge function (7) was adjusted during the calibration phase of the particle tracker in such a way that the observed historical, long-period groundwater table fluctuations of Fig. 3 are roughly matched. A detailed description of these and





**Figure 12.** Results of dynamic particle tracking over a total integration time of 22 years, a recurrence period of 1000 days, and using a conductivity of  $k=50$  m/day. The right inset shows the position of the initial free-surface groundwater table. The left inset illustrates the transient cyclic variation of the recharge source function, that mimics the changes from wet to dry years and vice versa.

other considerations that are required for the appropriate calibration and verification of the particle tracking model can be found in Koch et al. (1994) and Koch and Cekirge (1996) where a sensitivity study is also presented.

The envelopes of the extreme endpoints of all particle tracers on each side of the stream delineate the *dynamic water-lines* and 'sandwich' the maximal corridor of possible aquifer pollution caused by the industrial Fenholloway river. Fig. 12 illustrates that this particle tracking simulation (and numerous other ones discussed in Koch and Cekirge, 1996) result in 'pollution corridors' that are close to those obtained from the *static water-lines* that resulted from the transient MODFLOW simulations in the previous section. The 'worst-case' dynamic water lines of Fig. 12 should, therefore, provide water-planning agencies with realistic guidelines for where to draw the 'safest' limits of the proposed public water supply lines for the residents that are living along the Fenholloway river.

## 5. SUMMARY

Different hydrological modeling methods are applied in this study to analyze a possible contaminated corridor in the aquifer along both sides of the industrial Fenholloway river. Time series analysis and, in particular, ARIMA- and linear transfer models, statistically explain the main hydrological features within the data itself and the interrelation among the data series. For example, the autocorrelations of the river gage heights are significant only for shorter lag-periods than those for the groundwater table elevations which hints of the short time-scale of the surface river flow processes. The crosscorrelations between the river gage heights and the water table elevations show significant positive correlation for lags less than zero, indicating that a feedback exists between the groundwater table and river gage heights. A strong crosscorrelation is also found between the precipitation and the water table elevations. The feedback analysis shows that the river gage and the groundwater table are mutually dependent and, particularly, that the river stage heights are also strongly influencing the groundwater table. This implies, in turn, that the industrial river water may contaminate portions of the aquifer close to the river, especially during long dry seasons when the groundwater table may fall below the river gage elevations and sections of the industrial river may become influent.

Ultimately, extreme estimates of the possible spatial extensions of a contaminant plume emanating from the river over the short and the long term (worst-case scenarios) are established by two explicit modeling approaches. The first one is based on the use of transient MODFLOW simulations and mimics a drop of the groundwater table during a long dry season as has been observed in the area in the past. This approach defines the *static water-lines*. The second modeling option is based on a new model for dynamic stream/aquifer particle tracking, using a Green's function methodology. Using this technique, *dynamic water-lines* are defined by the end-locations of river particles tracked over a long time period for a specified dry- and wet season scenario. It is particularly shown, that the extent of lateral aquifer contamination is mostly affected by the periods of cycles for the wet-and-dry seasons and -years, with the maximum of river-particle migration into the surrounding aquifer for long drought intervals, when the groundwater table drops beneath the river gage level for a significant length of time. It was postulated that the longest cycles of periods of wet and dry climatic variations in Florida are related to the EL Niño/Southern Oscillation (ENSO), which appears to have a periodicity of about 3 to 5 years. During half of the regular ENSO-cycle an El Niño year changes to a La Niña year with, for Florida, a corresponding switch from anomalously high to low precipitation, respectively. Therefore, it is during extreme La Niña years that the potential for stream-aquifer pollution is the highest and the most extreme contaminated corridors, as delineated by the water-lines along the Fenholloway river are established..

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