An Aquifer-Test Preprocessor for the Ground-Water Flow Model Calibration Program MODOPTIM and its Application to a Well Field in Duval County, Florida

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Prepared in cooperation with the
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Preface

This report presents a computer program that serves as an aquifer-test preprocessor for the ground-water flow model calibration program MODOPTIM. The preprocessor generates the input files needed to run MODOPTIM to analyze aquifer-performance test data obtained from a production well that penetrates one or two aquifers in a confined aquifer system. The performance of this preprocessor has been tested with both hypothetical and actual aquifer performance tests; however, future applications of the program could reveal errors that were not detected in these tests. Users are requested to notify the USGS if errors are found in the report or in the preprocessor program.

Although this preprocessor program has been used by the USGS, no warranty, expressed or implied, is made by the USGS or the United States Government as to the accuracy and functioning of the program and related program material. Nor shall the fact of distribution constitute any such warranty, and no responsibility is assumed by the USGS in connection therewith.

The computer program documented in this report is available from the USGS at:
http://pubs.water.usgs.gov/sir/20055233.

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Conversion Factors and Datum

Multiply	By	To obtain
	Length	
inch (in.)	2.54	centimeter (cm)
foot (ft)	0.3048	meter (m)
mile (mi)	1.609	kilometer (km)
	Area	
square mile (mi^2)	2.590	square kilometer (km^2)
	Flow rate	
cubic foot per second (ft^3/s)	0.02832	cubic meter per second (m^3/s)
gallon per minute (gal/min)	0.00006309	cubic meter per second (m^3/s)
million gallons per day (Mgal/d)	0.04381	cubic meter per second (m^3/s)
	Hydraulic conductivity	
foot per day (ft/d)	0.3048	meter per day (m/d)
	Transmissivity*	
foot squared per day (ft^2/d)	0.09290	meter squared per day (m^2/d)
	Leakance	
foot per day per foot [(ft/d)/ft]	1	meter per day per meter [(m/d)/m)]

Temperature in degrees Fahrenheit (°F) may be converted to degrees Celsius (°C) as follows:

°C=(°F-32)/1.8

Horizontal coordinate information (latitude-longitude) is referenced to the North American Datum of 1983 (NAD 83).

Vertical coordinate information is referenced to the National Geodetic Vertical Datum of 1929 (NGVD 29); horizontal coordinate information is referenced to the North American Datum of 1927 (NAD 27).

*Transmissivity: The standard unit for transmissivity is cubic foot per day per square foot times foot of aquifer thickness [(ft^3/d)/ft^2]ft. In this report, the mathematically reduced form, foot squared per day (ft^2/d), is used for convenience.

Acronyms and Additional Abbreviations

APT	aquifer-performance test
FAS	Floridan aquifer system
ICU	intermediate confining unit
LFA	Lower Floridan aquifer
LFAM	Lower Floridan aquifer monitoring
MSCU	middle semiconfining unit
SCU	semiconfining unit
SAS	surficial aquifer system
UFA	Upper Floridan aquifer
UZLFA	upper zone of the Lower Floridan aquifer

List of Symbols

Roman

d	multiplicative factor used in geometric series, [dimensionless]
r_w	radius of the pumping well, [L]
R	total simulated radial distance, [L]

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Abstract

A method was developed to generate the input files needed to compute the hydraulic properties from aquifer-performance test data for confined aquifers (such as the Floridan aquifer system) by using an aquifer-test preprocessor for the computer program MODOPTIM. MODOPTIM is a non-linear, ground-water flow model calibration and management tool that uses MODFLOW-96 to simulate cylindrical or axisymmetric flow in the vicinity of a pumping well for any aquifer-well configuration. The preprocessor assumes that the production well penetrates either the Upper Floridan aquifer only, or penetrates both the Upper Floridan aquifer and Lower Floridan aquifer. The production well may fully or partially penetrate either aquifer. Input files needed to run MODOPTIM are generated by the aquifer-test preprocessor and the optimal hydraulic parameter values are computed by running MODOPTIM, which determines the set of parameter values that minimizes the sum-of-squared differences between simulated and measured drawdowns by using an iterative quasi-Newton algorithm.

Some field conditions that cannot be simulated with analytical solutions are analyzed by using MODOPTIM. A hypothetical aquifer-performance test is used to show how MODOPTIM can be used to compute hydraulic parameter values from drawdown generated by a well that fully penetrates the Upper Floridan aquifer and partially penetrates the upper zone of the Lower Floridan aquifer. The analysis of this hypothetical aquifer-performance test showed the hydraulic conductivities of the aquifers were correlated with each other. A flow log is needed to reduce the uncertainty of the hydraulic conductivities. The anisotropy of the upper zone of the Lower Floridan aquifer was the only parameter with a parameter sensitivity less than 0.01.

MODOPTIM was used to analyze the regional hydraulic parameter values for a well field in south central Duval County, Florida. The hydraulic conductivity of the Upper Floridan aquifer computed by MODOPTIM was 38 feet per day, based on the analyses of drawdown data recorded during an aquifer-performance test at a well field in Duval County, Florida. The hydraulic conductivity of the Upper Floridan aquifer, derived by using analytical solutions, was 86 feet per day. The difference in computed hydraulic conductivities of the Upper Floridan aquifer is because MODOPTIM simulated the storativity and leakance of the confining units above and below the aquifer—field conditions not considered by the analytical solutions used.

The computed hydraulic conductivity of the upper zone of the Lower Floridan aquifer by MODOPTIM was 42 feet per day based on the analysis of drawdown data for the study area. The computed anisotropy of the upper zone of the Lower Floridan aquifer, 0.14, was correlated to the hydraulic conductivity of the UZLFA, indicating that only the ratio of these two hydraulic parameters can be determined uniquely. There was a good match between the simulated and measured flow ratios to the wellbore from the Upper Floridan aquifer and upper zone of the Lower Floridan aquifer. The computed hydraulic conductivity for the middle semiconfining unit was about three orders of magnitude greater than that for the intermediate confining unit.

Introduction

The estimation of hydraulic parameter values from aquifer-performance test (APT) data usually is performed by fitting measured water levels in observation wells with specific type curves obtained from analytical solutions. The analytical solutions are derived from the ground-water flow equation, appropriate boundary conditions based on knowledge of the aquifer system, and the aquifer-well configuration. The aquifer-well configuration generally found in Duval County, Florida, however, is one where the production well penetrates most of the thickness of the Upper Floridan aquifer (UFA) and partially penetrates the upper zone of the Lower Floridan aquifer (UZLFA). Under these conditions, it is inappropriate to use analytical solutions to analyze APT data to compute hydraulic parameter values for the pumped aquifers. Other properties of the Floridan aquifer system, such as leaky confining units and the capability of these confining units to store water, make it more inappropriate to use existing analytical solutions to analyze APT data.

An alternative way to analyze APT data for a typical aquifer-well configuration in Duval County is to minimize the difference between the measured drawdowns and drawdowns simulated with a numerical model. The differences between simulated and measured drawdowns can be systematically minimized by changing the set of hydraulic parameter values used to compute the simulated drawdowns. Such simulation should account for any aquifer-well configuration and for the main characteristics of the confining units overlying and underlying the stressed aquifers.

The computer code MODOPTIM (K.J. Halford, U.S. Geological Survey, written commun., 2004) employs a systematic approach to minimize the differences between measured and simulated drawdowns. Specific instructions for MODOPTIM input files are provided in appendixes A, B, C, and D (K.J. Halford, U.S. Geological Survey, written commun., 2004). MODOPTIM uses iterative quasi-Newton algorithms that periodically revert to either a Gauss-Newton or Levenberg-Marquardt gradient-search minimization (Gill and others, 1981) based on the fact that the sum-of-squared differences between the measured and simulated drawdowns is a smooth and continuous function. MOPOPTIM simulates ground-water flow by using MODFLOW-96 (Harbaugh and McDonald, 1996a), and can thus be used to simulate transient drawdowns generated by a production well that fully or partially penetrates a one- or two-layered confined aquifer. In addition, both vertical and horizontal components of flow in the aquifers and confining units can be simulated. Most analytical solutions of the ground-water flow equation assume that flow in the confining units is strictly vertical.

A preprocessor for MODOPTIM to assist in the analysis of APT data for a typical aquifer-well configuration in Duval County, Florida, was developed by the U.S. Geological Survey in cooperation with the Jacksonville Electric Authority and the St. Johns River Water Management District during a 2-year study (2003-05). The aquifer-test preprocessor is illustrated through the analysis of (1) hypothetical APTs where the storativity is simulated in the confining units and flow is assumed to have both radial and vertical components, and (2) two APTs conducted in a well field in Duval County, Florida (fig. 1). In this report, MODOPTIM is used to analyze the APT data by deriving hydraulic parameter values for the specific aquifer-well configuration where the production well penetrates the UFA and partially penetrates the UZLFA. MODOPTIM and the preprocessor also can be used to analyze the APT data for the aquifer-well configuration where the production well fully or partially penetrates only one aquifer.

Purpose and Scope

This report describes the use of an aquifer-test preprocessor for a non-linear, ground-water flow model calibration and management tool developed by Halford (1992) that simulates flow with MODFLOW-96. A brief description of MODOPTIM input and output files is presented to help the reader interpret MODOPTIM results. The implementation of the preprocessor also is described. Data input for the preprocessor is illustrated through the analyses of hypothetical and actual APTs in a well field in Duval County, Florida. Hydraulic parameter values derived from the analysis are presented and compared with those obtained by using type curves derived from analytical solutions. The FORTRAN source code, a compiled version of the program suitable for use on most computer platforms, and all input and output files for the hypothetical and actual APTs are available at: http://pubs.water.usgs.gov/sir/2005/5233/.

The aquifer-test preprocessor presented in this report was specifically developed to generate the MODOPTIM input files needed to analyze the drawdown data recorded in the vicinity of a production well that penetrates one or two aquifers. In addition, the upper aquifer is assumed to be overlain and underlain by confining units. A no-flow or a constant-head boundary condition can be specified at the model top and/or

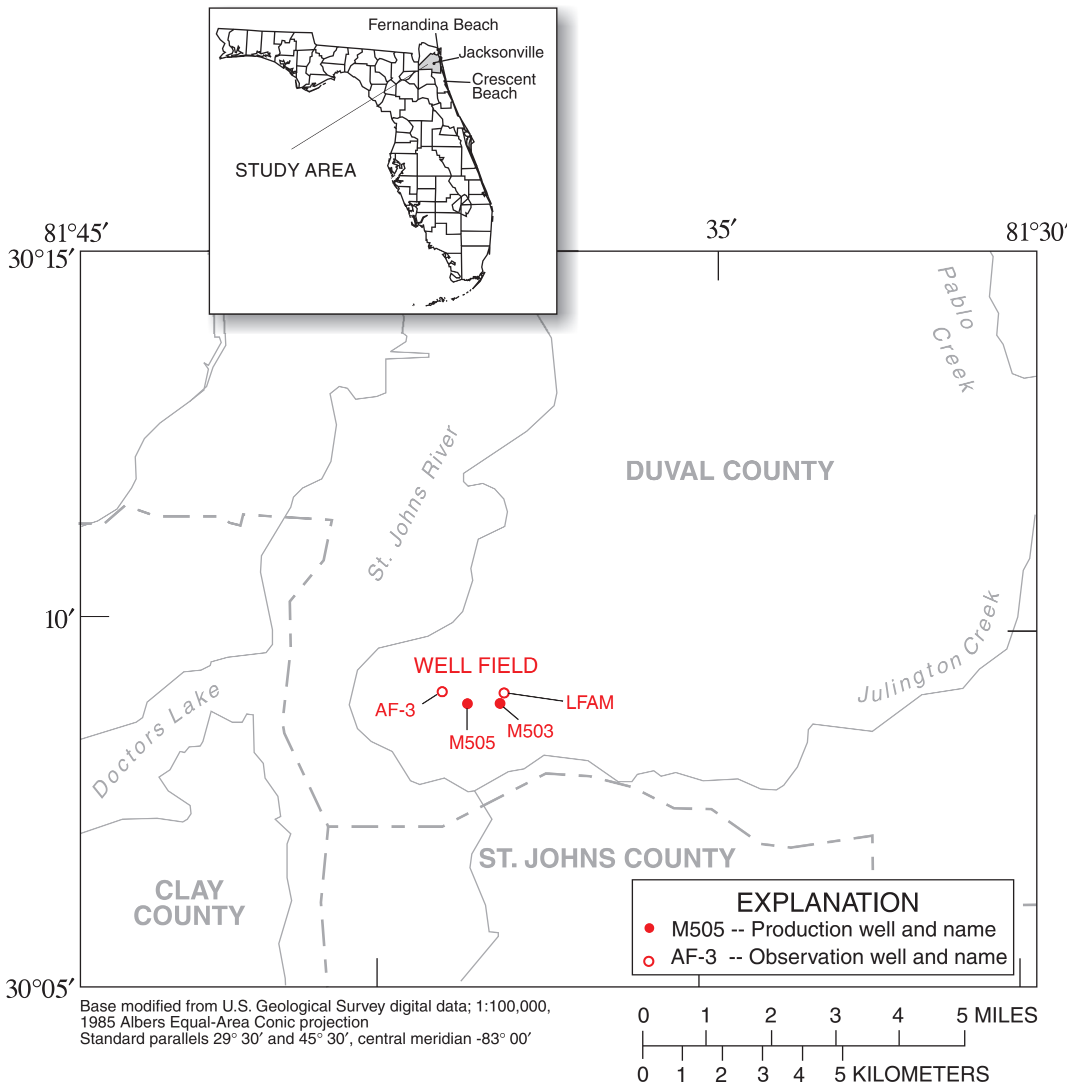

Figure 1. Locations of wells referenced in the aquifer-performance tests (APT) in Duval County, Florida.

bottom boundaries. Although MODOPTIM can solve a wide range of ground-water flow optimization problems, the aquifer-test preprocessor was not developed to generate the input files for the full spectrum of problems that MODOPTIM can solve. The preprocessor was developed to solve a need in northeast Florida. This computer program is useful to analyze data in other areas where the production well fully or partially penetrates one or two aquifers in a confined aquifer system.

Hydrogeologic Framework

The APTs performed as part of this study were conducted in an area underlain by a thick sequence of sedimentary rocks that overlie deeper volcanic, metamorphic, and sedimentary rocks. The primary water-bearing sediments are composed of limestone, dolomite, shell, and sand that range in age from late Paleocene to Holocene. Stratigraphic units and corresponding hydrogeologic units penetrated by wells in the study area are described in figure 2.

The principal water-bearing units in the study area are the surficial aquifer system (SAS) and the Floridan aquifer system (FAS). The SAS is the uppermost water-bearing unit and generally is unconfined, but may be semiconfined in areas where some beds of lower permeability are sufficiently thick and continuous. The intermediate confining unit (ICU) underlies the SAS and

Series	Stratigraphic unit	General lithology	Hydrogeologic unit			Hydrogeologic properties
Holocene	Undifferentiated surficial deposits	Discontinuous sand, clay, shell beds, and limestone	Surficial aquifer system (SAS)			Sand, shell, limestone, and coquina deposits provide local water supplies.
Miocene	Hawthorn Group	Interbedded phosphatic sand, clay, limestone, and dolomite	Intermediate confining unit (ICU)			Sand, shell, and carbonate deposits provide limited local water supplies. Low permeability clays serve as the principle confining beds for the Floridan aquifer system below.
Eocene	Ocala Limestone	Massive fossiliferous chalky to granular marine limestone	Floridan aquifer system (FAS)	Upper Floridan aquifer (UFA)		Public-water supply source. Water from some wells shows increasing salinity.
Eocene	Avon Park Formation	Alternating beds of massive granular and chalky limestone, and dense dolomite	Floridan aquifer system (FAS)	Middle semiconfining unit (MSCU)		Low permeability limestone and dolomite.
Eocene	Avon Park Formation	Alternating beds of massive granular and chalky limestone, and dense dolomite	Floridan aquifer system (FAS)	Lower Floridan aquifer (LFA)	Upper zone (UZLFA)	Public-water supply source. High permeability. Water from some wells shows increasing salinity.
Eocene	Oldsmar Formation	Alternating beds of massive granular and chalky limestone, and dense dolomite	Floridan aquifer system (FAS)	Lower Floridan aquifer (LFA)	Semiconfining unit (SCU)	Low permeability limestone and dolomite.
Eocene	Oldsmar Formation	Alternating beds of massive granular and chalky limestone, and dense dolomite	Floridan aquifer system (FAS)	Lower Floridan aquifer (LFA)	Fernandina permeable zone (FPZ)	Salinity increases with depth.
Paleocene	Cedar Keys Formation	Uppermost appearance of evaporites; dense limestones	Sub-Floridan confining unit			Low permeability; contains highly saline water.

Figure 2. Stratigraphic units, general lithology, and hydrogeologic units in Duval County, Florida (modified from Spechler, 1994).

primarily includes sediments of the Hawthorn Group of Miocene age. The unit consists of interbedded clay, silt, sand, limestone, and dolomite containing abundant amounts of phosphatic sand, granules, and pebbles. The ICU serves as a confining layer that restricts the vertical movement of water between the SAS and the UFA.

The FAS is composed of a sequence of highly permeable carbonate rocks of Eocene and Late Paleocene age and includes the following stratigraphic units in descending order: the Ocala Limestone, the Avon Park Formation, the Oldsmar Formation, and the upper part of the Cedar Keys Formation (fig. 2). The FAS is divided into two aquifers of relatively high permeability, referred to as the Upper Floridan and Lower Floridan aquifers. The water-bearing zones within the FAS consist of soft, porous limestone, generally in the UFA, and porous highly fractured dolomite beds, generally in the Lower Floridan aquifer (LFA). These aquifers are separated by a less permeable unit called the middle semiconfining unit (MSCU), that somewhat restricts the vertical movement of water within the aquifer. The LFA can be subdivided into two principal water-bearing zones, the UZLFA and the Fernandina Permeable Zone (FPZ), separated by a less permeable unit. The base of the FAS is defined by the occurrence of low permeability limestone and dolomite that contain considerable quantities of gypsum and anhydrites.

The UFA generally corresponds to the Ocala Limestone, and in some areas also includes the uppermost part of the Avon Park Formation. The top of the UFA averages about 450 feet (ft) below NGVD 29 at the well field. The MSCU separates the UFA and LFA and is composed of beds of less permeable limestone and dolostone of variable thickness. The MSCU occurs in the upper part of the Avon Park Formation, but also can include the lower part of the Ocala Limestone, which

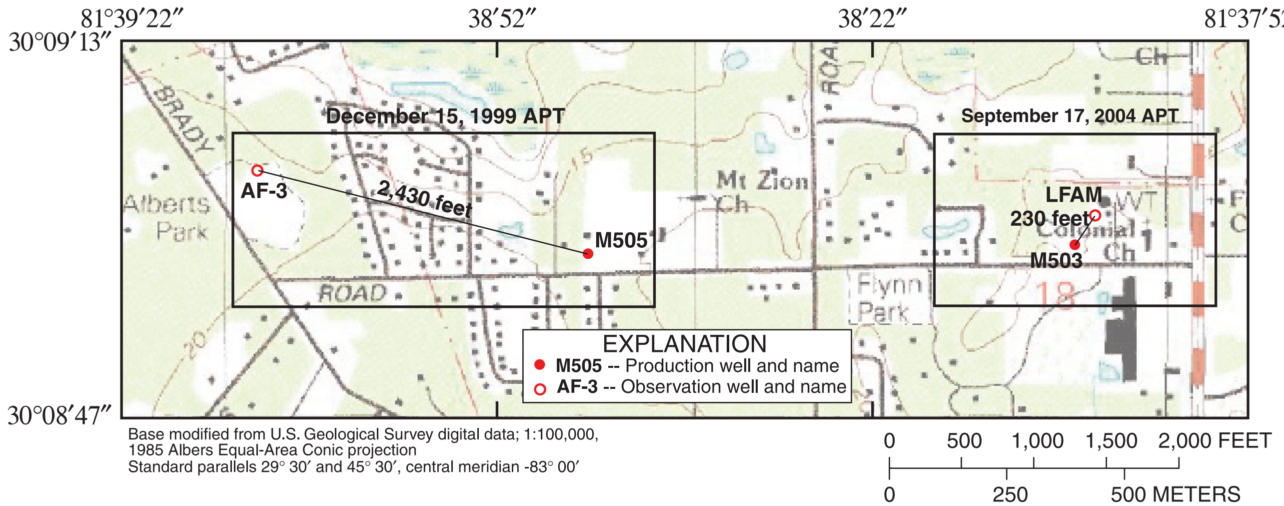

Figure 3. Locations and distances between production and observation wells referenced in the aquifer-performance tests (APT) conducted on December 15, 1999, and September 17, 2004, at the Duval County well field.

may consist of hard dolostone or limestone. The top of the MSCU is recognized by a decrease in flow observed on flowmeter logs. The contrast in permeability between the rocks of the MSCU and the permeable rocks above and below is less than that for any other middle confining unit in the FAS (Miller, 1986). Accordingly, the MSCU in Duval County is the leakiest confining unit known in the FAS. Thickness of the unit could range from about 135 to 165 ft at the well field based on flow meter logs.

The LFA underlies the MSCU and includes the lower part of the Avon Park Formation, all of the Oldsmar Formation, and the upper part of the Cedar Keys Formation. The aquifer is highly productive and is composed of alternating beds of limestone and dolomite. The two main water-bearing zones of the LFA, the UZLFA and the FPZ, are separated by a less-permeable semiconfining unit (SCU). The top of the UZLFA generally can be identified on flow logs as an interval contributing a noticeable increase in flow to the well. Permeability within this zone is related mostly to secondary porosity developed along bedding planes, joints, and fractures, developed by repeated episodes of active dissolution of the rock matrix (Phelps and Spechler, 1997). The sub-Floridan confining unit, which underlies the LFA, typically is characterized by low permeability and serves as the hydraulic base of the FAS. Total thickness of the LFA at the site, including the SCU and the FPZ, was estimated to be about 1,250 ft (Sepúlveda and Spechler, 2004).

Hydrogeology of Duval County Well Field

The local hydrogeology at the Duval County well field (fig. 3) is described and based on lithologic data from one production and one monitoring well in the well field. The altitudes of the contacts between hydrogeologic units penetrated by production well M505 (fig. 4) were determined by R.M. Spechler (U.S. Geological Survey, written commun., 2003) based on geophysical logs (fig. 5) and gamma, fluid resistivity, and temperature logs published by CH2MHill (1999). The flow log under pumping conditions for production well M505 (fig. 5) shows that little or no flow is contributed to the wellbore from 950 to 1,100 ft below land surface. Considering that land-surface altitude at this well is 20 ft (NGVD 29), no flow to the wellbore occurs at altitudes below -930 ft. Thus, the effective open

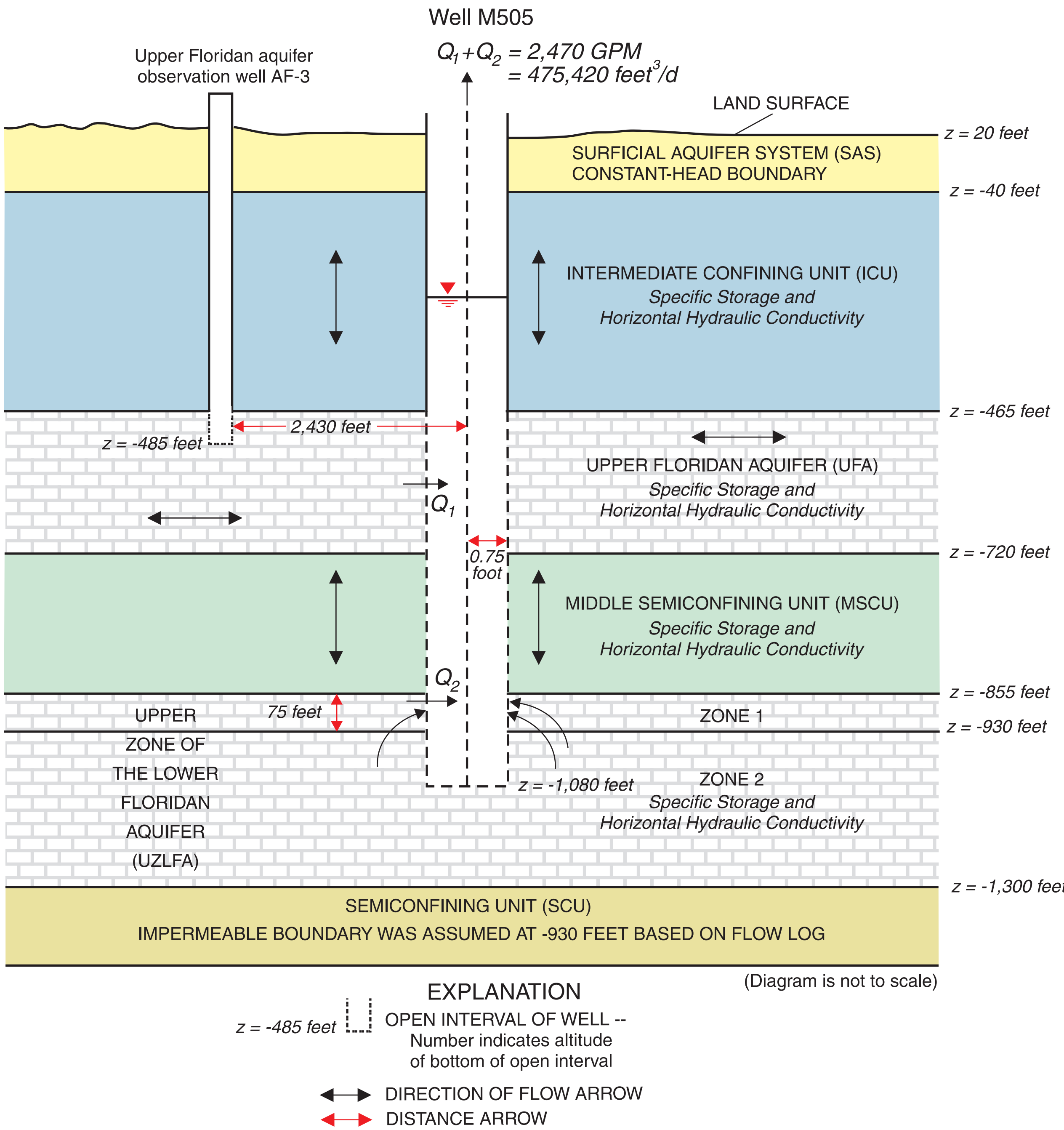

Figure 4. Hydrogeologic units penetrated by well M505 and depth of open interval of well AF-3.

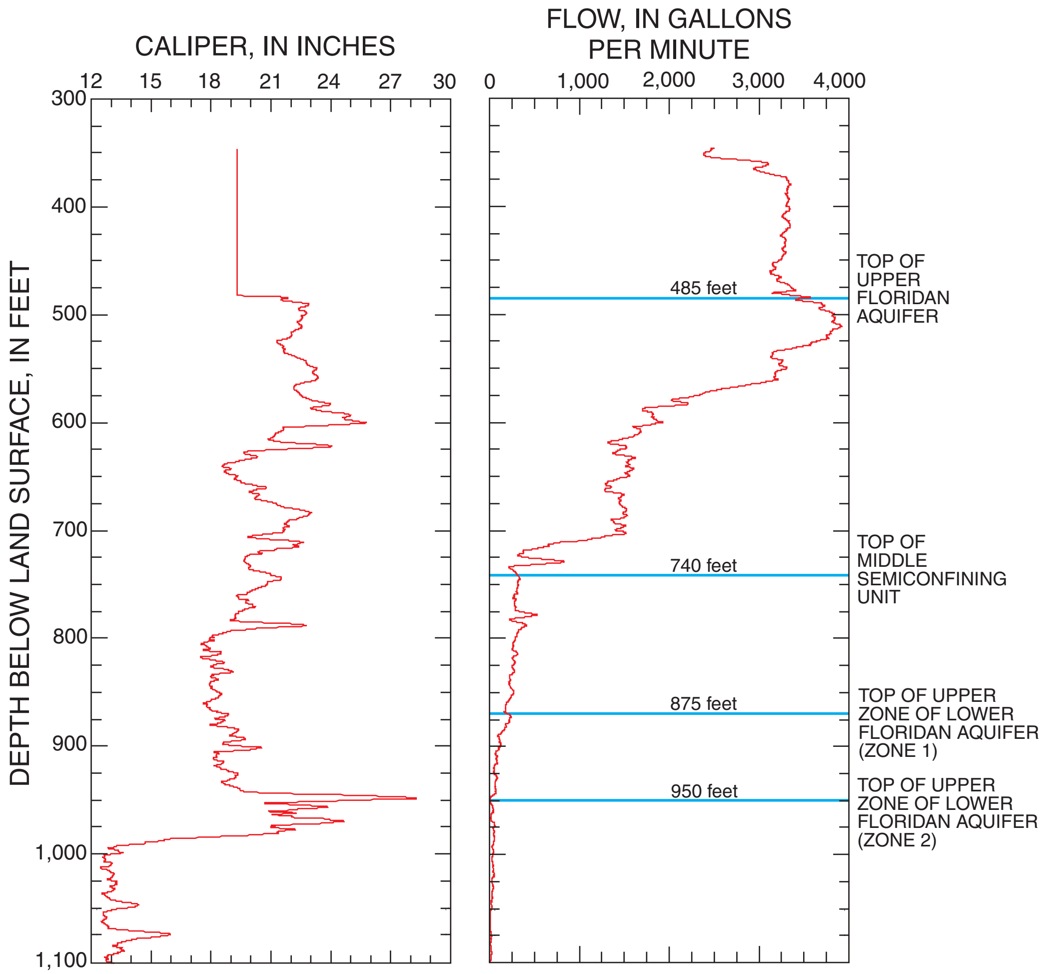

Figure 5. Caliper log, flow log under pumping conditions, and hydrogeologic units for well M505 (modified from CH2MHill, 1999).

interval of well M505 extends from altitudes of -465 to -930 ft, making well M505 mostly a UFA well. The zone beginning at the bottom of the MSCU (altitude -855 ft) and ending at altitude -930 ft is referred to as zone 1 of the UZLFA in this report (fig. 4). Zone 2 of the UZLFA is defined as the interval from -930 ft to the top of the SCU (-1,300 ft). There is no substantial flow to well M505 in zone 2.

The altitudes of the contacts between hydrogeologic units penetrated by the LFA monitoring (LFAM) well (fig. 6) also were determined by R.M. Spechler (U.S. Geological Survey, written commun., 2003) using temperature and fluid-resistivity logs in addition to caliper and flow logs. Because there is no flow log available for well M503, it was assumed that the flow zones delineated for well LFAM are a good approximation to the flow zones on well M503 (located 230 ft to the southeast, fig 1). The top of the UZLFA was estimated to be at an altitude of -855 ft. The thickness of the UZLFA, based on figures 5 and 7, was estimated to be 445 ft (Sepúlveda and Spechler, 2004). The flow log under pumping conditions for well LFAM (fig. 7) shows about 55 percent of the flow to the well coming from zone 2 of the UZLFA and about 45 percent from the UFA. A substantial contribution of water to the wellbore occurs at an altitude of about -1,150 ft (NGVD 29), a depth not tapped by well M505. Zones 1 and 2 of the UZLFA were delineated as shown in figures 5 and 7 because well M505 does not receive much flow from the aquifer at altitudes below -930 ft (or 950 ft below land surface).

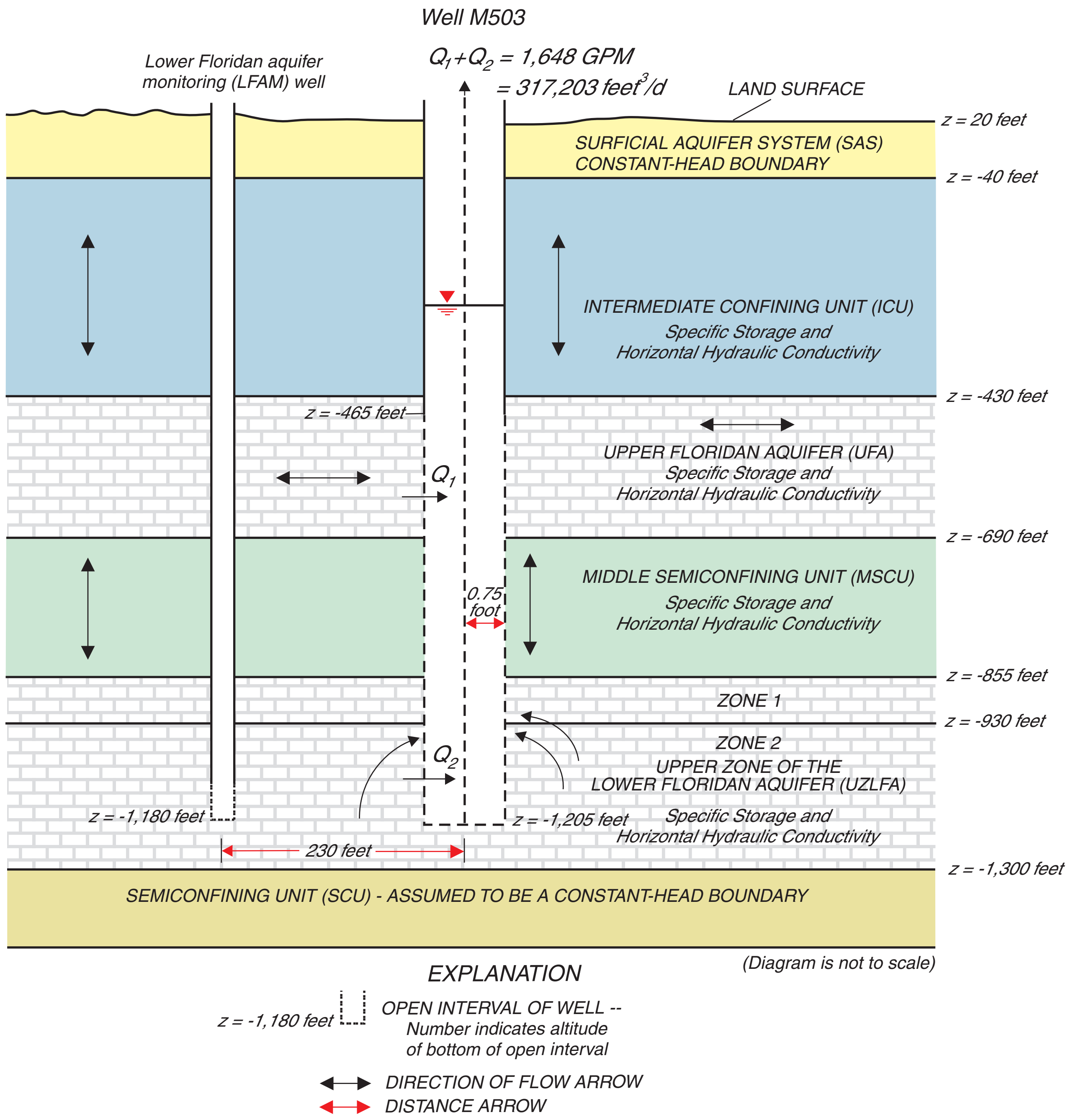

Figure 6. Hydrogeologic units penetrated by well M503 and depth of open interval of well LFAM.

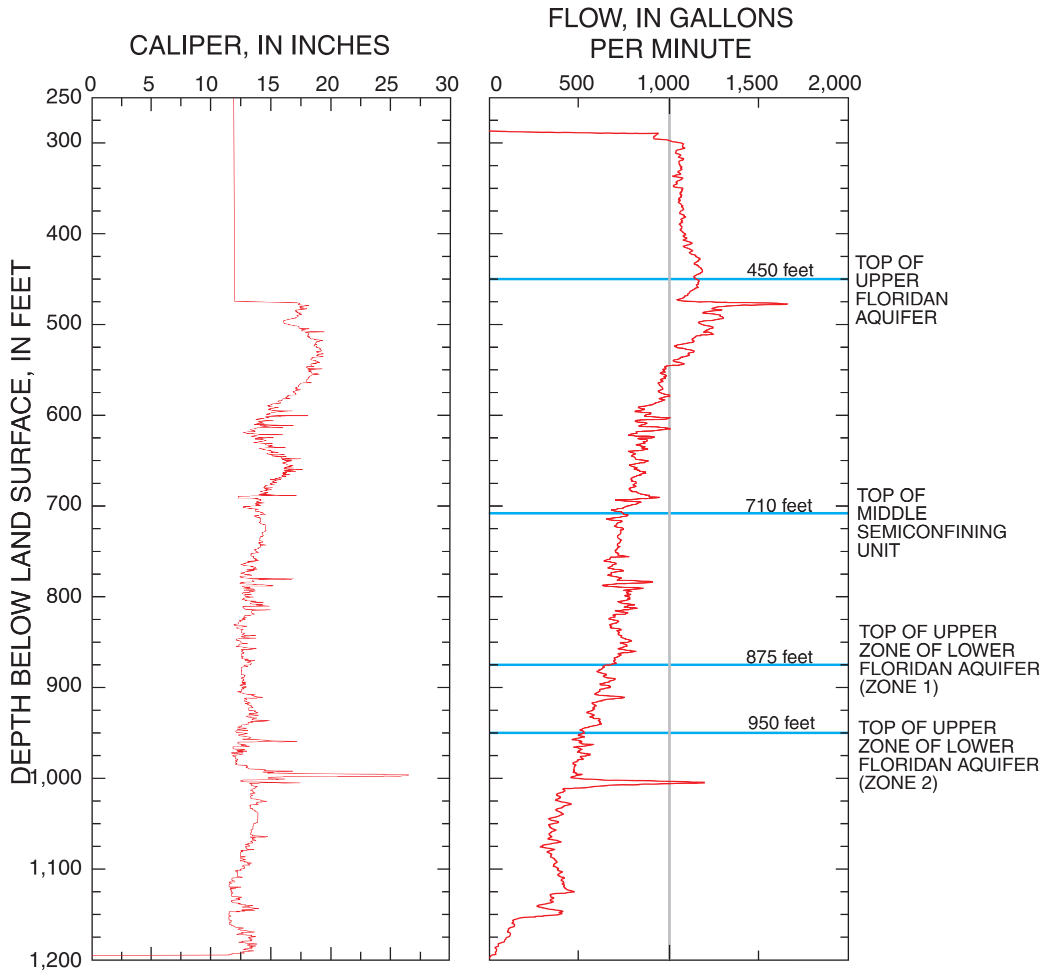

Figure 7. Caliper log, flow log under pumping conditions, and hydrogeologic units for well LFAM (modified from CH2MHill, 2001).

Figures 5 and 7 indicate two production zones within the UZLFA. Given the specific and local aquifer-well configuration of wells M505 and LFAM, production zones 1 and 2 in the UZLFA have been delineated to facilitate the analysis of the APT data. This zone identification, however, is not necessarily valid elsewhere in Duval County. Figures 5 and 7 indicate that a small amount of flow originates from zone 1 of the UZLFA and that there is a contrast between the flows originating from zone 2 in wells M505 and LFAM. This contrast is explained by the fact that well M505 only taps a small vertical interval of zone 2. The APTs at wells M503 and M505 are used to compute the hydraulic conductivities of zones 1 and 2 of the UZLFA.

Previous Studies

Type curves generated from analytical solutions commonly are used to analyze APT data. A classical type curve (Theis, 1935) assumes the well-discharge rate is constant, the well is of infinitesimal diameter and fully penetrates the aquifer, the confining units underlying and overlying the aquifer are not leaky, and flow from the well is derived exclusively from storage in the aquifer. Cooper and Jacob (1946) developed a linearized version of the solution by Theis. Papadopulos and Cooper (1967) derived an analytical solution for drawdown generated by a well of finite diameter assuming the flow from the well is derived from aquifer storage and the wellbore.

Hantush (1961) derived a drawdown solution for a configuration where the well is of infinitesimal diameter and partially penetrates the aquifer.

Hantush and Jacob (1955) presented an analytical solution for the drawdown generated by a well of infinitesimal diameter that fully penetrates an aquifer overlain, or underlain, everywhere by a leaky confining unit of uniform thickness and vertical hydraulic conductivity. Their solution assumed that no water was released from storage in the confining unit. Hantush (1964) extended Hantush and Jacob (1955) solution to work for wells of infinitesimal diameter that partially penetrate the aquifer. Hantush (1960) derived a drawdown solution for the configuration where the well fully penetrates an aquifer with leaky overlying and underlying confining units. The latter solution was valid only for early and late times. Moench (1985) derived a drawdown solution valid for all times based on the numerical inversion of the Laplace transform. An analytical solution for the aquifer drawdown generated by a well that penetrates most of the upper aquifer (such as the UFA) and partially penetrates the lower aquifer (such as the LFA) is yet to be derived.

The drawdown data obtained from the APT conducted on December 15, 1999, were analyzed by CH2MHill (2000) to compute the transmissivity and storativity of the UFA and the vertical leakance attributed to the ICU. CH2MHill used the analytical solutions presented by Theis (1935), Cooper and Jacob (1946), and Hantush and Jacob (1955) to compute these hydraulic parameters independently of the method used. Based on the APT data from production well M505 and from observation well AF-3, the average transmissivity of the UFA was about 22,000 feet squared per day, the average specific storage of the UFA was 1.0 x 10^{-6} per foot, and the leakance for the ICU, derived from the solution by Hantush and Jacob (1955), was 6.3 x 10^{-5} feet per day per foot (CH2MHill, 2000). The average transmissivity of the UFA of 22,000 feet squared per day is equivalent to a horizontal hydraulic conductivity of about 86 feet per day. The average pumping rate at the well was 2,470 gallons per minute. Field conditions that were not considered in the derivation of these properties were that well M505 penetrates the MSCU and that both the ICU and MSCU have storative and leakage properties. No drawdown data were available at the time to compute hydraulic properties for the UZLFA.

Acknowledgments

The author would like to thank the Jacksonville Electric Authority for their assistance in conducting the APT in the well field on September 17, 2004. The author also wants to thank Keith J. Halford of the U.S. Geological Survey for providing the appendixes and for his assistance with the MODOPTIM code.

Description of MODOPTIM

The computer code MODOPTIM uses MODFLOW-96 (Harbaugh and McDonald, 1996b) in axisymmetric or radial-geometry mode. MODOPTIM conceptualizes ground-water flow to a pumping well as a single model layer. Radial distance increases with increasing column indices, and depth increases with increasing row indices. The model columns extend from the well center to a point sufficiently far away from the pumping well to minimize potential boundary effects. The model rows span the thicknesses of the hydrogeologic units tapped by the production well. The large horizontal hydraulic gradients in the vicinity of the well are simulated by decreasing radial distances of model columns in the direction of the well center. Hydraulic conductivities and storages of the i^{th} column are multiplied by $2\pi r_i$ to simulate radial flow; where r_i is the distance from the outer edge of the first column to the center of the i^{th} column.

MODOPTIM, a non-linear, ground-water model calibration and management tool, developed by K.J. Halford (U.S. Geological Survey, written commun., 2004), simulates flow with MODFLOW-96 as a subroutine. Using an iterative quasi-Newton algorithm to estimate changes in parameter values from initial values, MODOPTIM can compute optimal parameter values for a wide range of problems. In particular, MODOPTIM can compute optimal aquifer hydraulic parameter values from measured drawdowns in the vicinity of pumping wells by using basic aquifer-well configuration data and by systematically reducing the sum-of-squared differences between simulated and measured drawdowns.

Hydraulic parameter values obtained with MODOPTIM from the analysis of the APT data measured in the vicinity of a production well that penetrates most of the UFA and partially penetrates the UZLFA may not constitute a unique solution to the ground-water flow in the vicinity of the production well. As the sum-of-squared differences between simulated and measured drawdowns decrease, however, the best fit of the measured data indicates the optimal solution among the non-unique solutions of the ground-water flow.

The confining units are simulated in MODOPTIM as "aquifers" because both radial and vertical flows are simulated. The vertical hydraulic conductance values among cells in rows located along the hydrogeologic unit contacts are used to determine the leakance between units. This implies that a fraction of the well discharge may originate from a confining unit penetrated by the production well.

Parameters Used to Generate MODOPTIM Input Files

The main parameters used to compute the optimal hydraulic parameter values from APT data are compiled in a spreadsheet—table 1 is an example. Initial values used for some hydraulic parameters must be specified in this table for each MODOPTIM run because of the effect these values may have on the convergence process to an optimal solution. Initial values for specific storage and anisotropy were assigned internally in the aquifer-test preprocessor for MODOPTIM. An initial value for specific storage for all hydrogeologic units, equal to 1.0×10^{-6} per foot, was found not to affect the convergence of the solution to the optimal specific storage values of the units. The initial ratio of vertical to horizontal hydraulic conductivity of the hydrogeologic unit being partially penetrated by the pumping well, set to 0.10, was found not to affect the convergence to the optimal anisotropy value of the unit.

There are other parameters used by the computer program MODOPTIM but not listed in table 1. Values for these parameters were coded in the preprocessor program because it was assumed that they would not change from one APT to another. These parameters were: (1) the total radial distance to be simulated in the ground-water flow model, assumed to be 400,000 ft to minimize model boundary effects during pumping; (2) the minimum reduction in sum-of-squares objective function, assumed to be 0.01; and (3) a threshold correlation coefficient of 0.95 for which all parameter pairs exceeding this correlation coefficient are listed in the parameters output file. In addition, all weighting factors assigned to sets of measured drawdowns are set equal to 1 by the aquifer-test preprocessor. A batch file was written to run the preprocessor and MODOPTIM.

The name of the input file for MODOPTIM's preprocessor, generatefiles.txt, is established in line 1 of the spreadsheet. This text file can be generated from the same spreadsheet file by clicking the button labelled "WRITE TXT FILE", located in the spreadsheet. The common part of most of MODOPTIM input and output file names is specified by the six-character name specified in line 2, often the site name or identifier. The initial values for the horizontal hydraulic conductivities of the hydrogeologic units are specified in lines 3 through 6. The assessment of potentially non-unique hydraulic parameter solutions can be done by changing the initial values specified in lines 3 through 6, and noticing how these changes affect the optimal parameter values at the end of the MODOPTIM run. The radius of the well screen, in inches, is entered in line 7; the well discharge, in gallons per minute, is entered in line 8. The well screen top and bottom altitudes, in feet and using a consistent datum, are specified in lines 9 and 10. For the purpose of illustrating the use of altitudes in this spreadsheet file, the datum of NGVD 29 is used, however, any datum could be used. The altitudes of the hydrogeologic unit contacts are specified in lines 11 through 15 (table 1).

The boundary conditions to be applied at the top and bottom of the model are specified in lines 16 and 17, respectively. A negative integer is used to specify a constant-head source and a nonnegative integer is used to specify a no-flow boundary. The maximum number of iterations to be performed by MODOPTIM is specified by the user in line 18. The number specified in line 18 should be at least 3 times the number of parameters being computed to allow for the solution to converge. The number of drawdown time series obtained from the observation wells and recorded during the APT is specified in line 19. The information for each one of the drawdown time series available for the APT analysis is specified in the next group of four lines in table 1. Each group of four lines (lines 20-23 and lines 24-27) specifies a code name used to designate the observation well name, the radial distance (in feet) from the production well, the average altitude of the open interval in the observation well, and the name of the file that contains the drawdown time series. The use of the average altitude of the open interval in the observation well is recommended in MODOPTIM because it is assumed that the simulated head at the row and column for the average altitude of the open interval closely approximates the average simulated head of the entire open interval, which is not computed by MODOPTIM.

Initial values used for specific storage and anisotropy change after the first iteration. Several other initial values were chosen for these variables to determine the effect these would have on the optimal solution computed by MODOPTIM. The initial values listed above for specific storage and anisotropy did not affect the calculation of the optimal values computed by MODOPTIM nor the number of iterations.

Table 1. Example of spreadsheet file used to generate the input files needed by MODOPTIM.

[ICU, intermediate confining unit; UFA, Upper Floridan aquifer; MSCU, middle semiconfining unit; LFA, Lower Floridan aquifer; ft, feet; d, day; NGVD 29, datum used as example]

Line number	Parameter value or field name	Parameter value or field description
1	generatefiles	Used to name the text file to be generated and should not be changed
2	COMHAL	Prefix name to be used for input and output files, exactly 6 characters in length
3	0.0030	Initial horizontal hydraulic conductivity of the ICU, in ft/d
4	35.0	Initial horizontal hydraulic conductivity of the UFA, in ft/d
5	0.250	Initial horizontal hydraulic conductivity of the MSCU, in ft/d
6	1.0	initial horizontal hydraulic conductivity of the LFA, in ft/d
7	9.0	Radius of well screen, in inches
8	2470.0	Well discharge, in gallons per minute
9	-465.0	Altitude of the top of the well screen, in ft NGVD 29
10	-930.0	Altitude of the bottom of the well screen, in ft NGVD 29
11	-40.0	Altitude of the top of the ICU, in ft NGVD 29
12	-465.0	Altitude of the top of the UFA, in ft NGVD 29
13	-720.0	Altitude of the top of the MSCU, in ft NGVD 29
14	-855.0	Altitude of the top of the LFA, in ft NGVD 29
15	-930.0	Altitude of the bottom of the LFA, in ft NGVD 29, not used if well screen does not tap LFA
16	-1	Constant-head (negative) or no-flow (nonnegative) condition imposed at the top of model
17	0	Constant-head (negative) or no-flow (nonnegative) condition imposed at the bottom of model
18	15	Maximum number of iterations to be performed by MODOPTIM, an integer
19	2	Number of (time, drawdown) data files generated during the aquifer performance test
20	M505	Name code to designate observation well 1, exactly 4 characters in length
21	0.75	Radial distance from center of pumping well to observation well 1, in ft
22	-576.0	Average altitude of open interval for observation well 1, in ft NGVD 29
23	INPUT_CH05.txt	Name of (time, drawdown) data file for well 1, up to 20 characters in length, in (days, feet)
24	AF-3	Name code to designate observation well 2, exactly 4 characters in length
25	2430.0	Radial distance from center of pumping well to observation well 2, in ft
26	-576.0	Average altitude of open interval for observation well 2, in ft NGVD 29
27	INPUT_UFA.txt	Name of (time, drawdown) data file for well 2, up to 20 characters in length, in (days, feet)

Radial and vertical grid refinement was implemented in the preprocessor. The total radial distance R, assumed to be 400,000 ft, simulated in the two-dimensional axisymmetric model was discretized into model columns by using the equation:

$$R = r_w + r_w d + r_w d^2 + \ldots + r_w d^{NCOL-1} = \frac{r_w(d^{NCOL} - 1)}{d - 1} \quad , \qquad (1)$$

where

r_w is the radius of the pumping well,

$NCOL$ is the assigned number of radial columns in the model,

d is the multiplicative factor computed from equation (1) and known parameters r_w, R, and $NCOL$, and

$r_w d^i$ is the radial distance of column index $i + 1$ for $i = 1, 2, \ldots, NCOL - 1$.

The value of *NCOL* was chosen as the number that minimizes the numerical error associated with the finite differences algorithm of MODFLOW. This was accomplished by calculating the sum-of-squared differences between the simulated and analytical heads for the hypothetical APTs (fig. 8). Analytical heads were computed from Moench's solution (1985). The chosen value of *NCOL*, 150, was that number for which no significant reduction in the sum-of-squared differences was obtained for any larger number. The value of *d* was computed by solving equation (1) using Newton's iterative algorithm. Similarly, the number of time steps (90) and the time step multiplier (1.10) used to simulate the APT were chosen to reduce the sum-of-squared differences.

The number of rows used in the model was chosen depending on the thickness of each hydrogeologic unit and the well screen interval. The top of the ICU, the top of the UFA, the top of the well screen, the bottom of the UFA, the bottom of the well screen, the top of the UZLFA, and the bottom of the LFA were the altitudes used to compute the total number of rows in the model. These seven altitudes were ordered from highest to lowest and the resulting six intervals were assigned a number of rows to span each thickness. The maximum row thickness, about 15 ft, also was selected to minimize the sum-of-squared differences for the APT (fig. 8). This assured that the top of the well screen began at the top of a given row and the bottom of the well screen ended at the bottom of another row.

The main contents of the input files generated by MODOPTIM's preprocessor are listed in table 2. The input data needed by MODOPTIM is read from three primary files (lines 1-3) that define the optimization problem, the MODFLOW-96 model, and the model grid data. Detailed specifications of general structural requirements of MODOPTIM's input files are listed in appendix A (K.J. Halford, U.S. Geological Survey, written commun., 2004). The format of input files listed in lines 1 to 3 of table 2 is explained in detail in appendixes B, C, and D, respectively (K.J. Halford, U.S. Geological Survey, written commun., 2004). Additional files, specifying output controls, solvers, and specified stresses are used by MODFLOW-96, but are not used directly by MODOPTIM's optimization routine (table 2, lines 4-7). The optimization file, the combined MODOPTIM/MODFLOW-96 input file, and the model grid file are referred to by the suffixes OPT, INP, and GR3, respectively, in table 2. This naming convention was adopted for file identification by MODOPTIM and the preprocessor.

Weighting factors assigned by the preprocessor to all drawdown measurements are assumed to be 1.0. These factors may be used to prioritize the reliability of the drawdown data. If weighting factors different than 1.0 are to be assigned to some drawdown files, based on additional field assumptions, then these would need to be edited accordingly in the OPT input file generated by MODOPTIM's preprocessor.

MODOPTIM Output Files

Results from MODOPTIM are written to a master optimization output file, a residual-and-sensitivities output file, and a parameter-estimates output file. The master optimization output file contains pertinent data from MODOPTIM's OPT input file along with parameter estimates from each optimization iteration. The residual-and-sensitivity file contains simulated and measured drawdowns, weighting factors, residuals, and weighted-sensitivity coefficients for the simulation with the smallest sum-of-squared differences (or model error). The parameter-estimates file contains optimization statistics and parameter estimates for the set of parameters with the smallest sum-of-squares error. The MODOPTIM output file names and a brief file contents description are listed in table 3. Several MODFLOW-96 (Harbaugh and McDonald, 1996b) input files also are generated as output from MODOPTIM. These files (lines 4-9, table 3) generally are not of interest to the parameter estimation or optimization process. Files in lines 10 and 11 (table 3) are used by MODOPTIM but are not of interest to either the parameter estimation or optimization process.

Aquifer-Parameter Sensitivity and Non-Uniqueness of Solution

Parameter sensitivity is a measure of how important the parameter is for representing the observations. Parameter sensitivity can be used as a guide to determine which parameters should be estimated. More sensitive parameters have steeper slopes of model error versus parameter changes than less sensitive parameters. One should not attempt to estimate insensitive parameters because the variations in the sum of the square differences between the observed and simulated drawdowns as these parameters change is essentially zero. Parameter sensitivity is reported by MODOPTIM in terms of the relative sensitivity (Cooley and Naff, 1990; Poeter and Hill, 1997; and Hill and others, 1998).

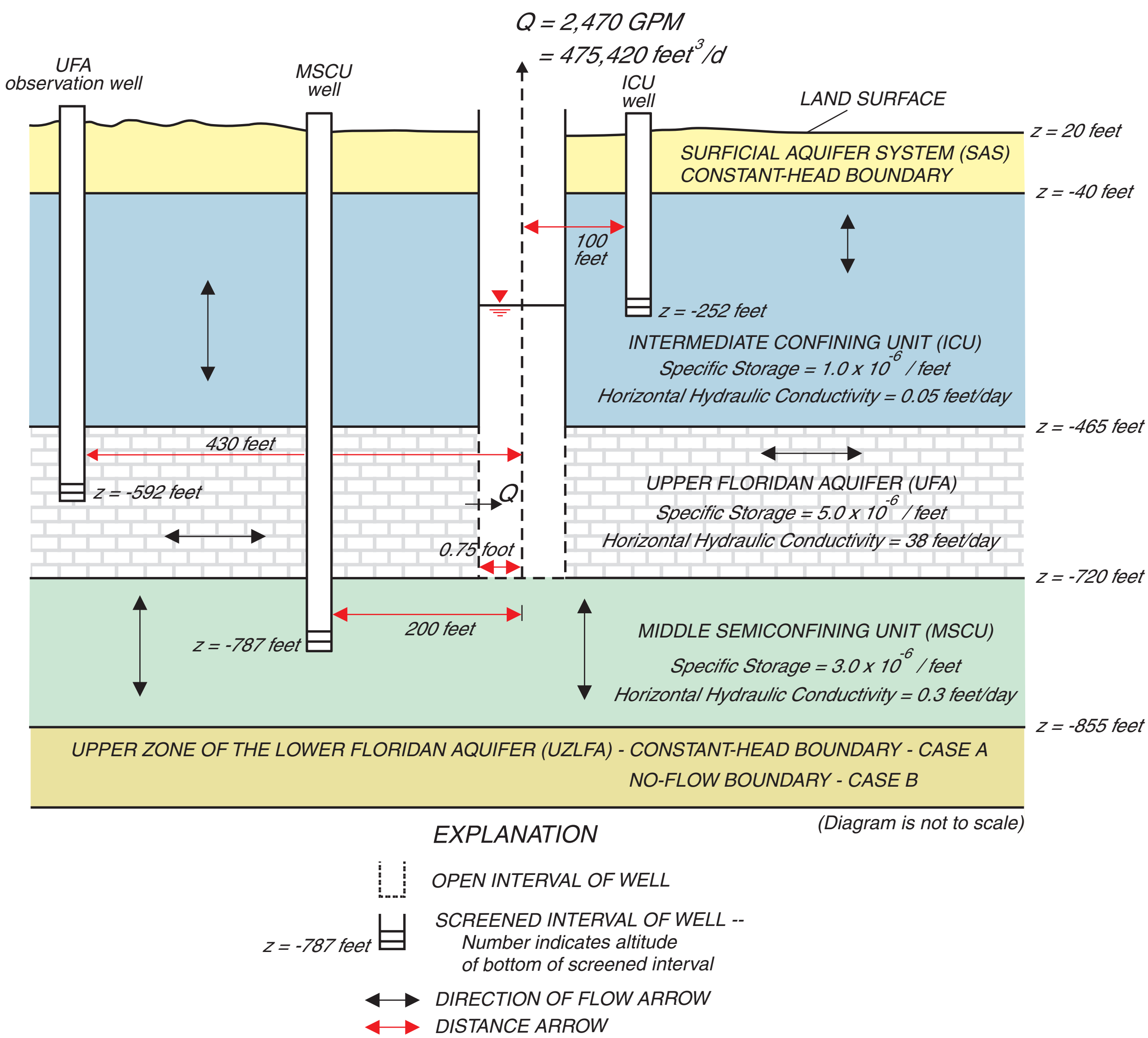

Figure 8. Hydrogeologic units penetrated by production and observation wells in a hypothetical aquifer-performance test with true hydraulic parameter values and two cases (case A, constant-head boundary; case B, no-flow boundary) used to illustrate the capabilities of MODOPTIM.

Table 2. List of input file names generated by the aquifer-test preprocessor and brief descriptions of files used to run MODOPTIM.

[COMHAL, code name given by the user and used to form input file names (table 1, line 2); MODFLOW-96, (McDonald and Harbaugh, 1988); BAS, Basic package file; BCF, Block centered flow package file]

Line number	Input file name	Description of input file contents
1	INPUT_COMHAL.OPT.txt	File specifications, convergence criteria for optimization, optimization control variables, initial or updated optimization parameter values, and observation data
2	INPUT_COMHAL.INP.txt	Data needed to build BAS and BCF, stress-periods input data, MODFLOW-96 file names and unit numbers, starting head values, and cell-by-cell flow specifications
3	INPUT_COMHAL.GR3.txt	Column widths and row thicknesses for the radial coordinate system
4	INPUT_COMHAL.OC.txt	Output control input file, as required in MODFLOW-96
5	INPUT_COMHAL.PCG.txt	Preconditioned conjugate gradient 2 input file, as required in MODFLOW-96
6	INPUT_COMHAL.WEL.txt	Well package input file, as required in MODFLOW-96
7	INPUT_COMHAL.ZONES.txt	Integer array indicating zone numbers with implied boundary condition notations

Table 3. List of output file names and brief descriptions of files generated by MODOPTIM.

[COMHAL, code name given by the user and used to form input file names (table 1, line 2); MODFLOW-96, (McDonald and Harbaugh, 1988)]

Line Number	Output file name	Description of output file contents
1	OUTPUT_COMHAL.Parameters.txt	Optimization statistics and parameter estimates with the smallest sum-of-squares error
2	OUTPUT_COMHAL.Resi&Sens.txt	Measured, simulated, time of measured value, residuals, weights, spatial coordinates, and weighted-sensitivity coefficients to each parameter for optimal parameter values
3	OUTPUT_COMHAL.MAIN-OPT.txt	Input from the optimization file and parameter estimates from each iteration
4	OUTPUT_COMHAL.MODFLOW-LIST.txt	MODFLOW-96 list output file
5	OUTPUT_COMHAL.BAS.txt	MODFLOW-96 Basic package file
6	OUTPUT_COMHAL.BCF.txt	MODFLOW-96 Block centered flow package file
7	OUTPUT_COMHAL.CBC	MODFLOW-96 unformatted file with calculated cell-by-cell flows
8	OUTPUT_COMHAL.UFH	MODFLOW-96 unformatted file with calculated head values
9	OUTPUT_COMHAL.VAR1.txt	Anisotropy data file
10	OUTPUT_old.grd.txt	Grid coordinates data file
11	OUTPUT_SHD.txt	Matrix of zero values to reset heads for all cells in the model

Parameters with a relative sensitivity of less than 0.01 should not be estimated (Hill, 1998).

Weighted and unweighted sum-of-squares, root-mean squares, and average errors are reported by drawdown file and for the complete set of drawdown files listed at the end of the OPT input file. Parameter estimates are ranked and reported by relative sensitivity in the optimization statistics and parameter-estimates output file.

Beginning several MODOPTIM runs with different initial parameter values could help determine the uniqueness of the optimized parameter values. If the optimized parameter values differ from each other by values that are small relative to their computed standard deviations, the optimization is likely to be unique (Hill and others, 2000, p. 18). If this is not the case, the optimal parameter values are not unique. Non-uniqueness is indicated by pairs of parameters that are correlated. Lack of uniqueness could be indicated by local minima in the objective function, that is, the sum-of-squared differences between measured and simulated drawdowns. In this case, it may be possible to identify the global minimum of the objective function by running MODOPTIM with different initial parameter values. The global minimum may be the set of estimated parameter values that produces the smallest value of the objective function. If non-uniqueness is caused by extreme parameter correlation, the sum-of-squares value for each optimized set of parameters is likely to be similar and at least one pair of parameters will have a correlation coefficient close to 1.0 or -1.0. It follows that only the ratio of the parameter values that are correlated can be computed.

Application of Aquifer-Test Preprocessor for MODOPTIM

This section shows how the aquifer-test preprocessor is used to generate the necessary input files to run MODOPTIM to analyze hypothetical APTs. The preprocessor also is used to generate the input files for the analysis of the APTs conducted at the well field in Duval County on December 15, 1999, and September 17, 2004. The optimal hydraulic parameter values computed by MODOPTIM were compared to those obtained by using the approach of fitting type curves to measured drawdown to provide the best fit. An explanation of the differences between each set of parameters is given based on the implicit assumptions associated with the numerical and analytical solutions.

Use of Aquifer-Test Preprocessor

The application of MODOPTIM's preprocessor is illustrated first by generating the input files needed to analyze hypothetical APT data for the aquifer-well configuration shown in figure 8. The hydraulic conductivity and the specific storage values for this hypothetical APT were assumed to be as shown in figure 8; these values are referred to as the true hydraulic parameter values. The expected drawdown at the UFA, ICU, and MSCU observation wells (fig. 8) were computed from Moench's solution (1985) by using the true hydraulic parameter values. The spreadsheet file described in table 4 was used to write the input text file needed by the preprocessor. Steps needed to run MODOPTIM with the preprocessor are shown in figure 9. The optimal hydraulic parameter values computed with MODOPTIM were compared to the true values to provide the reader with an assessment of MODOPTIM's capabilities to estimate the true values. The optimal hydraulic parameter values computed with MODOPTIM compared reasonably well to the true hydraulic parameter values for the aquifer-well configuration (fig. 8) with each set of boundary conditions (table 5).

As the relative sensitivity of a parameter increases, the optimal value is more likely to be close to the true value, and conversely, the lower the value of the relative sensitivity, the less likely the optimal value will be close to the true value. Thus, the relative sensitivity of the optimal parameter should be considered when assessing the reliability of the optimal parameter value. For boundary cases A and B (fig. 8), the relative sensitivity of all hydraulic parameters was at least 0.15 (table 5), allowing the optimal value to be close to the true value. Drawdowns in these hypothetical APTs were most sensitive to the hydraulic conductivity of the UFA. The specific storage and horizontal hydraulic conductivity of the ICU was the only pair of correlated parameters for cases A and B, indicating that only the ratio of these parameters can be determined uniquely but not each parameter separately. Note that the ratio of the hydraulic conductivity and specific storage of the ICU for the true values is equal to that ratio for the optimal values from MODOPTIM, in part because of the large relative sensitivity values of these parameters.

Table 4. Spreadsheet file used to generate the input files to run MODOPTIM for a hypothetical aquifer test with the aquifer-well case A configuration shown in figure 8.

[ICU, intermediate confining unit; UFA, Upper Floridan aquifer; MSCU, middle semiconfining unit; LFA, Lower Floridan aquifer; ft, feet; d, day; NGVD 29, datum used as example]

Line number	Parameter value	Parameter or field description
1	generatefiles	Used to name the text file to be generated and should not be changed
2	CHTEST	Prefix name to be used for input and output files, exactly 6 characters in length
3	0.010	Initial horizontal hydraulic conductivity of the ICU, in ft/d
4	20.0	Initial horizontal hydraulic conductivity of the UFA, in ft/d
5	1.0	Initial horizontal hydraulic conductivity of the MSCU, in ft/d
6	10.0	Initial horizontal hydraulic conductivity of the LFA, in ft/d
7	9.0	Radius of well screen, in inches
8	2470.0	Well discharge, in gallons per minute
9	-465.0	Altitude of the top of the well screen, in ft NGVD 29
10	-720.0	Altitude of the bottom of the well screen, in ft NGVD 29
11	-40.0	Altitude of the top of the ICU, in ft NGVD 29
12	-465.0	Altitude of the top of the UFA, in ft NGVD 29
13	-720.0	Altitude of the top of the MSCU, in ft NGVD 29
14	-855.0	Altitude of the top of the LFA, in ft NGVD 29
15	-930.0	Altitude of the bottom of the LFA, in ft NGVD 29, not used if well screen does not tap LFA
16	-1	Constant-head (negative) or no-flow (nonnegative) condition imposed at the top of model
17	-1	Constant-head (negative) or no-flow (nonnegative) condition imposed at the bottom of model
18	20	Maximum number of iterations to be performed by MODOPTIM, an integer
19	3	Number of (time, drawdown) data files generated during the aquifer performance test
20	UFA1	Name code to designate observation well 1, exactly 4 characters in length
21	430.0	Radial distance from center of pumping well to observation well 1, in ft
22	-592.0	Average altitude of open interval for observation well 1, in ft NGVD 29
23	CHTEST.UFA.txt	Name of (time, drawdown) data file for well 1, up to 20 characters in length, in (days, feet)
24	ICU1	Name code to designate observation well 2, exactly 4 characters in length
25	100.0	Radial distance from center of pumping well to observation well 2, in ft
26	-252.0	Average altitude of open interval for observation well 2, in ft NGVD 29
27	CHTEST.ICU.txt	Name of (time, drawdown) data file for well 2, up to 20 characters in length, in (days, feet)
28	MSCU	Name code to designate observation well 3, exactly 4 characters in length
29	200.0	Radial distance from center of pumping well to observation well 3, in ft
30	-787.0	Average altitude of open interval for observation well 3, in ft NGVD 29
31	CHTEST.MSCU.txt	Name of (time, drawdown) data file for well 3, up to 20 characters in length, in (days, feet)

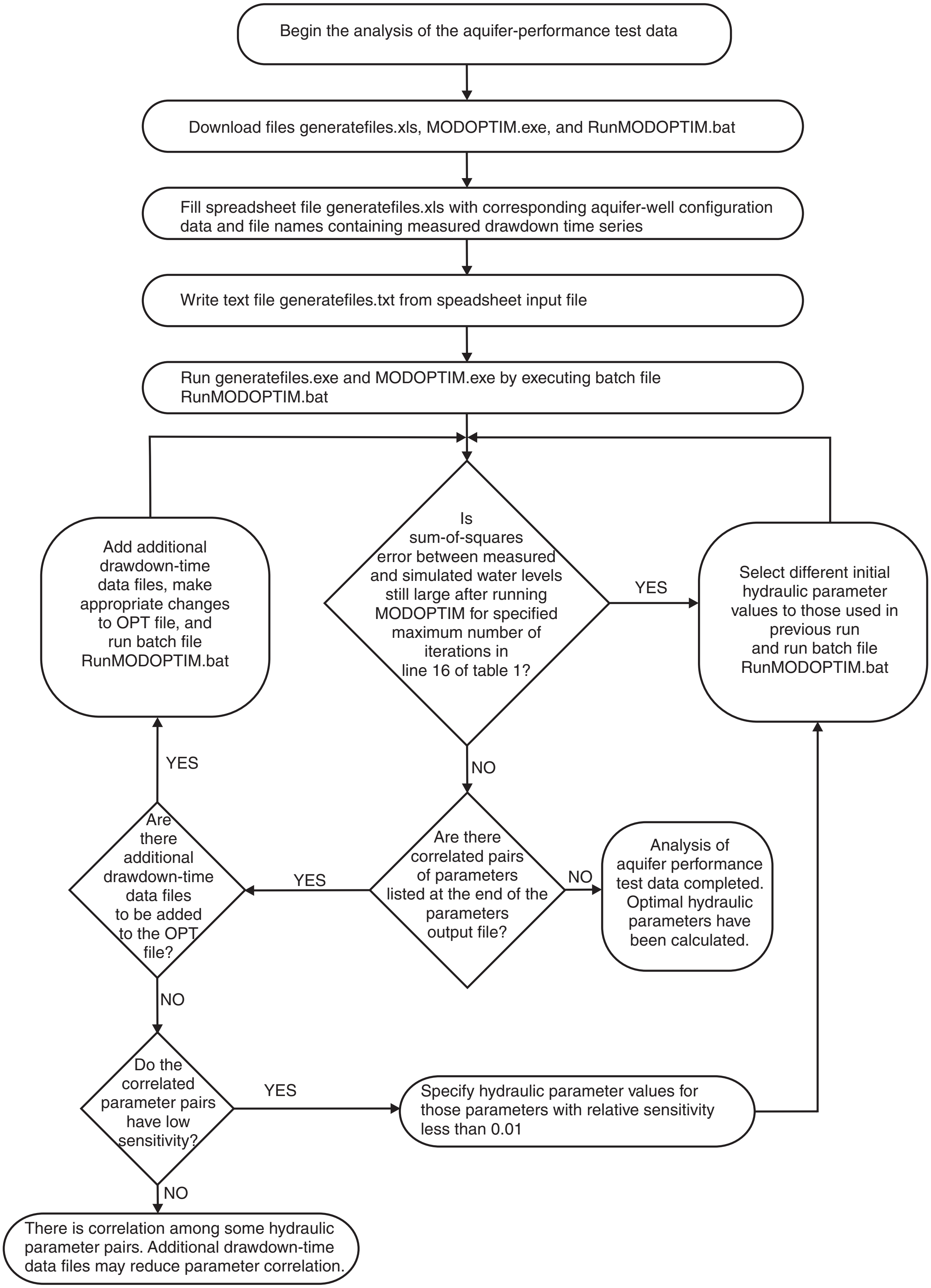

Figure 9. Steps needed to run MODOPTIM using the aquifer-test preprocessor.

Table 5. Hydraulic parameter values computed by MODOPTIM based on the aquifer-well configurations shown in figure 8 and the true values used to compute the predicted drawdowns.

[K, horizontal hydraulic conductivity in feet/day; S, specific storage in 1/feet; ICU, intermediate confining unit; UFA, Upper Floridan aquifer; MSCU, middle semiconfining unit]

Hydraulic parameter	True value	MODOPTIM value, case A	Relative sensitivity, dimensionless	MODOPTIM value, case B	Relative sensitivity
K-UFA	38.0	36.4	1.00	37.9	1.00
S-UFA	5.0×10^{-6}	5.0×10^{-6}	.31	5.1×10^{-6}	.29
K-MSCU	.30	.34	.22	.32	.19
S-MSCU	3.0×10^{-6}	3.3×10^{-6}	.15	3.1×10^{-6}	.22
K-ICU	5.0×10^{-2}	4.9×10^{-2}	.24	1.7×10^{-2}	.18
S-ICU	1.0×10^{-6}	9.8×10^{-7}	.25	3.4×10^{-7}	.18
Parameter pairs with correlation higher than 0.95: (S-ICU, K-ICU) in cases A and B					

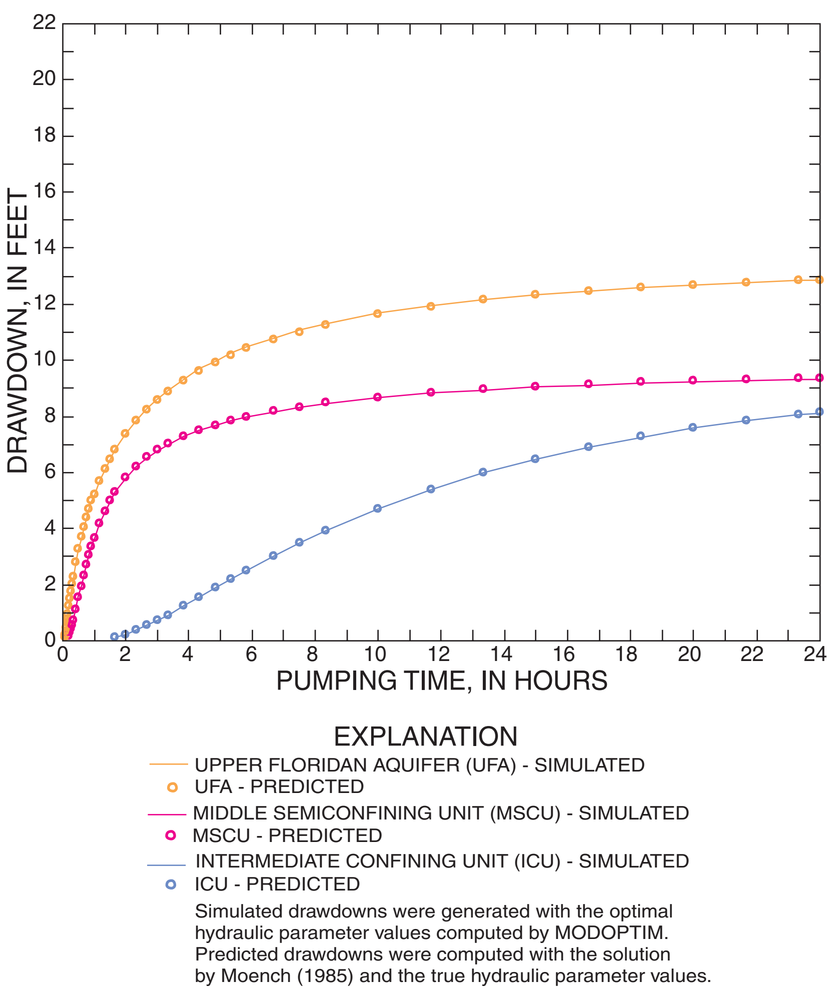

Figure 10. Predicted and simulated drawdowns in the production and observation wells for case A (fig. 8).

The drawdowns at the UFA, ICU, and MSCU wells computed by MODOPTIM compared reasonably well (figs. 10 and 11) with the “true” drawdowns computed using the analytical solution of Moench (1985). Although an optimal parameter value from MODOPTIM may be off by a factor, as it happens for the specific storage of the ICU in case B (table 5), simulated drawdowns may not be significantly different from analytical drawdowns if the ratio of the values of the correlated parameters is close to the ratio of the true values. The use of a type-curve matching technique also would result in the calculation of only the ratio of the true values.

A second hypothetical APT was used to assess MODOPTIM’s capability to derive optimal parameter values for a typical aquifer-well configuration in Duval County, where the production well fully penetrates the UFA and MSCU, and partially penetrates the UZLFA (fig. 12). The purpose of this hypothetical APT was to determine if the hydraulic conductivities and specific storages of the ICU, UFA, MSCU, and UZLFA can be determined uniquely from drawdowns recorded at these units. Table 6 describes the contents of the spreadsheet file used to generate MODOPTIM’s input files for the aquifer-well configuration shown in figure 12.

Table 6. Spreadsheet file used to generate the input files to run MODOPTIM for a hypothetical aquifer test with the aquifer-well configuration shown in figure 12.

[ICU, intermediate confining unit; UFA, Upper Floridan aquifer; MSCU, middle semiconfining unit; LFA, Lower Floridan aquifer; ft, feet; d, day; NGVD 29, datum used as example]

Line number	Parameter value or field name	Parameter or field description
1	generatefiles	Used to name the text file to be generated and should not be changed
2	CHTEST	Prefix name to be used for input and output files, exactly 6 characters in length
3	0.0050	Initial horizontal hydraulic conductivity of the ICU, in ft/d
4	30.0	Initial horizontal hydraulic conductivity of the UFA, in ft/d
5	0.10	Initial horizontal hydraulic conductivity of the MSCU, in ft/d
6	30.0	Initial horizontal hydraulic conductivity of the LFA, in ft/d
7	9.0	Radius of well screen, in inches
8	2500.0	Well discharge, in gallons per minute
9	-430.0	Altitude of the top of the well screen, in ft NGVD 29
10	-1205.0	Altitude of the bottom of the well screen, in ft NGVD 29
11	-40.0	Altitude of the top of the ICU, in ft NGVD 29
12	-430.0	Altitude of the top of the UFA, in ft NGVD 29
13	-690.0	Altitude of the top of the MSCU, in ft NGVD 29
14	-855.0	Altitude of the top of the LFA, in ft NGVD 29
15	-1300.0	Altitude of the bottom of the LFA, in ft NGVD 29, not used if well screen does not tap LFA
16	-1	Constant-head (negative) or no-flow (nonnegative) condition imposed at the top of model
17	1	Constant-head (negative) or no-flow (nonnegative) condition imposed at the bottom of model
18	15	Maximum number of iterations to be performed by MODOPTIM, an integer
19	5	Number of (time, drawdown) data files generated during the aquifer performance test
20	PW-1	Name code to designate observation well 1, exactly 4 characters in length
21	0.75	Radial distance from center of pumping well to observation well 1, in ft
22	-560.0	Average altitude of open interval for observation well 1, in ft NGVD 29
23	CHTEST.UFA1.txt	Name of (time, drawdown) data file for well 1, up to 20 characters in length, in (days, feet)
24	UFAO	Name code to designate observation well 2, exactly 4 characters in length
25	2430.0	Radial distance from center of pumping well to observation well 2, in ft
26	-560.0	Average altitude of open interval for observation well 2, in ft NGVD 29
27	CHTEST.UFA2.txt	Name of (time, drawdown) data file for well 2, up to 20 characters in length, in (days, feet)
28	ICUW	Name code to designate observation well 3, exactly 4 characters in length
29	100.0	Radial distance from center of pumping well to observation well 3, in ft
30	-235.0	Average altitude of open interval for observation well 3, in ft NGVD 29
31	CHTEST.ICU.txt	Name of (time, drawdown) data file for well 3, up to 20 characters in length, in (days, feet)
32	MSCU	Name code to designate observation well 4, exactly 4 characters in length
33	200.0	Radial distance from center of pumping well to observation well 4, in ft
34	-772.0	Average altitude of open interval for observation well 4, in ft NGVD 29
35	CHTEST.MSCU.txt	Name of (time, drawdown) data file for well 4, up to 20 characters in length, in (days, feet)
36	LFAW	Name code to designate observation well 5, exactly 4 characters in length
37	230.0	Radial distance from center of pumping well to observation well 5, in ft
38	-1130.0	Average altitude of open interval for observation well 5, in ft NGVD 29
39	CHTEST.LFA.txt	Name of (time, drawdown) data file for well 5, up to 20 characters in length, in (days, feet)

Simulated drawdowns at the UFA production well and at the UFA, ICU, MSCU, and UZLFA observation wells (files listed in lines 23, 27, 31, 35, and 39, table 6) were generated by using MODFLOW-96 and the true values listed in figure 12. Predicted drawdowns at these locations were computed using Moench (1985) solution using the true values. The hydraulic parameter values computed by MODOPTIM were very close to the true values (table 7). Three pairs of hydraulic parameters were correlated. The relative sensitivities of the hydraulic parameters of the ICU and MSCU were lower than those obtained in the hypothetical APTs (fig. 8).

Hydraulic conductivities of the UFA and UZLFA were correlated in the hypothetical APT of figure 12, indicating these two parameters cannot be determined uniquely. A flow log from the wellbore would be needed to determine the flow rates to the well originating from each penetrated hydrogeologic unit. Such a flow log would allow the hydraulic conductivities of the UFA and UZLFA to be determined reliably with MODOPTIM by calibrating for the hydraulic conductivities that simulates the closest flow ratio of each aquifer to the well.

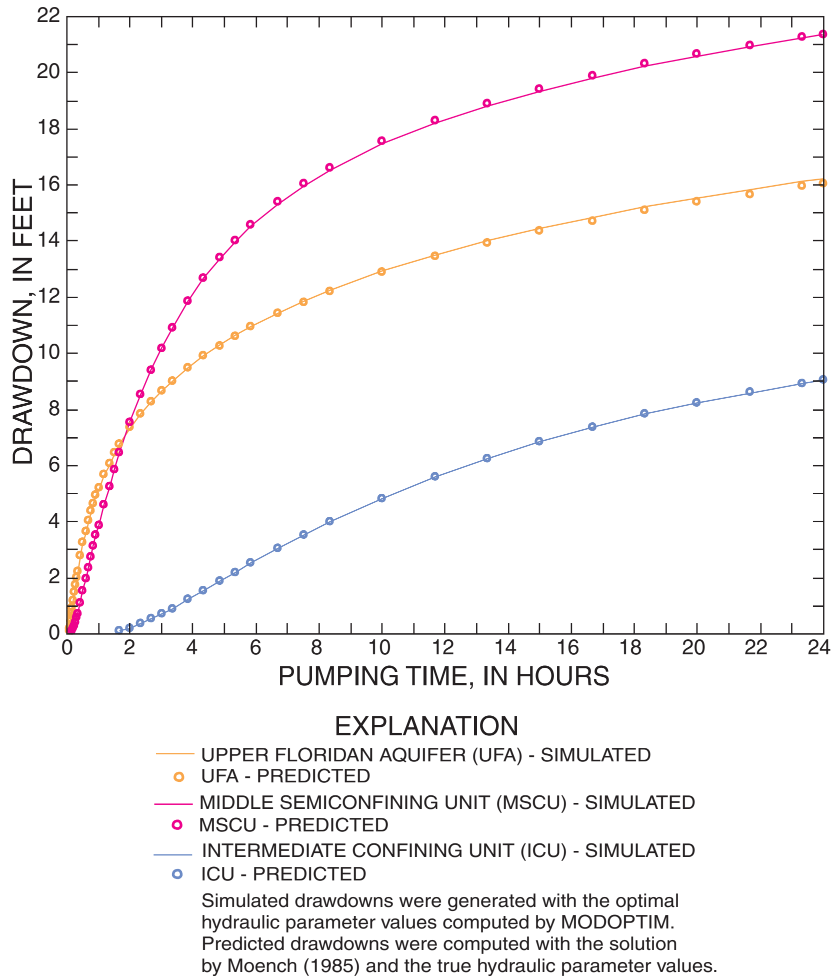

Figure 11. Predicted and simulated drawdowns in the production and observation wells for case B (fig. 8).

Table 7. Hydraulic parameter values computed by MODOPTIM based on the aquifer-well configuration shown in figure 12 and the true values used to compute the predicted drawdowns.

[K, horizontal hydraulic conductivity in feet/day; S, specific storage in 1/feet; ICU, intermediate confining unit; UFA, Upper Floridan aquifer; MSCU, middle semiconfining unit; LFA, Lower Floridan aquifer; A, anisotropy]

Hydraulic parameter	True value	MODOPTIM value	Relative sensitivity, dimensionless
K-UFA	38.0	36.3	0.52
S-UFA	5.0 x 10-6	5.1 x 10-6	.06
K-MSCU	.30	.24	.06
S-MSCU	3.0 x 10-6	2.4 x 10-6	.06
K-ICU	5.0 x 10-2	3.9 x 10-2	.07
S-ICU	1.0 x 10-6	8.3 x 10-7	.06
K-LFA	46.0	47.1	1.00
S-LFA	7.0 x 10-6	7.5 x 10-6	.11
A-LFA	.1	.1	.00

Parameter pairs with correlation higher than 0.95: (S-ICU, K-ICU); (S-MSCU, K-MSCU); and (K-LFA, K-UFA)

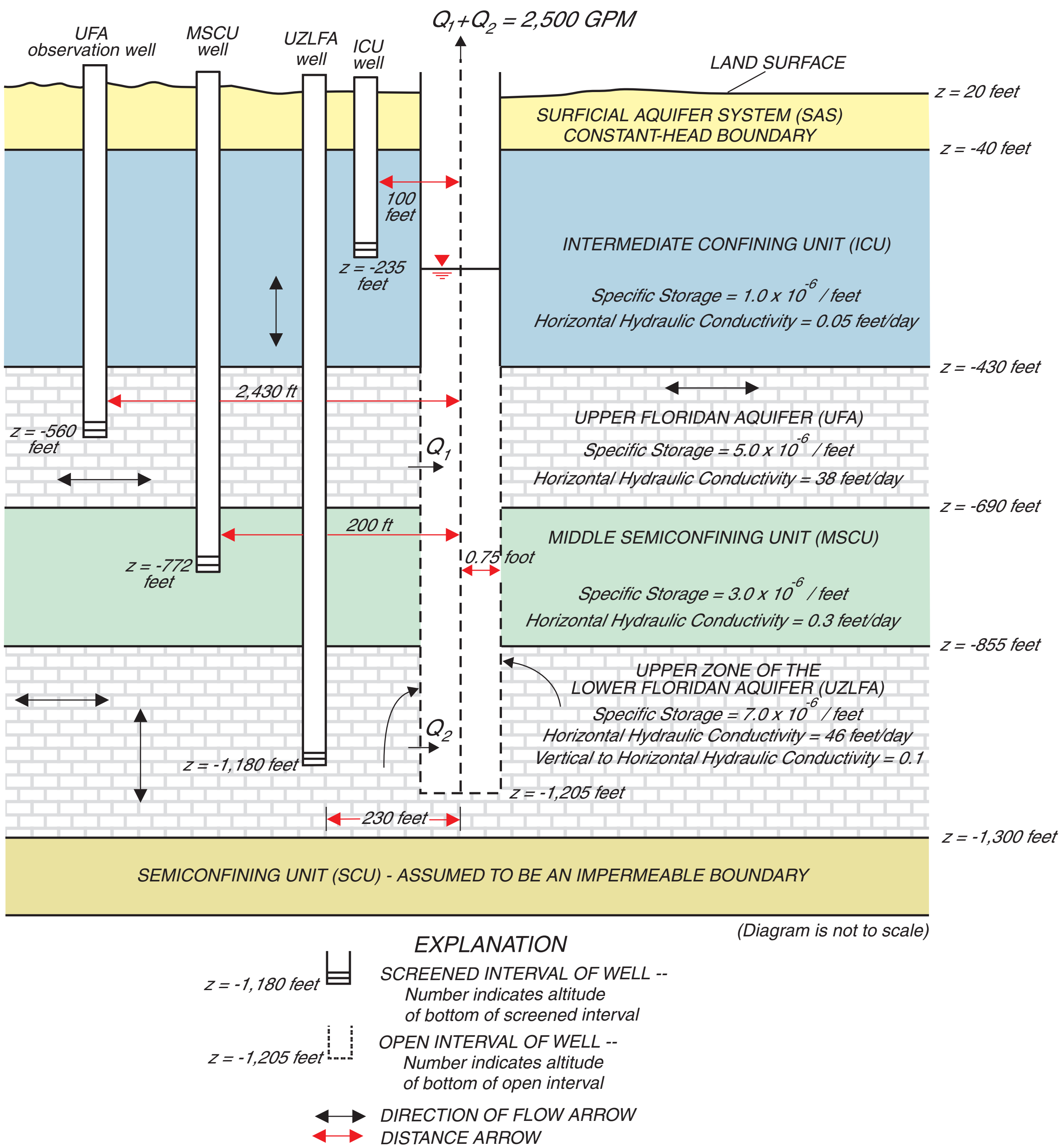

Figure 12. Hydrogeologic units penetrated by production and observation wells in a hypothetical aquifer-performance test with true hydraulic parameter values and boundary conditions used to illustrate the capabilities of MODOPTIM.

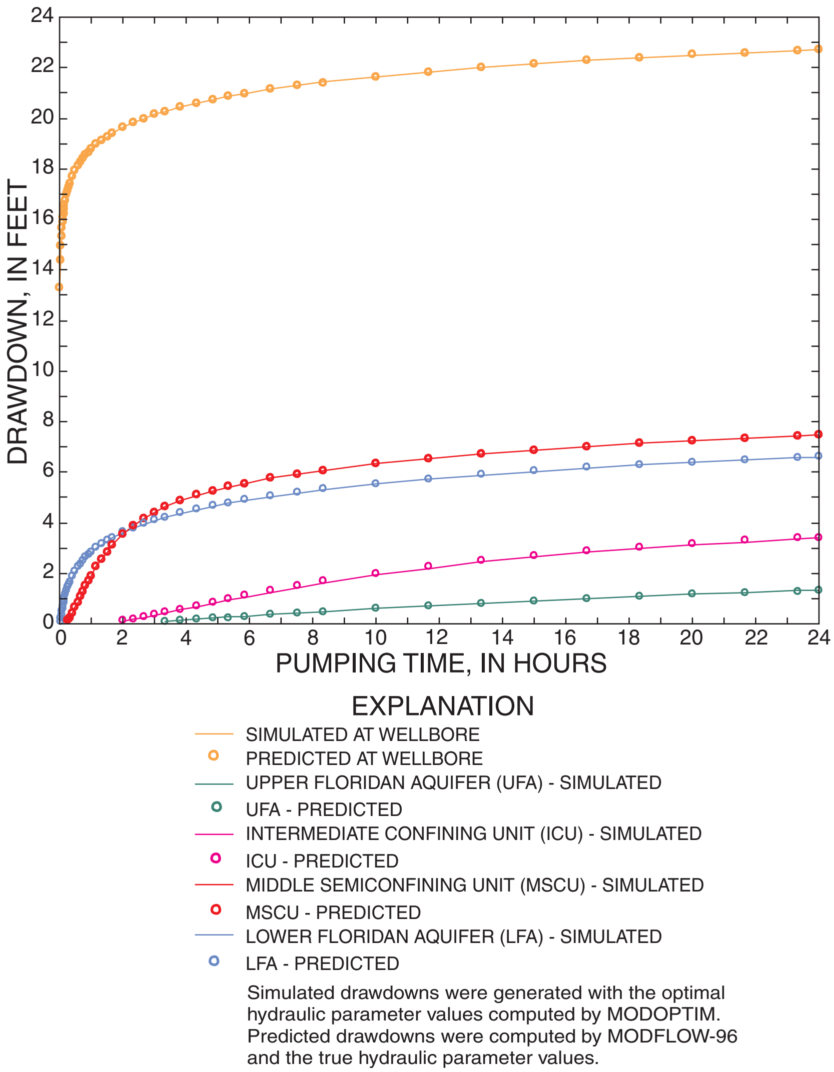

Figure 13. Predicted and simulated drawdowns in the production and observation wells in the aquifer-well configuration shown in figure 12.

Table 8. Drawdown data recorded at well AF-3 during the December 15, 1999, aquifer test performed at well M505.

[Time, time after pumping began in well M505; drawdown, recorded at well AF-3 open from -475 to -485 ft; drawdown is relative to equilibrium]

Time, in minutes	Draw-down, in feet	Time, in minutes	Draw-down, in feet
30	0.10	750	4.29
60	.60	780	4.34
90	1.06	810	4.39
120	1.45	840	4.43
150	1.78	870	4.47
180	2.06	900	4.51
210	2.31	930	4.55
240	2.51	960	4.59
270	2.70	990	4.63
300	2.87	1,020	4.67
330	3.02	1,050	4.72
360	3.17	1,080	4.76
390	3.30	1,110	4.81
420	3.42	1,140	4.87
450	3.53	1,170	4.92
480	3.63	1,200	4.98
510	3.73	1,230	5.04
540	3.82	1,260	5.10
570	3.90	1,290	5.17
600	3.97	1,320	5.24
630	4.04	1,350	5.31
660	4.11	1,380	5.36
690	4.17	1,410	5.40
720	4.23	1,440	5.43

Only the ratios of the hydraulic conductivities and specific storages from the ICU and MSCU can be computed as these parameter pairs also were correlated. Simulated drawdowns at the production and observation wells computed with MODOPTIM by using the optimal hydraulic parameter values compared reasonably well (fig. 13) with the predicted drawdowns. The anisotropy of the UZLFA could not be computed because the optimization process was insensitive to this parameter.

Analysis of Aquifer-Test Data From Well Field in Duval County, Florida

MODOPTIM was used to analyze the drawdown data from the APTs of December 15, 1999, and September 17, 2004. Hydraulic properties for the ICU, UFA, MSCU, and zone 1 of the UZLFA were obtained from the December 15, 1999, APT data from wells AF-3 and M505 (tables 8 and 9, respectively). Results from

Table 9. Drawdown data recorded at well M505 during the December 15, 1999, aquifer test performed at well M505.

[Time, time after pumping began in well M505; drawdown, recorded at well M505 with a casing radius of 0.75 ft and open from -465 to -1,080 ft; drawdown is relative to equilibrium]

Time, in minutes	Drawdown, in feet	Time, in minutes	Drawdown, in feet	Time, in minutes	Drawdown, in feet	Time, in minutes	Drawdown, in feet
0.22	8.92	0.91	45.05	9.40	54.23	140.00	60.14
.23	11.05	.92	45.47	9.60	54.26	160.00	60.22
.24	17.77	.94	45.64	9.80	54.28	180.00	60.33
.26	18.82	.95	45.99	10.00	54.59	200.00	60.46
.27	20.63	.96	45.85	12.00	54.94	220.00	60.76
.30	21.94	.98	46.04	14.00	55.21	260.00	61.00
.32	24.48	.99	46.28	16.00	55.37	300.00	61.08
.33	26.47	1.20	47.88	18.00	55.52	320.00	61.24
.35	27.84	1.40	48.90	22.00	55.72	340.00	61.32
.37	31.13	1.60	49.57	24.00	56.15	360.00	61.54
.40	32.98	1.80	49.97	26.00	56.47	400.00	61.72
.42	34.68	2.00	50.54	28.00	56.58	420.00	61.76
.43	35.76	2.40	50.81	30.00	56.66	440.00	61.84
.45	36.64	2.60	51.17	32.00	56.72	460.00	62.05
.48	37.15	3.00	51.60	36.00	56.98	500.00	62.11
.50	37.56	3.20	51.75	42.00	57.15	580.00	62.16
.52	37.40	3.40	52.13	44.00	57.20	640.00	62.32
.53	37.47	3.60	51.88	46.00	57.39	680.00	62.34
.55	38.24	3.80	52.13	48.00	57.68	720.00	62.43
.58	39.58	4.20	52.19	50.00	57.93	740.00	62.49
.60	40.36	4.40	52.27	52.00	57.96	860.00	62.56
.63	41.65	4.60	52.61	56.00	58.12	920.00	62.69
.65	41.78	4.80	52.62	62.00	58.17	980.00	62.75
.68	42.32	5.00	52.75	64.00	58.27	1,040.00	62.81
.71	42.40	5.20	52.80	68.00	58.44	1,120.00	62.83
.72	42.91	5.40	52.89	70.00	58.51	1,140.00	62.84
.73	43.14	5.60	53.08	72.00	58.71	1,160.00	62.99
.75	43.38	5.80	53.15	74.00	58.36	1,220.00	63.11
.76	43.60	6.40	53.26	78.00	58.63	1,280.00	63.13
.78	43.78	6.80	53.32	80.00	58.78	1,300.00	63.15
.81	43.83	7.00	53.66	86.00	58.85	1,320.00	63.23
.82	44.13	8.00	53.82	94.00	58.89	1,380.00	63.27
.84	44.43	8.20	53.86	96.00	59.00	1,440.00	63.40
.85	44.50	8.40	53.89	98.00	59.06		
.86	44.86	8.80	54.02	100.00	59.11		
.88	44.97	9.00	54.07	120.00	59.66		

Table 10. Drawdown data recorded at well LFAM during the September 17, 2004, aquifer test performed at well M503.

[Time, time after pumping began in well M503; drawdown, recorded at well LFAM located 230 feet from M503 and open from -1,080 to -1,180 ft; drawdown is relative to equilibrium; pumping well M503 open from -465 to -1,205 ft]

Time, in minutes	Drawdown, in feet	Time, in minutes	Drawdown, in feet	Time, in minutes	Drawdown, in feet
17.0	0.18	42.0	1.16	115.0	1.86
17.5	.21	43.0	1.16	120.0	1.89
18.0	.24	44.0	1.19	125.0	1.89
18.5	.27	45.0	1.19	130.0	1.92
19.0	.29	46.0	1.22	135.0	1.94
19.5	.32	47.0	1.25	140.0	1.97
20.0	.35	48.0	1.25	145.0	1.97
20.5	.38	49.0	1.28	150.0	2.00
21.0	.41	50.0	1.31	155.0	2.00
21.5	.50	51.0	1.31	160.0	2.03
22.0	.50	52.0	1.34	165.0	2.06
22.5	.50	53.0	1.34	170.0	2.06
23.0	.53	54.0	1.34	175.0	2.06
23.5	.56	55.0	1.37	180.0	2.09
24.0	.58	56.0	1.37	185.0	2.12
24.5	.64	57.0	1.39	190.0	2.12
25.0	.64	58.0	1.42	195.0	2.15
25.5	.64	59.0	1.42	200.0	2.15
26.0	.67	60.0	1.42	205.0	2.15
26.5	.70	62.0	1.45	210.0	2.18
27.0	.70	64.0	1.48	215.0	2.18
27.5	.73	66.0	1.48	220.0	2.20
28.0	.73	68.0	1.51	225.0	2.20
28.5	.79	70.0	1.54	230.0	2.20
29.0	.82	72.0	1.57	235.0	2.20
29.5	.82	74.0	1.57	240.0	2.23
30.0	.82	76.0	1.60	245.0	2.23
31.0	.84	78.0	1.63	250.0	2.23
32.0	.87	80.0	1.63	255.0	2.26
33.0	.93	82.0	1.65	260.0	2.26
34.0	.93	84.0	1.65	265.0	2.26
35.0	.96	86.0	1.68	270.0	2.26
36.0	.99	88.0	1.71	275.0	2.26
37.0	1.05	90.0	1.71	280.0	2.26
38.0	1.08	95.0	1.74	285.0	2.29
39.0	1.10	100.0	1.77	290.0	2.29
40.0	1.13	105.0	1.80	295.0	2.29
41.0	1.13	110.0	1.83	299.0	2.29

this analysis were used to compute hydraulic properties for zone 2 of the UZLFA using the APT data from well LFAM for September 17, 2004 (table 10). This was done because (1) no reliable drawdown data were available from a UFA observation well from the APT of September 17, 2004, (2) no drawdown data were available from the UZFA for the test of December 15, 1999, and (3) well M505 only penetrates the UFA, MSCU, and UZLFA (zone 1) hydrogeologic units because flow to the wellbore from zone 2 of the UZLFA is negligible.

The APT data of December 15, 1999, was re-analyzed with MODOPTIM to assess the differences between the hydraulic parameter values obtained by using the analytical solutions described earlier and those computed with MODOPTIM when the storative and leakage properties of the ICU and MSCU are considered. The input files for MODOPTIM were generated by the preprocessor, using the spreadsheet file shown in table 1. The preprocessor described in this report was then used to generate the input files needed to run MODOPTIM to compute the optimal hydraulic parameter values in the vicinity of the well field using the December 15, 1999, APT data. Drawdown data used in this analysis were the recorded drawdowns at wells AF-3 and M505 (fig. 3, tables 8 and 9).

The results of the analysis of the APT data are shown in table 11. There were very small differences between measured and simulated drawdowns at production well M505 and observation well AF-3 (fig. 14). No anisotropy for the UFA was computed by MODOPTIM from the analysis of the APT data of December 15, 1999, because the recorded drawdown data were insensitive to this parameter. No two hydraulic parameters were

Table 11. Hydraulic parameter values computed from analytical methods and by MODOPTIM for the well field in Duval County based on the aquifer tests conducted on December 15, 1999, and September 17, 2004.

[K, horizontal hydraulic conductivity, in feet per day; S, specific storage, in 1/feet; ICU, intermediate confining unit; UFA, Upper Floridan aquifer; MSCU, middle semiconfining unit; LFA, Lower Floridan aquifer; a-LFA, anisotropy in the LFA; --, value was not computed; CJ, Cooper and Jacob (1946); TH, Theis (1935); HJ, Hantush and Jacob (1955). Average analytical values were computed by CH2MHill (2000)]

Hydraulic parameter	Average analytical value	Analytical method(s) used	MODOPTIM value	Relative sensitivity, dimensionless
December 15, 1999				
K-UFA	86[a]	CJ, TH, HJ	38	1.00
S-UFA	1.0×10^{-6} [a]	CJ, TH, HJ	4.4×10^{-7}	.03
K-MSCU	--	--	.12	.05
S-MSCU	--	--	7.3×10^{-6}	.06
K-ICU	.03[b]	HJ	3.1×10^{-3}	.02
S-ICU	--	--	1.3×10^{-6}	.02
K-LFA (zone 1)	--	--	.21	.03
S-LFA (zone 1)	--	--	1.3×10^{-5}	.05
Parameter pairs with correlation higher than 0.95: None				

[a]Indicates values were calculated from thickness of UFA shown in figure 4.

[b]Indicates value was calculated from vertical leakance assuming no anisotropy and the ICU thickness shown in figure 4.

Hydraulic parameter	MODOPTIM value	Relative sensitivity, dimensionless
September 17, 2004		
K-LFA (zone 2)	42	.97
S-LFA (zone 2)	2.0×10^{-5}	1.00
a-LFA (zone 2)	.14	.61
Parameter pairs with correlation higher than 0.95: (K-LFA, a-LFA)		

correlated at the 0.95 level or higher and all hydraulic parameters had a relative sensitivity of 0.02 or higher.

An APT was performed at production well M503 on September 17, 2004. Drawdown data recorded at well LFAM (table 10), resulting from pumping well M503 (fig. 3) at an average rate of 1,648 gal/min, were used for the analysis of the APT data. Drawdown data were available at well LFAM only 17 minutes after pumping well M503 (table 10). A constant-head boundary was used at the SCU (fig. 6) because upward flow from the FPZ—through the SCU to the UZLFA—occurs in the well field (Sepúlveda and Spechler, 2004). The calculation of the hydraulic parameter values for zone 2 of the UZLFA was performed by using MODOPTIM to analyze the APT data of September 17, 2004, with the transmissivity and specific storage values for the ICU, UFA, MSCU, and zone 1 of the UZLFA fixed as determined from the analysis of the December 15, 1999, APT data (table 11). This was accomplished by changing the "status" of parameters for the ICU, UFA, MSCU, and UZLFA (zone 1) hydrogeologic units from "Active" to "Modify" in the OPT input file generated by the preprocessor. The hydraulic conductivity, specific storage, and anisotropy of zone 2 of the UZLFA were the only parameters assigned with the status of "Active" and thus allowed to change in the optimization scheme executed by MODOPTIM.

There were very small differences between recorded and simulated drawdowns at well LFAM (fig. 15). The hydraulic conductivity of zone 2 of the UZLFA was

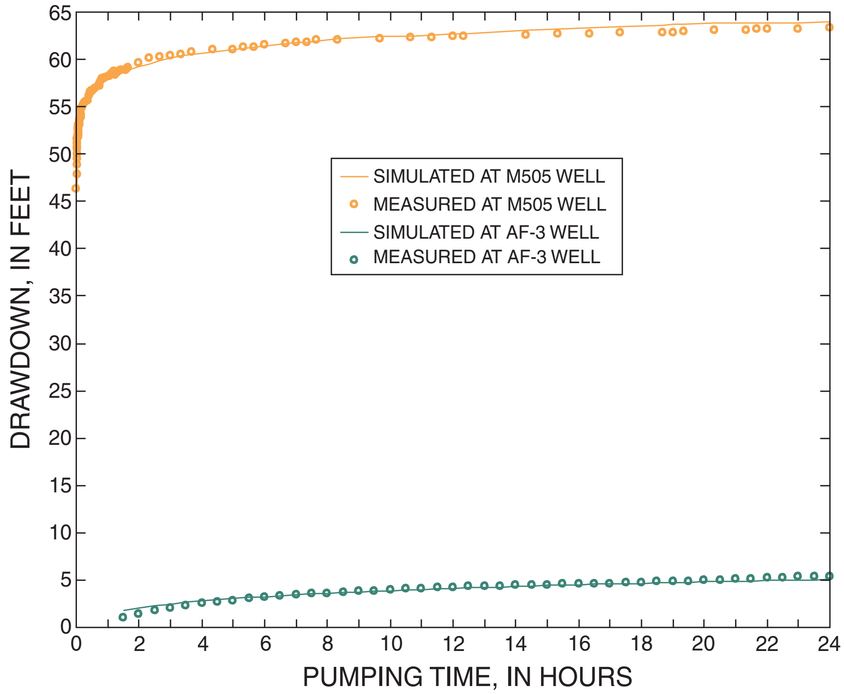

Figure 14. Measured drawdowns in production well M505 and observation well AF-3 on December 15, 1999, and simulated drawdowns using the optimal hydraulic parameter values computed by MODOPTIM.

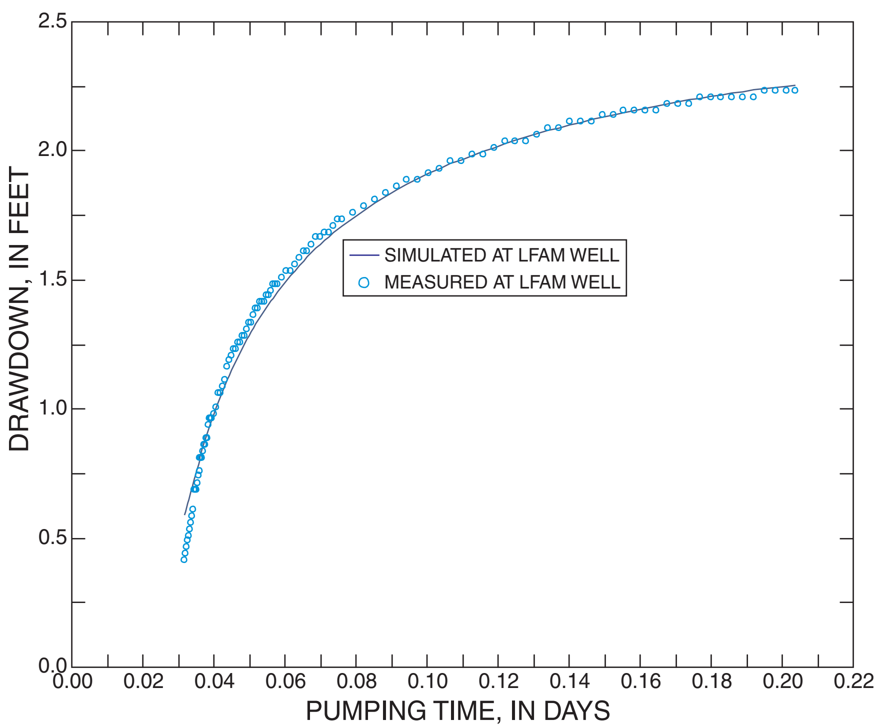

Figure 15. Measured drawdowns in well LFAM on September 17, 2004, and simulated drawdowns using the optimal hydraulic parameter values computed by MODOPTIM.

greater than that for the UFA (table 11). The parameter pair of hydraulic conductivity and anisotropy for zone 2 were correlated in this analysis, indicating that only the ratio of hydraulic conductivity to anisotropy for zone 2 can be estimated reliably. Several sets of initial values were used, and the optimal values shown are those that resulted in the minimum sum-of-squared differences between measured and simulated drawdowns.

Flows from storage in the UFA and zone 2 of the UZLFA decrease as time of pumping increases, while flows from storage from the ICU and the MSCU increase (fig. 16). If the storativity properties of the confining units were not simulated, the hydraulic conductivities of the aquifers would be overestimated because the aquifers would be the only hydrogeologic units accounting for the additional source of water from the confining units. The simulated flows to the wellbore from the UFA and zone 2 agree reasonably well with the flow log for well LFAM (fig. 7). Flows to the wellbore from the confining units are negligible, indicating these flows are not expected to cause significant differences in hydraulic properties values in the well field. About 60 percent of the simulated flow to the wellbore originated from zone 2, and about 40 percent originated from the UFA. This good match between simulated and measured flows to the wellbore from the UFA and from zone 2 at well M503 reduces the uncertainty of the simulated ratio of hydraulic conductivity to anisotropy for zone 2.

Although the general perception has been that the transmissivity of the LFA is at least one order of magnitude larger than that for the UFA in northeastern Florida, the results shown in this report for the well field in Duval County, Florida, show such perception may not always be the case. Factors like fractures and cavities may contribute to the differences in permeabilities between the two aquifers. Zone 1 of the

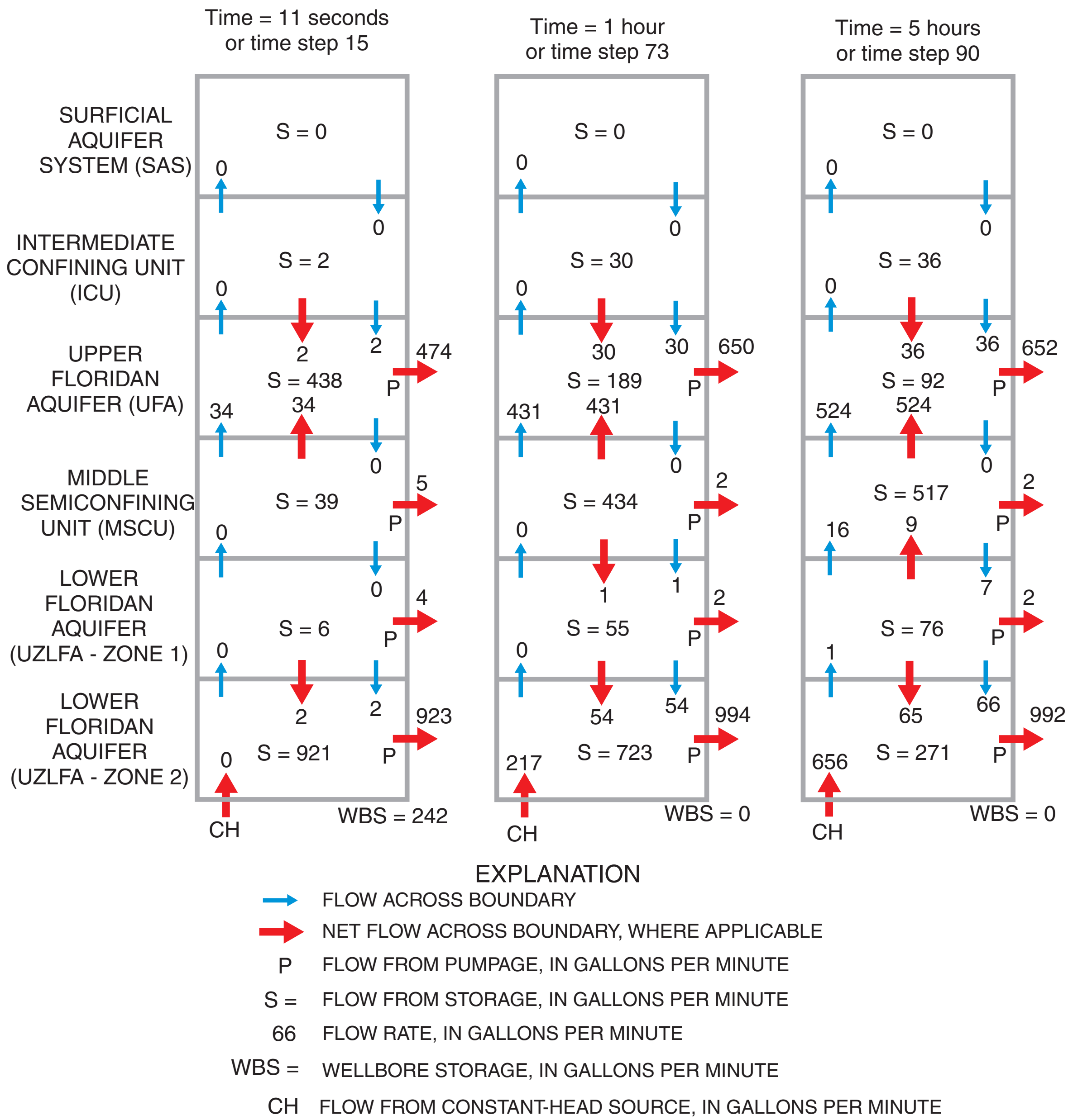

Figure 16. Simulated volumetric flow budget of the surficial and Floridan aquifer systems 11 seconds, 1 hour, and 5 hours after pumping started at well M503 at 1,648 gallons per minute during the September 17, 2004, aquifer test.

UZLFA in the well field (figs. 5 and 7) is generally much less permeable than zone 2 because of secondary porosity features like fractures and dissolution-enlarged cavities in hard dolomite in zone 2. Deeper zones in the LFA may be much more permeable, however, than the depths tapped by wells M505 and M503 because of potential fractures and cavities.

Comparison Between MODOPTIM and Analytically-Derived Values

The difference between the hydraulic conductivities of the UFA obtained by MODOPTIM and from analytical solutions (table 11) can be explained by differences in assumptions made in both analyses. The average hydraulic conductivity of the UFA derived by analytical solutions was 86 feet per day (CH2MHill, 2000). The hydraulic conductivity of the UFA derived by MODOPTIM was 38 feet per day (table 11). The analytical solutions used do not account for the storativity properties of the ICU and MSCU, whereas MODOPTIM does account for water storage in the confining units. The stored water in the confining units represents an additional source to the aquifer, which results in less drawdown compared to that generated when no storage in the confining units is considered (all other hydraulic parameter values being equal). Thus, the computed hydraulic conductivity from the method that considers storage in the confining units will be lower than the one computed from the method that does not consider storage to match the same measured drawdown. The hydraulic conductivity computed from the analysis of drawdown generated from a production well generally is overestimated when no storage in the confining units is considered.

MODOPTIM simulates a fraction of the well discharge, however small, originating from the confining unit open to the wellbore, which causes the discharge from the aquifer to be less than the total well discharge. Discarding the possibility that some discharge comes from the confining units is equivalent to overestimating the hydraulic conductivity of the aquifer because a larger discharge from the aquifer would have to be compensated with an increase in hydraulic conductivity. Figure 16 indicates that flow from the ICU and MSCU to the wellbore could not have caused the hydraulic conductivity of the UFA to be overestimated.

If wellbore storage in the production wells is neglected in the analysis of the drawdown data, then the specific storage of the aquifer would be overestimated because the average specific storage of the well and the aquifer in the vicinity of the well is higher than the specific storage of the aquifer. The measured drawdown in the well accounts for the wellbore storage. These are the basic reasons the hydraulic conductivity of the UFA was overestimated by the analysis of the APT data using the analytical solutions.

The transmissivity of the UFA was about 9,700 feet squared per day, the value of the optimal hydraulic conductivity obtained by MODOPTIM (38 feet per day) multiplied by the estimated thickness of 255 ft for the UFA (fig. 4). Based on an estimated thickness of zone 2 of the UZLFA of about 370 ft in the well field (fig. 6), and a MODOPTIM-computed hydraulic conductivity of zone 2 of 42 feet per day, the transmissivity of zone 2 of the UZLFA was about 15,500 feet squared per day. The hydraulic conductivity of the MSCU, 0.12 feet per day, was at least one order of magnitude higher than that for the ICU, computed to be 3.1×10^{-3} feet per day. The computed specific storage of zone 2 of the UZLFA was 2×10^{-5} per foot. This large value for specific storage for zone 2 of the UZLFA was perhaps due to the large radius of well LFAM, coupled with the large volume of water stored in the wellbore prior to the aquifer test. The computed ratio of vertical to horizontal hydraulic conductivity in zone 2 of the UZLFA, 0.14, indicates that the estimated vertical hydraulic conductivity of this zone is about 5.9 feet per day.

Limitations and Advantages of MODOPTIM

Ground-water flow simulations generally are based on conceptual models that are simplified representations of complex heterogeneous ground-water flow systems. MODOPTIM uses MODFLOW-96 to simulate ground-water flow and thus is subject to errors made in ground-water flow simulation stemming from the simplified representations of the real ground-water flow system. Assumptions such as isotropy, vertical homogeneity within each row, and the absence of preferential flow zones or dissolution cavities are examples of simplified representations that can be sources of error in a ground-water flow simulation.

MODOPTIM is a calibration and management tool that can be used to solve a wide range of optimization problems (K.J. Halford, U.S. Geological Survey, written commun., 2004). The preprocessor presented in this report, however, was developed for the specific analysis of APT data obtained for a production well that penetrates one or two aquifers. The upper aquifer has underlying and overlying confining units. The boundary conditions specified at the top and bottom of the simulated area can either be a constant-head source or a no-flow boundary.

The solution of the ground-water flow equation through a finite-difference approximation has a round-off error associated with the grid refinement. Analytical solutions to the ground-water flow equation do not have this round-off error associated with grid refinement. Analytical solutions, however, are not available for the specific aquifer-well configuration in which the production well fully penetrates an aquifer confined above and below by leaky units that can store water, and partially penetrates the aquifer below. Such a problem can be solved numerically by using MODOPTIM. Flow into the wellbore from the confining units can occur; this process can be simulated by MODOPTIM but not by analytical solutions.

The calculation of optimal hydraulic parameter values using MODOPTIM results in the analysis of the sensitivity of these parameters, providing a tool to quantify the relative capability of each parameter to reduce the sum of the square differences between the measured and simulated drawdowns. Optimal hydraulic parameter values can be obtained from APT data using MODOPTIM with reliable accuracy, particularly parameters for which the model shows a high relative sensitivity.

Summary and Conclusions

An aquifer-test preprocessor for MODOPTIM was developed to facilitate the calculation of optimal hydraulic parameter values from drawdown data recorded in the vicinity of a pumping well that fully or partially penetrates one or two aquifers. The aquifer-test preprocessor presented generates the input files needed to analyze drawdown data from such aquifer-well configuration using MODOPTIM. MODOPTIM, which uses MODFLOW-96, can be used to compute optimal hydraulic parameter values from the analysis of aquifer-performance test data by using a cylindrical or axisymmetric flow model in the vicinity of a pumping well. MODOPTIM's performance and the use of the preprocessor were illustrated for three hypothetical aquifer performance tests (APTs). Two of these tests used the drawdown in the aquifer and confining units computed from an analytical solution derived by Moench (1985) as "measured" drawdown. Another hypothetical APT used the drawdown in the aquifer and confining units computed from MODFLOW-96 as measured drawdown. The true hydraulic parameter values were compared to the optimal values computed by MODOPTIM for several sets of boundary conditions.

The analyses of the hypothetical APT data in which the production well penetrates only one aquifer indicated that the storativity and hydraulic conductivity of one confining unit were correlated, precluding the calculation of all hydraulic parameter values uniquely. The analyses of the hypothetical APT data in which the production well fully penetrates the upper aquifer and partially penetrates the lower aquifer indicated an increase in the number of correlated hydraulic parameter pairs, making more difficult the calculation of all hydraulic parameter values uniquely. The availability of flow-log data allows the hydraulic conductivities of the penetrated aquifers to be determined reliably with MODOPTIM by calibrating the hydraulic conductivities that simulate the closest flow ratio of each aquifer to the well. The lack of a flow log restricts the calculation of the hydraulic conductivities of the penetrated aquifers to only its ratio.

The aquifer-test preprocessor was used to generate the input files needed to analyze APT data conducted in a well field in Duval County, Florida, using MODOPTIM. The computed hydraulic conductivity of the Upper Floridan aquifer (UFA) in the well field was 38 feet per day, whereas that for the upper zone of the Lower Floridan aquifer (UZLFA) was 42 feet per day. The computed hydraulic conductivity for the middle semi-confining unit (MSCU) was 0.12 feet per day, whereas that for the intermediate confining unit (ICU) was about two orders of magnitude lower, or 3.1×10^{-3} feet per day. The hydraulic conductivity of the UFA derived from analytical solutions was 86 feet per day, more than twice the MODOPTIM value. The hydraulic conductivity derived by MODOPTIM is an improved value because it accounts for complexity not considered in the derivation of the analytical solutions. In addition, MODOPTIM has the benefit of generating estimates of parameter sensitivity and correlation.

The anisotropy of zone 2 of the UZLFA by MODOPTIM was 0.14. The analysis of the APT data from well M505 was performed neglecting the flow from zone 2 of the UZLFA to the wellbore. This resulted in no pairs of correlated hydraulic parameters. The analysis of the APT data from well M503 indicated that the hydraulic conductivity and anisotropy of zone 2 of the UZLFA were correlated. The flow log from well LFAM allowed the matching of the flows to the wellbore from the UFA and zone 2 of the UZLFA at well M503.

There are advantages and disadvantages of using analytical versus numerical solutions for the ground-water flow equation when drawdown data are analyzed to compute hydraulic parameter values. An advantage of using an analytical solution is that round-off errors associated with grid resolution are eliminated. A disadvantage of using an analytical solution for the analysis of drawdown data is the overestimation of the hydraulic conductivity of the aquifer if the storativity and hydraulic conductivity of the confining units are neglected. Potentially, another cause of overestimation is the assumption that no flow to the wellbore could come from the confining units tapped by the production well, although this was not a factor in the analyses of the APT data analyzed in this report. If wellbore storage is not accounted for, the specific storage of an aquifer computed from matching an analytical solution also can be overestimated. An overestimation occurs because the drawdown recorded at the well is the result of an average specific storage between the wellbore and the aquifer, which is greater than the specific storage of the aquifer alone.

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MODOPTIM Input File Descriptions

Appendixes

By Keith J. Halford

Appendix A. Input Structures Used in MODOPTIM Files

Data are read from MODOPTIM input files as 2,048 character wide, alphanumeric cards to facilitate the addition of comments within the model input files and the use of keys to identify input variables. All integer, real, and character variables are read from the alphanumeric cards. The cards are initially read by the subroutine NCREAD. Cards that precede with a '#' sign in the first column are treated as comment cards, are not passed to any other routines, and are discarded. Once NCREAD has acquired a valid data card, the card is checked for a '!' sign. If a '!' sign is detected, the '!' sign and all text right of the '!' sign are removed from the card before passing it to any other routines.

The subroutine QREAD extracts numeric values as real numbers from the input cards acquired by NCREAD and will read all numeric values that are followed by a trailing blank or comma. Numeric values will be read from the card regardless of the presence or absence of text on the card which allows for text only descriptors to be embedded next to the input variables. All integer variables are read as real numbers and converted to integers to avoid reading errors if the user specifies the variable as a real number.

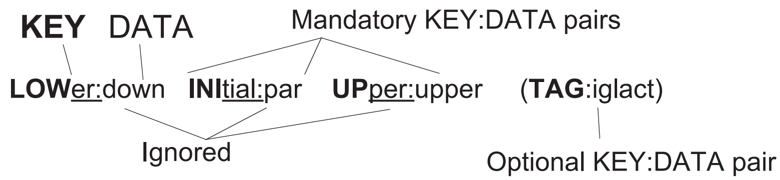
The typical functioning of the subroutines NCREAD and QREAD are best illustrated by example. If the following is read from an input file by NCREAD:

```
#   Closure Criteria for:
#          Iterations, Net Parameter Change, & SS Error Reduction
#
   maxit=4 smin 0.001    dermin=0.05! Try dermin= -1.0E6 to ignore oversteps
#
```

NCREAD returns the stripped input card (maxit = 4 smin 0.001   dermin=0.05) to the routine and the subroutine QREAD extracts three values (4, 0.001, and 0.05).

Array data are read with the subroutine GETMAT which utilizes the subroutines NCREAD and QREAD. As such, arrays can contain comment cards and text identifiers within the field of the array but all numeric entries must be separated by blank, comma, or tab delimiters. Row numbers can be denoted in the input by placing the values beyond the rightmost edge of the matrix and preceding the value with a '!' sign. Array data entry is terminated with an '<end>' flag.

Alphanumeric strings are used in MODOPTIM to identify variables (keys) and make logical decisions (flags). Specification of these keys and flags is case insensitive because all letters are capitalized before performing any logical tests. Keys precede the variable to be read. Logical decisions are based on the presence (true) or absence (false) of a flag. Data entry with key:data pairs will be presented as follows



where,

Bold, upper-case letters denote the part of the key that is tested by MODOPTIM,

Key:data pairs that are not delimited by parentheses are mandatory and must be included, and

Key:data pairs that are delimited by parentheses are optional because default values exist if they are not specified.

I/O Redirection

The three primary MODOPTIM files (Appendices B, C, and D) can be subdivided into smaller files with I/O redirection. I/O can be redirected from the primary file to an auxiliary input file by inserting an I/O redirect statement at any location in the file. Multiple I/O redirect statements can be used in a file. I/O redirection can only occur from a primary MODOPTIM file and not from an auxiliary input file.

1. DATA: **REDIRECT** : Filename
TYPE: Alphanumeric header card

REDIRECT:Filename= The filename of the auxiliary input must follow the colon. The entire key **REDIRECT** switches the I/O from the primary file to the auxiliary file and all 8 characters must be present.

Sample input of an element of GROUP 1 data:

```
#
Tag:PERM             Layer:1
       10    1.000    (6e13.5)                -7
Redirect to file:sem_bos.array
Tag:VCON             Layer:1
        0    1.000    (6e13.5)                -7
```

Appendix B. Input for Main Optimization File

DATA GROUP 1 -- FILE SPECIFICATIONS

Read 6 lines with file name and unit number that specify:

1A. The composite MODFLOW/MODOPTIM file for building BAS, BCF, and other MODFLOW files with parameters to be estimated.
1B. Main MODOPTIM output file.
1C. MODOPTIM update file that contains residuals and sensitivities.
1D. Name of MODFLOW-BAS file that is generated by MODOPTIM.
1E. Name of standard MODFLOW output file.
1F. MODOPTIM update file that contains best parameter estimates.

DATA GROUP 2 -- CLOSURE CRITERIA FOR OPTIMIZATION

NOTE: Cards 2A and 2B are mutually exclusive.

2A. DATA:	Maxit	Smin	Dermin	CCmin
TYPE:	Integer	Real	Real	Real

Maxit = Maximum number of parameter estimation iterations
If Maxit < 0, Sensitivity arrays for each optimization parameter are computed and optimization is not performed.
Smin = Minimum overall parameter change
Dermin = Minimum reduction in Sum-of-Squares objective function
CCmin = All parameter pairs with correlation coefficients greater than CCmin are explicitly shown in the MODOPTIM parameter-estimate file (PAREST).

2B. DATA:	**SENSITIVITY** PLOT	Points	Multiply
TYPE:	Alphanumeric header card		

SENSITIVITY PLOT a flag that causes U-plot sensitivity profiles to be computed for each active parameter and causes optimization to not be performed.
Points = Number of RMS points to be computed along an error profile.
Multiply = Defines range of parameter profile as a multiple of the initial value. For example, the sensitivity profile for a parameter with an initial value of 20 and *multiply* equal to 5 would range from 4 to 100.

DATA GROUP 3 -- OPTIMIZATION CONTROL VARIABLES

3. DATA:	Smax	Stfrc	Frcsec	Rkmin	Cfi	(**LIMIT**:Choice)
TYPE:	Real	Real	Real	Real	Real	Logical choice

SMAX = the maximum step length for all parameters. A typical value is 0.5
STFRC = the maximum fraction any given parameter can change between its lower and upper limits. A typical value is 0.25

FRCSEC = determines Levenberg-Marquardt type value to constrain step length of the search vector and direction of search if the BFGS updates fail. Values of FRCSEC > 1 cause the search vector to be short and oriented along a steepest-descent path. Values of FRCSEC < 0.01 generally produce an unconstrained Gauss-Newton solution.

RKMIN = is the threshold below which a diagonal value is treated as zero. For many problems, RKMIN should be greater than 0.001 and a value of 0.01 is more honest.

CFI = is the perturbation factor or influence coefficient for calculating gradients. Typically CFI = 0.01 and should not be less than 0.001 because of rounding errors that occur while updating MODFLOW input files.

LIMIT:Choice = is a switch (REMove/Keep) that determines if parameter estimation will be attempted during successive iterations after a parameter is constrained by either its lower or upper limit. MODOPTIM defaults to keep attempting to estimate all parameters with every iteration.

DATA GROUP 4 -- DEFINITION OF PARAMETER-WEIGHT MATRICES

OPTIONAL: If a weight matrix header is not read, no parameter-weight matrices will be defined and estimated parameters cannot be modified by a parameter-weight matrix.

REPEAT THE FOLLOWING DATA IN SEQUENCE FOR EACH PARAMETER-WEIGHT MATRIX -- Weight matrix entry is terminated if the key [WEIGHT] is not present on data line 4A.

4A. **KEY:**DATA **WEIGHT**:wtag (**NORM**alize:Y/N) (**TYPE**:iwp) (**INPUT**:Entry)

TYPE: Alphanumeric header card

WEIGHT:wtag = each parameter-weight matrix is identified by an alphanumeric tag. Only a capitalized version of the first 4 letters is retained for parameter-weight matrix identification.

NORMalize:Y/N **=** parameter-weight matrix is normalized by dividing matrix values by the standard deviation of all values in the matrix, including values in inactive cells.

OPTIONAL -- A parameter-weight matrix is normalized by default.

TYPE:iwp = specifies if the parameter-weight matrix is spatial or temporal. If it is spatial, *iwp* indicates the number of spatial dimensions and the spatial orientation of the matrix in an XYZ coordinate system. The following keys are used to specify *iwp*.

X = a one-dimensional, NCOL matrix

Y = a one-dimensional, NROW matrix

Z = a one-dimensional, NLAY matrix

XY = a two-dimensional, NCOL by NROW matrix

XZ = a two-dimensional, NCOL by NLAY matrix

YZ = a two-dimensional, NROW by NLAY matrix

XYZ = a three-dimensional, NCOL by NROW by NLAY matrix

SP = a one-dimensional, NPER matrix

OPTIONAL -- XYZ is the default setting.

INPUT:Entry = First character of entry controls how a parameter-weight matrix will be defined by MODOPTIM. The choices are:

Polarize = a spatial parameter-weight matrix is constructed from an iso-value contour that is described by a series of <x,y> pairs. A temporal parameter-weight matrix is constructed by interpolating the time at the end of each stress period to a schedule defined by the <time,y> pairs. (Typically, one might be defining a production schedule for wells). Data entry is terminated with the <end> flag. The polarized parameter-weight matrix is filled with positive distances from the iso-value contour on one side and negative values on the other side.

Absolute = a parameter-weight matrix is constructed with only positive distances from the iso-value contour. Data entry is the same as for the Polarize option.

Direct = read in a parameter-weight matrix of the dimensions specified in *iwp* directly.

OPTIONAL -- Direct entry is the default setting.

4B. DATA weight
TYPE: Matrix reader

Weight = parameter-weight matrix is read directly or as <x,y> pairs that define either an iso-value line or a temporal schedule. (Data entry is defined by the options selected on line 4A). Data entry to the matrix reader is terminated with a '<end>' flag on the line that follows the last value read.

DATA GROUP 5 -- DEFINITION OF OPTIMIZATION PARAMETERS

REPEAT THE FOLLOWING DATA IN SEQUENCE FOR EACH PARAMETER -- Parameter entry is terminated if the key [PARA] is not present on data line 5A or <end> is detected.

5A. **KEY:**DATA **PARAM**eter:ptag **TAG**:ptype (**STATUS**:istatus) **TYPE**:pinfo
TYPE: Alphanumeric header card

PARAMeter:ptag = An arbitrary and unique 4 character descriptor assigned to each parameter. Parameters are tracked and reported with this variable.

TAG:ptype = identifies which variables in MODFLOW the parameter ptag will modify. The MODFLOW variables are identified by the corresponding variable *pname* in the MODFLOW files. the identifiers *ptype* and *pname* are user-defined.

STATUS:istatus = First character is the key that determines how a parameter will be defined by MODOPTIM. The choices are:

Active = parameter is modified and estimated.

Modify = parameter is modified but is NOT estimated.

Inactive = parameter definition is ignored.

OPTIONAL -- Active is the default setting.

TYPE:pinfo = defines how a parameter modifies MODFLOW input and has 4 components that are composed of the first letter of the choices listed. For example, input of TYPE:Parallel,None,Exp,No will be stored in *pinfo* as ‘PNEN’.

B.5A Options that can be specified for the *PINFO* variable.

Modifier type	Zero Limits	Operator	Scaling
Parallel	Lower	Exponential	Scale
Series	Upper	Multiplicative	No scaling
	None	Additive	

5B. **KEY:**DATA **LOW**er:down **INI**tial:par **UP**per:upper (**TAG**:iglact)

TYPE: Alphanumeric data input card

LOWer:down = lower limit of parameter estimate

INItial:par = initial parameter estimate

UPper:upper = upper limit of parameter estimate

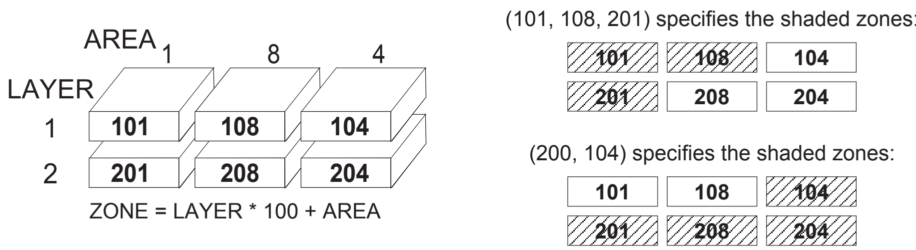
TAG:iglact = an alphanumeric tag that identifies a weight matrix defined in the data group 4 input. If *iglact* is not defined, a uniform weight of one will be used.

5C. DATA parb *(igbact) [igbsp]

TYPE: Alphanumeric data input card

parb = a global multiplier that modifies the parameter across the zones specified by *igbact* and the stress periods specified by *igbsp*. This multiplier can be used to change units and does not change during parameter estimation.

igbact = the zones to be modified by the parameter. Zones can be assigned individually and as groups in the same manner as room numbers in a multi-story building or street numbers within a block. If the areas of the model domain are assigned integer identifiers, zones can be specified by $zones = layer \times step + area$ where *step* is a value of 10, 100, or 1,000 and is larger than the greatest area identifier. For example,



igbsp = the stress periods during which the parameter will be modified. Stress periods are identified individually [1, 3, 4, 5] and as ranges [2 to 8]. A ‘TO’ placed between two stress periods denotes that MODFLOW input in all stress periods between the two limits will be modified by this parameter. For example, [2 to 5] specifies the MODFLOW input in stress periods 2, 3, 4, and 5 will be modified by the parameter.

5C cards can be repeated up to *mgb* times, where *mgb* is the maximum number of global multipliers as defined in the compiled program.

Sample input of an element of GROUP 5 data:

```
#
  Parameter:Klow   Tag:PERM    Status:Active    Type:Parallel,None,Exp,NoScaling
Lower:1.00       Initial:20.        upper:500.0
#   Multiplier*(Zones)[SP] a '(' sign is mandatory to indicate zone input
3.0*( 100 )
0.4*( 31, 41, 51 )
#
Parameter:Khi Tag:PERM    Status:Active    Type:Parallel,None,Exp,NoScaling
Lower:1.00       Initial:100.        upper:500.0
#   Multiplier*(Zones)[SP] a '(' sign is mandatory to indicate zone input
1.0*( 200 )
#
Parameter:Rspg Tag:RECH Status:Active    Type:Parallel,None,Exp,NoScaling
Lower:1.00       Initial:9.        upper:50.0
#   Multiplier*(Zones)[SP] a '(' sign is mandatory to indicate zone input
1.0*( 100 )[1, 3, 5 to 9, 14]

Parameter:Rfal Tag:RECH Status:Active    Type:Parallel,None,Exp,NoScaling
Lower:1.00       Initial:2.        upper:50.0
#   Multiplier*(Zones)[SP] a '(' sign is mandatory to indicate zone input
1.0*( 100 )[2, 4, 10 to 13]
#
<end>
#  ................ End Parameter Input .....................
```

DATA GROUP 6 -- GENERAL OBSERVATION MODIFIERS

OPTIONAL: All input before reading the observations have default values.

6. **KEY:**DATA — The following observation modifiers can be entered in any order and on however many lines that the user needs.

TYPE: Alphanumeric data input cards

START:timref = Identifies time 0 of simulation in time units of data input. Default is 0.

SCALE:timscl = Scales time units of data input to time units that are used within the MODFLOW simulation. Default is 1.

PURPOSE: allows user to modify observation times in data input by: $t_{MODFLOW} = (t_{INPUT} - timref)timscl$. This option has been used to facilitate analyzing aquifer-test data.

OFFSET:wlref = Shifts datum of water levels in units of data input. Default is 0.

MULT:wlmlt = Scales water-level units of data input to units that are used within the MODFLOW simulation. Default is 1.

PURPOSE: allows user to modify observation values in data input by: $WL_{MODFLOW} = (WL_{INPUT} - wlref)wlmlt$. This option has been used to facilitate analyzing aquifer-test data.

INTIME = if either the fragment '**SS**' or '**NO TIME**' are found before the first observation site is read from the MODOPTIM input file, simulated water levels and flow rates will not be interpolated in time to the observation time. Default is to interpolate simulated values in time.

PURPOSE: Temporal interpolation is not appropriate if a steady-state or series of steady-state flow systems are being simulated.

ADJUST-WEIGHT = a flag that normalizes weights for each observation type to the first observation type by standard deviation of each measurement type. Default is to leave weights unadjusted.

PURPOSE: Provides an initial estimate for scaling different observation types to sensitivities of similar magnitude.

FLOW:qtest = specifies the descriptor and number of characters that will be used to identify flow-rate observations. The text string specified in *qtest* is compared to *otype* which is defined on card 7A. If *qtest* is not specified, the default descriptor is 'FLOW' for all flow-rate comparisons.

PURPOSE: Allows for multiple flow-rate observation types to be classified.

MULT-Q:qmlt = Scales flow units of data input to units that are used within the MODFLOW simulation. Default is 1.

QUALITY:qwtest = specifies the descriptor and number of characters that will be used to identify water-quality observations. The text string specified in *qwtest* is compared to *otype* which is defined on card 7A. If *qtest* is not specified, the default descriptor is 'CONC' for all water-quality comparisons.

PURPOSE: Allows for multiple water-quality observation types to be classified.

MULT-QW:qwmlt = Scales water-quality units of data input to units that are used within the MODFLOW simulation. Default is 1.

COST:liftst = specifies the descriptor and number of characters that will be used to identify lift-cost observations. The text string specified in *liftst* is compared to *otype* which is defined on card 7A. If *liftst* is not specified, the default descriptor is 'LIFT' for all lift-cost comparisons.

PURPOSE: Allows for multiple lift-cost observation types to be classified.

MULT-LIFT:cstmlt = Scales lift units of data input to units that are used within the MODFLOW simulation. Default is 1.

OUTPUT:wminoc = minimum weight an observation can have and still be printed to the output file of residuals. Default value of *wminoc* = 0.

BLANK = a flag that indicates blank lines should be printed between sites in the output file of residuals. Default is no blank lines.

DATA GROUP 7 -- OBSERVATIONS

NOTE: The sequence of water-level, flow-rate, water-quality, lift-cost, or subsidence observation entries are arbitrary. The user can enter flow-rate and water-level observations in whatever fashion the user deems reasonable. All observations will be normalized to the first observation type.

REPEAT THE FOLLOWING SEQUENCE FOR EACH OBSERVATION SITE --

7A. **KEY:**DATA **OTYPE**(:flowkey) (**Z-INTER**:Y/N)(**ABSOL**ute)**LOCKEY**:coordinate **SITE**:well
TYPE: Alphanumeric header card

OTYPE = a 4-character descriptor that identifies the values to be compared as either water-level, flow-rate, water-quality, or lift-cost observations. *Otype* is set to the first 4 non-blank characters read from card 7A. For flow-rate, water-quality, or lift-cost observations, *otype* must begin with the text string specified in *qtest*, *qwtest*, or *liftst*, respectively. If *otype* does not begin with the descriptor specified for *qtest*, *qwtest*, or *liftst* the observations from that site are assumed to be water levels.

(:flowkey)= character strings that identify the flow components to be compared. This is only needed for flow-rate observations. Flowkey is set to MNW for water-quality and lift-cost observations. The flowkeys and flow components are listed below:

B.7A List of flow components from MODFLOW modules that can be compared to specified discharge rates.

FLOWKEY	Flow component from MODFLOW module
STORage	Storage from SBCF5S
WEL or MNW	Specified discharge from WEL5BD and MNW1BD
DRAIn	Head dependent discharge from DRN5BD
RIVEr or STREam	Head dependent discharge from RIV5BD and STR5BD
ET	Evapotranspiration from EVT5BD
CHD or SPECified head	Specified heads from SBCF5F
GHB	General head boundary from GHB1BD
RECHarge	Specified recharge from RCH5BD

(**Z-INTER**polation:Y/N)**=**simulated water levels can either be or not be interpolated between layers.
OPTIONAL -- Default condition is to NOT interpolate water levels between layers.

(**ABSOL**ute) **=** simulated flow rates for a site are the summation of the absolute value of all flow terms. The **ABSOL**ute switch allows a penalty to be imposed on the overall magnitude of stresses if the observation sums both sink and source terms.
OPTIONAL -- The default condition is to sum positive and negative flow rates.

(**LOCKEY:**) = identifies discrete locations for water-level, water-quality, and lift-cost observations or zones that define a volume for summing flow-rate and lift-cost observations and flow-rate-weighted averaging of water quality observations. For discrete observations, 3 variables are read according to the table below. Simulated water levels are interpolated to the measured water level location. Discrete water-quality and lift-cost observations are compared at the node with a pumping well. Observations that are summed or averaged over a volume are defined by up to 8 zones that correspond to zone assignments in the IOBFLX array.

B.7B List of LOCKEY variables for identifying the method of specifying observation locations.

LOCKEY:	Coordinate	OTYPE	Number of variables
XYZ:	Cart-X, Cart-Y, Cart-Z	Water Level, Water Quality, Subsidence, and Lift Cost	3
XYK:	Cart-X, Cart-Y, Layer		3
XJZ:	Cart-X, Row, Cart-Z		3
XJK:	Cart-X, Row, Layer		3
IYZ:	Column, Cart-Y, Cart-Z		3
IYK:	Column, Cart-Y, Layer		3
IJZ:	Column, Row, Cart-Z		3
IJK:	Column, Row, Layer		3
ZONE:	Zone identifiers specified in the IOBFLX array	Flow Rate, Water Quality, and Lift Cost	1 - 8

SITE:well = an alphanumeric descriptor that is used to identify an observation site.

7B. **KEY:**DATA wellbore **STOR**age Kxy Lscreen Rw **TAG**:*pname*

TYPE: Alphanumeric data input card

OPTIONAL: This card is optional and is only read if it immediately follows card 7A. Cards 7B and 7C are mutually exclusive.

wellbore **STOR**age = indicates wellbore storage effects in the observation wells will be simulated and the required variables will be read from this card.

Kxy = lateral hydraulic conductivity of the material around the wellbore.

Lscreen = the length of the well screen.

rw = the radius of the well casing

The three variables (Kxy, Lscreen, rw) are reduced to one variable by $\beta = \dfrac{L_{SCREEN}K_{XY}}{2\ln\left(\dfrac{L_{SCREEN}}{r_w}\right)r_w^2}$ which is

used in the equation

$hw_m = \dfrac{\beta\Delta t(h_m + h_{m-1} - hw_{m-1}) + hw_{m-1}}{1 + \beta\Delta t}$ to estimate the water-level in the observation well

TAG:*pname* = is the name of the MODFLOW variable that is to be tracked if β is to be estimated independently or if β is co-estimated with the hydraulic conductivity distribution that surrounds the well screen.

7C. **KEY:**DATA **PUMP**ing well losses T Rw **TAG**:*pname*

TYPE: Alphanumeric data input card

OPTIONAL: This card is optional and is only read if it immediately follows card 7A. Cards 7B and 7C are mutually exclusive. Use of this option forces the observation to the nearest node which is presumably being stressed by a well.

PUMPing well losses= indicates head losses between node and pumping well will be simulated and the required variables will be set from this card.

T = lateral transmissivity of the material around the wellbore.

Rw = the radius of the well casing

The two variables (T, rw) are reduced to one variable by

$\beta = \frac{2\pi T}{\ln(r_o / r_w)}$ where $r_o = 0.14\sqrt{\Delta x^2 + \Delta y^2}$, Δx is the width of the column, and Δy is the width of the row. The equivalent radius of the pumping cell (r_o) was defined by Peaceman (1983). The difference in head between the well node and the wellbore is estimated by $\Delta h = Q/\beta$ where Q is the rate of water withdrawal or injection.

TAG:*pname* = is the name of the MODFLOW variable that is to be tracked if β is to be estimated independently or if β is co-estimated with the hydraulic conductivity distribution that surrounds the well screen.

7D. DATA time observation (**<**,**>**) (-weight) (+weight) (**Default**) (**Reference**)

TYPE: Alphanumeric data input card

time = is the time the observation was made.

observation = is either a measured water level or flow rate. Flow rates use the same sign convention used in MODFLOW. Negative values denote discharge from the ground-water flow system.

(**<**,**>**) = is an optional flag. Parameter estimates are only affected by positive residuals (**>**) or negative residuals (**<**).

(-weight) = is the weight assigned to negative residuals. A user-defined default weight is assigned if left blank. The default weight is 1 if no weight was specified.

(+weight) = is the weight assigned to positive residuals and defaults to *-weight* if it is not specified.

(**Default**) = reassigns weight entry on this card as the new default value for the current observation type.

(**Reference**) = allows for the comparison of differences between current observation and a reference observation. Observations such as water-level, discharge, water-quality, and lift-cost pairs can be differenced.

DXyz**:***well2, time2* = identifies the location and time of reference observation. If *time2* is not specified, *time2* defaults to *time*.

DT = the observation read from the previous card is the reference observation. If **DT** is specified for the first observation at a site, no comparison will be made and the weight is set to zero.

NO comparison sets *-weight* and *+weight* to 0.00 for sites that are reference observations.

OFFSET sets this observation as the reference observation for all subsequent observations until a new site is specified. Simulated and measured observations are both set to zero for this entry which does not affect the objective function.

DATA GROUP 8 -- DEFINITION OF SUMMED AND FLOW-RATE AVERAGED OBSERVATION ZONES

OPTIONAL: If flow zones are not defined in data group 8, the flow zones in the IOBFLX array are set equal to the parameter zones in the IZCUBE array.

8A. **KEY:**DATA **FLUXZONES** **Dimension**:size (**BY**:step)
TYPE: Alphanumeric header card

FLUXZONES = the flag that signals data group 8 will be read.
Dimension:size = denotes if the matrix read to define the flow zones are 1, 2, or 3-dimensional and the orientation of the matrix in an XYZ coordinate system as denoted by the type flags:
GLOBAL = a single value
Z = a one-dimensional, NLAY matrix
XY = a two-dimensional, NCOL by NROW matrix
XYZ = a three-dimensional, NCOL by NROW by NLAY matrix
OPTIONAL -- XYZ is the default setting.
(**BY**:step) = increases zone values by $zones = layer \times step + izn$ where *step* is typically a value of 10, 100, or 1,000 and is larger than the greatest area identifier. Allows zones to be modified by the parameter.

8B. DATA iobflx
TYPE: Matrix reader

iobflx = zones for summing flow-rate and lift-cost observations and averaging flow-rate weighted water quality observations. Data entry to the matrix reader is terminated with a ‘<end>’ flag on the line that follows the last value read.

Sample input with elements of GROUP 7 and 8 data:

```
# ----- GROUP 7 DATA ------
HEAD         IJK: 14  9   4     Site:p-cell
    1.00            100
HEAD         IJK: 14  9   4     Site:p-well
  PUMPing well losses:  T= 500  Rw= 0.5      TAG:PERM
    1.00            100
HEAD         XYZ:  16583.   2024.    13.0     Site:1
    1.00            95.21
HEAD         XYZ:   9886.  15334.    80.0     Site:A-11
    1.00           103.13
HEAD         XYZ:  13496.  13199.    32.0     Site:w-70
    1.00           105.72
WLDZ         XYk:   14510   17091       1     Site:74-L1
    1.00            98.65               No comparison
WLDZ         XYk:   14515   17096       4     Site:74-L4
    1.00            97.33          dxyz:74-L1
CONC         IJK:  3   3     1        Site:QW-1
      0.     250.0     0.001    10.0     W-Default
    180.     250.0
LIFT         IJK:  6   6    1        Site:Lift-1pt
      0.     1.0E6    0.001      0.5      W-Default
     90.     1.0E6
    180.     1.0E6
HEAD         IJK:  7   8    2        Site:WL-lay2
      0.     130.0     2.0     0.0001     W-Default
    180.     125.0
#
# ----- GROUP 8 DATA ------
#  Can define a new array to define zones for flow components
#  Trip reader by adding: FLUXZONE      dimension:Z, XY, or XYZ
FLUX ZONES        dimension:Z
1 2 3 4 5
#    End input of flow component zones .........
# ----- GROUP 7 DATA ------
flow:chd                 zone:1,2       site:CHD_1&2
   1.0      -40892.9      5.0
flow:River               zone:1           site:rivers
   1.0     -164528.      5.0
flow:River, well, chd, drains         zone:1, 2, 3, 4, 5      site:combo
   1.0     -623998.      0.00000001
flow:MNW           Zone:1       site:Wells
      0.    -8.0E5     4.0    25.0
     60.    -8.0E5     5.0    10.0       W-Default
    120.    -8.0E5   !  Target production rate is 6 MGD (800,000 ft3/d)
    180.    -8.0E5
CONC:MNW              zone:1      site:QW-AVG
      0.     200.0      0.1      4.0      W-Default
     60.     200.0
    120.     200.0
    180.     200.0
flow:Drains              zone:1      site:Drain
    -1.e5   -6.0E5
      0.    -6.0E5
     60.    -6.0E5
    120.    -6.0E5
    180.    -6.0E5
LIFT:MNW                   zone:1        Site:Total-Cost
      0.    25.0E6    0.05    20.00      New Default
     90.    25.0E6
    180.    25.0E6
<end>
```

Appendix C. Input for Composite MODFLOW/MODOPTIM File with Parameters to be Estimated

---

DATA GROUP 1 -- General data for building MODFLOW / BAS file

1A. DATA txt
TYPE: Alphanumeric header card

txt = is the model description and is read on 2 cards

1B. **KEY:**DATA File with 3D grid definition**:** filename
TYPE: Alphanumeric data input card

filename = is the name of the file with the column, row, and layer dimensions, the column and row widths, a reference location, the thickness of the model cells, and the elevation of the model nodes.

1C. DATA itmuni
TYPE: integer

itmuni = specifies the time unit in MODFLOW. ITMUNI can range from 0 to 5 to specify time as undefined, seconds, minutes, hours, days, or years, respectively. If ITMUNI is not specified or is not in the range of 0 to 5, it is set to 4.

DATA GROUP 2 -- Specification of stress period and time step lengths

2A. DATA perlen nstp tsmult
TYPE: Matrix reader

perlen = stress period length
nstp = number of time steps in a stress period
tsmult = time step multiplier as defined by McDonald and Harbaugh (1988)
NOTE: variables are read until a ‘<end>’ flag is encountered. The number of variables read must be divisible by 3 or MODOPTIM will halt and report the error.

DATA GROUP 3 -- SPECIFY MODFLOW FILES AND UNIT NUMBERS

3A. **KEY**:DATA **FILE**:filename **MODKEY**:unit
TYPE: Alphanumeric data input card

FILE:filename = name of MODFLOW data input file to be opened.

MODKEY:unit = the unit number associated with the filename. MODKEY identifies the MODFLOW module that will read data from the file and the IUNIT location it is assigned in the BAS package. MODFLOW data input files that will be built by MODOPTIM must be assigned a unit number between 10 and 39, inclusive. Unit numbers 40 through 69, inclusive, are reserved by MODOPTIM. The recognized MODKEYs and MODFLOW modules are listed below:

C.3A List of MODKEY flags that identify a MODFLOW module.

MODKEY	MODFLOW module	IUNIT
BCF	Block Centered Flow	1
WEL	Wells	2
DRN	Drains	3
RIV	River	4
EVT	Evapotranspiration	5
TLK	Transient Leakage	6
GHB	General head boundary	7
RCH	Recharge	8
SIP	Strongly Implicit Procedure	9
DE4	Direct Solver	10
SOR	Slice Successive Over Relaxation	11
OC	Output Control	12
PCG2	Pre-Conditioned Gradient	13
GFD	General Finite Difference	14
HFB	Horizontal Flow Barrier	16
RES	Reservoir	17
STR	Stream Routing	18
IBS	Inter-Bed Storage	19
CHD	Time-Dependent Specified head	20
FHB	Flow and Head Boundary	21
VAR1	Time-Dependent BCF	22
MNW	Multi-Node, drawdown-limited wells	23

NOTE: Files are read, assigned unit numbers, and opened until an ‘<end>’ statement is encountered.

3B. **KEY**:DATA **FILE**:filename **<**unit**>**
TYPE: Alphanumeric data input card

FILE:filename = name of unformatted MODFLOW data output file to be opened.
<unit**>** = the unit number associated with the filename.
NOTE: Files are read, assigned unit numbers, and opened until an ‘<end>’ statement is encountered.

Sample input of GROUP 3 data:

```
# Identify packages and file name
FILE:t.bcf                BCF:10
FILE:3d_ss.oc             OUT:71
FILE:3d_ss.riv            RIV:73
FILE:t.rch               RECH:12
FILE:3d_ss.pcg           PCG2:74
FILE:t.wel               WELL:15
FILE:3d_ss.chd            CHD:76
FILE:3d_ss.drn          DRAIN:77
<END>   file input
# Specify additional files and their associated unit numbers to be opened
# in an unformatted format.
  File:t.ufh       <89>
  File:t.cbc       <90>
#
<END>  unformatted  file input
```

DATA GROUP 4 -- Specification of MODFLOW variables IAPART and ISTRT

4A. DATA	iapart	istrt
TYPE:	integer	integer

iapart = indicates whether array BUFF is separate from array RHS. If *iapart* = 0, arrays BUFF and RHS occupy the same space (McDonald and Harbaugh, 1988)

istrt = indicates whether starting heads are to be saved. If *istrt* = 0, starting heads are not saved. (McDonald and Harbaugh, 1988)

NOTE: If these values are not on this card, iapart defaults to 0 and istrt defaults to 1.

DATA GROUP 5 -- PARAMETER ZONES / IBOUND ARRAYS

Read either cards 5A and 5B or cards 5C, 5D, and 5E. Direct entry and polygon entry are mutually exclusive of one another.

If zones are defined directly as integer arrays, read cards 5A and 5B once--

5A. **KEY:**DATA	**DIRECT**	(**BY**:step)
TYPE:	Alphanumeric header card	

DIRECT = specifies that either 1, *nlay*, *ncol* by *nrow*, or *ncol* by *nrow* by *nlay* values be read and that the *IBOUND* and *IZCUBE* arrays will have 1 value, uniform values in each layer, unique areal zones, or unique zones throughout the model volume.

BY:step = increases zone values by $zones = layer \times step + izn$ where *step* is typically a value of 10, 100, or 1,000 and is larger than the greatest area identifier. This is valid only for a *ncol* by *nrow* array of integers.

5B. DATA	izcube
TYPE:	Matrix reader

izcube = is an array of zone values. Data entry to the matrix reader is terminated with a '<end>' flag on the line that follows the last value read.

If zones are defined by polygons, card 5C can be used to reassign the default zone number.

5C. **KEY:**DATA **GLOB**al**:**igbzn

TYPE: Alphanumeric header card

GLOBal**:**igbzn = **GLOB** is the key that identifies a new default zone identifier. *Igbzn* is the default zone identifier that was specified by the user. If card 5C is not read, the default zone identifier is 0.

Each polygon is specified with repeated sets of cards 5D and 5E--

5D. **KEY:**DATA **ZONE:**izn **LAYER**:layers (**BY**:step)

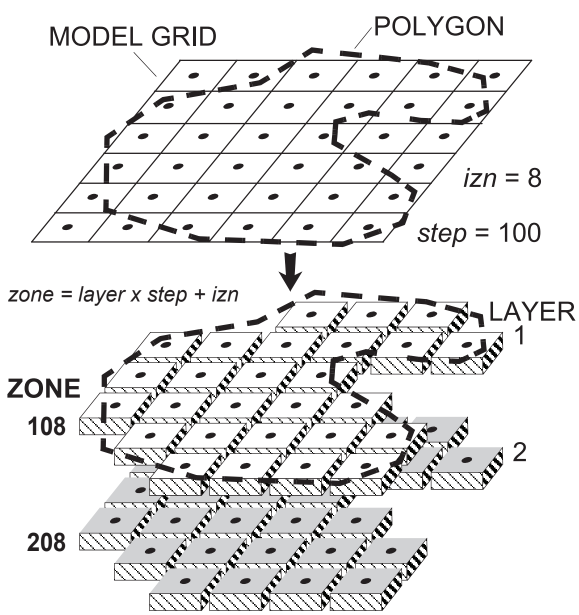
TYPE: Alphanumeric header card

ZONE:izn = **ZONE:** is the key that identifies the zone specified by a polygon. *Izn* specifies an element of the zone identifier used in *ibound* and *izcube*. If **BY**:step is not used, *izn* is equal to the zone number. Positive values of *izn* are used to assign zone numbers to nodes inside of the polygon while negative values of *izn* indicate that zone numbers will be assigned to nodes outside of polygon with the absolute value of *izn*.

LAYER:layers = specifies layers where polygon will define zone. Negative value for layer serves to flag specified head in ibound.

BY:step = increases zone values by $zones = layer \times step + izn$ where *step* is typically a value of 10, 100, or 1,000 and is larger than the greatest area identifier.

EXAMPLE: Usage of polygons to delineate zones is illustrated below:



5E. DATA izcube

TYPE: Matrix reader

izcube = is an array of <x,y> pairs that define a polygon. Data entry to the matrix reader is terminated with a ‘<end>’ flag on the line that follows the last value read.

NOTE: Zone values also can be modified on a cell-by-cell basis if the WEL1, WEL2, CHD, DRN, GHB, RIV, STR, or VAR packages are constructed by MODOPTIM.

DATA GROUP 6 -- INACTIVE CELL AND STARTING HEAD VALUES

6A. DATA `hnoflo`

TYPE: real

hnoflo = head value assigned to inactive cells. Default value of *hnoflo* is 1234567.

6B. **KEY:**DATA (**UNIT:**iohed) (**GLOBAL:**globe) **FILE:***name*

TYPE: Alphanumeric data input card

(**UNIT:**iohed) = specifies unit number for file with starting head values. The default assignment of *iohed* is 39. If *iohed* is less than 0, it is assumed the starting heads are stored in an unformatted file.

(**GLOBAL:**globe) = is a global starting head value that is assigned to all nodes if a file of starting heads does not already exist. This is an OPTIONAL assignment.

FILE:*name* = is the name of the file with the starting head values to be read by MODFLOW.

General description of DATA GROUPS 7, 8, 9 and 10

Data groups 7, 8, 9, and 10 describe the construction of MODFLOW files with parameters to be estimated. Much of the input for data groups 7, 8, 9, and 10 is similar to the input for a MODFLOW simulation without optimization. The MODFLOW files are constructed from the composite MODFLOW/MODOPTIM file to facilitate the placement of name tags (variable *pname*) that identify the hydraulic characteristics and stresses to be modified. The hydraulic characteristics and stresses in MODFLOW that can be estimated by MODOPTIM are read from files as *ncol* by *nrow* arrays (storage, transmissivity, vertical leakance, recharge, evapotranspiration) or as cell-by-cell lists (general head boundaries, rivers, specified heads, drains, wells).

DATA GROUP 7 -- Header for Packages with Hydraulic Properties to be Estimated

7A. **KEY:**DATA **PACKAGE =** MODKEY

TYPE: Alphanumeric header card

PACKAGE = MODKEY The MODFLOW module to be constructed is identified by the *MODKEY* variable which must equal one of the identifiers specified in table C.3A.

7B. DATA `text`

TYPE: Alphanumeric card

text Data sets that are needed in MODFLOW but are not needed by MODOPTIM. These cards are read and echoed into the MODFLOW packages. These cards are read and echoed until a *pname* tag or an <end> flag is read.

NOTE: cards are read and entered in the package constructed until an <end> flag is encountered.

DATA GROUP 8 -- Additional Data Needed to Construct a BCF Package

These cards are only read if *MODKEY* is equal to BCF.

8A. **KEY:**DATA Trans **CBC:**unit

TYPE: Alphanumeric data input cards

TRANS = a transient BCF package will be constructed if the fragment '**TRAN**' is detected. Otherwise, the default assumption is that a steady-state model is being simulated.

CBC:unit = specifies unit number for cell-by-cell output from BCF package to unformatted file.

8B. DATA Laycon

TYPE: integer

Laycon = specifies layer type and data sets to be read. LAYCON values: 0 - confined, 1 - unconfined, 2 - confined/unconfined with transmissivity held constant, and 3 - fully convertible between confined/unconfined (McDonald and Harbaugh, 1988) Any unspecified layer will be assumed to be confined (*laycon* = 0).

8C. DATA Trpy

TYPE: real

Trpy = specifies an anisotropy factor for each layer in terms of a column to row ratio ($Trpy = K_Y/K_X$) (McDonald and Harbaugh, 1988). Any unspecified values of *TRPY* will be assumed to be equal to 1.

Card 8D is optional and terminates further entry for the BCF package.

8D. **KEY:**DATA AUTO (LUMP)

TYPE: Alphanumeric data input cards

AUTO = automatically creates a BCF package from the vertical discretization that was specified in the GR3 file if the fragment '**AUTO'** is detected. Transmissivity arrays are assigned a *pname* of PERM. Vertical leakance arrays are assigned a *pname* of VCON. Storage coefficient arrays are created and assigned a *pname* of STOR only if the simulation is transient.

(LUMP) = assigns a *pname* of PERM to both transmissivity and vertical leakance arrays so they can be estimated as a single parameter. This is an OPTIONAL assignment.

NOTE: The widths of the columns and rows are not read because they were specified previously on card C.1B.

DATA GROUP 9 -- Identifying hydraulic properties or stresses to be estimated that are stored in a *ncol* by *nrow* array

9A. **KEY:**DATA **TAG:***pname* **Layer:**laypro (**SP:**itime)

TYPE: Alphanumeric data input cards

TAG:*pname* = is the user defined, 4-character tag that corresponds to the *ptype* variable defined on card B.5A in the OPT input file. *Pname* denotes if the property to be varied is a hydraulic conductivity, recharge, vertical leakance, or any other array of a hydraulic property or stress.

Layer:laypro = identifies the model layer for comparing IZONE numbers to the zone numbers that are specified in the *igbact* array before an optimization parameter can modify the MODFLOW array.

Layer numbers can be greater than the number of model layers.

SP:itime (OPTIONAL) identifies the stress period that corresponds to the stress periods specified in the *igbsp* array before an optimization parameter can modify the MODFLOW array. If *itime* is not specified, *itime* is set equal to 1.

9B. DATA Locat Cnstnt Fmtin Iprn

TYPE: Alphanumeric data input card

Locat is a flag. If *Locat* = 0, all elements are set equal to *Cnstnt* and card 9C is NOT read (McDonald and Harbaugh, 1988). If *Locat* > 0, *ncol* by *nrow* values are read. *Locat* is not used as a unit number. The unit number written to the constructed MODFLOW package is equivalent to the unit number assigned in card 3A.

Cnstnt = Constant to which all array values are set if *Locat* is equal to zero or by which all array values are multiplied if *Locat* is not equal to zero (McDonald and Harbaugh, 1988).

Fmtin = Format under which arrays are written and read from the constructed MODFLOW file. A format that maintains at least 5 significant figures should be used.

Iprn = MODFLOW code for format to be used when printing arrays (McDonald and Harbaugh, 1988).

9C. DATA work

TYPE: Real array

work = *ncol* by *nrow* values are read free-formatted into the temporary work array and are written in fixed format to the constructed MODFLOW package.

NOTE: Cards 9A and 9B are read for every array that contains hydraulic properties or stresses to be modified by optimization parameters.

If the RADIAL flag was set on card D.1A, all arrays to be estimated will be multiplied by 2π times an array of the X-coordinate of the columns.

DATA GROUP 10 -- Identifying hydraulic properties or stresses to be estimated that are stored in cell-by-cell lists.

10A. **KEY:**DATA**TAG:***pname* **Field:**Lf **SP:**itime

TYPE: Alphanumeric data input card

TAG:*pname* = is the user defined, 4-character tag that corresponds to the *ptype* variable defined on card B.5A in the OPT input file. *Pname* denotes if the property to be varied is a pumping rate, riverbed conductance, specified head, or any other cell-by-cell list of hydraulic properties or stresses.

Field: Lf = The presence of the **Field** flag instead of the **Layer** flag indicates that a cell-by-cell list follows. The variable *Lf* identifies the field of the cell-by-cell list input file that is to be modified. For example, flow rates that are specified in the well package are in the 4th field and riverbed conductances that are specified in the river package are in the 5th field.

SP:itime (OPTIONAL identifies the stress period that corresponds to the stress periods specified in the *igbsp* array before an optimization parameter can modify the MODFLOW array. If *itime* is not specified, *itime* is set equal to 1.

10B. Data ITMP

TYPE: Integer

ITMP is a flag. If $ITMP \leq 0$, cell-by-cell data from a previous stress period will be reused and input from item 10C will not be read. If $ITMP > 0$, it is the number of records of cell-by-cell data that will be read for the current stress period.

10C. DATA txt (**ZONE:**mz) (**KOFF:**koff)

TYPE: Alphanumeric data input card

txt is a cell-by-cell data entry. Values are read free-formatted to the *Lf*th field specified. The first three values (Layer, row, and column indices) are written to a (I10) format and the remaining values to the *Lf*th field specified are written to a (G10.4) format.

(**ZONE:**mz) Modifies non-zero zone assignments in *izcube* array to *mz* for each entry.

(**KOFF:**koff) Assigns an offset of *koff* to cell-by-cell layer assignment which allows for cell-by-cell entries in multiple layers to be specified by a single layer.

NOTE: Card 10A is only read ONCE for each cell-by-cell list MODFLOW package. It is assumed that only one field will be estimated in any package and that the same field will be estimated for all stress periods.

Input item 10C consists of one card for each cell-by-cell property specified. If ITMP is zero or less, item 10C is not read

Appendix D. Input for Grid Discretization File

DATA GROUP 1 -- Width of columns and reference for the X-coordinate

1A.DATA ncol (xref) (ixref) (**MULT**) (**RADIAL**)
TYPE: Alphanumeric header card

ncol is the number of model columns in the X-coordinate.
(xref) is the X-coordinate at the node in model column *ixref*. Default reference is X = 0 at the left-edge of the model.
(ixref) is the column of the reference node that coincides with the X-coordinate (*xref*).
(**MULT**) is a flag that indicates the last value read in the *dxm* array is the width of the model (the sum of *dxm* values from 1 to *ncol*). If the **MULT** flag is set, between 2 and *ncol*-1 values will be read. The remaining columns are filled by a uniform multiplier which successively increases the widths of the following columns until the total model width is equal to the last value read in the *dxm* array.
(**RADIAL**) is a flag that indicates the model will simulate radial flow. A radial model can have only 1 row or 1 layer. The reference of the X-coordinate is set to the default setting of X = 0 at the left-edge of the model. All arrays that are estimated in the BCF package are multiplied by an array of 2π times the X-coordinate of the columns.

1B. DATA dxm
TYPE: Matrix reader

dxm is the width of the model columns. Typically, one uniform value is read or an array of *ncol* values is read. If the **MULT** flag is set, between 2 and *ncol*-1 values will be read. (See **MULT**-flag explanation) Data entry to the matrix reader is terminated with a ‘<end>’ flag on the line that follows the last value read.

DATA GROUP 2 -- Width of rows and reference for the Y-coordinate

2A.DATA nrow (yref) (iyref) (**MULT**)
TYPE: Alphanumeric header card

nrow is the number of model rows in the Y-coordinate.
(yref) is the Y-coordinate at the node in model row *iyref*.
(iyref) is the row of the reference node that coincides with the Y-coordinate (*yref*).
(**MULT**) is a flag that indicates the last value read in the *dym* array is the height of the model (the sum of *dym* values from 1 to *nrow*). If the **MULT** flag is set, between 2 and *nrow*-1 values will be read. The remaining columns are filled by a uniform multiplier which successively increases the widths of the following rows until the total model width is equal to the last value read in the *dym* array.

2B. DATA dym
TYPE: Matrix reader

dym is the width of the model rows. Typically, one uniform value is read or an array of *nrow* values are read. If the **MULT** flag is set, between 2 and *nrow*-1 values will be read. (See **MULT**-flag explanation) Data entry to the matrix reader is terminated with a ‘<end>’ flag on the line that follows the last value read.

DATA GROUP 3 -- Thickness of layers and elevation of nodes

Data groups 3, 4, and 5 are mutually exclusive methods of defining vertical discretization.

3A.DATA nlay (izpls) (q3dthk)
TYPE: Alphanumeric header card

nlay is the number of model layers in the Z-coordinate.
(izpls) is the number of layers in excess of model layers that will be specified for defining parameter zones.
(q3dthk) is the gap between layers that must be exceeded before water-level and subsidence observations are interpolated with a quasi-3D interpretation of vertical leakances.

3B.DATA dzm
TYPE: Matrix reader

dzm is a *ncol* by *nrow* by *nlay* array of cell thicknesses. Either 1, *nlay*, or *ncol* x *nrow* x *nlay* values are read by the matrix reader. A uniform thickness is assigned to all cells if 1 value is read and to each layer if *nlay* values are read. Otherwise each cell thickness is assigned individually if *ncol* x *nrow* x *nlay* values are read. If the number of values read is not equal to 1, *nlay*, or *ncol* x *nrow* x *nlay*, MODOPTIM will halt and the error will be reported. Data entry to the matrix reader is terminated with a ‘<end>’ flag on the line that follows the last value read.

3C.DATA zc
TYPE: Matrix reader

zc is a *ncol* by *nrow* by *nlay* array of model node elevations. Either 1, *nlay*, *ncol* x *nrow*, or *ncol* x *nrow* x *nlay* values are read by the matrix reader. If 1 or *ncol* x *nrow* values are read, the array read is used as the top of the uppermost layer and the elevation of each node is computed by assuming all layers are contiguous. If *nlay* values are read, a uniform elevation is assigned to all nodes within each layer. If *ncol* x *nrow* x *nlay* values are read, the elevation of each node is assigned individually. If the number of values read is not equal to 1, *nlay*, *ncol* x *nrow*, or *ncol* x *nrow* x *nlay*, MODOPTIM will halt and the error will be reported. Data entry to the matrix reader is terminated with a ‘<end>’ flag on the line that follows the last value read.

DATA GROUP 4 -- Contacts of layers

4A.DATA nlay (izpls) CONTACT
TYPE: Alphanumeric header card

nlay is the number of model layers in the Z-coordinate. Nlay can be specified as 0 and will be counted by MODOPTIM.
(izpls) is the number of layers in excess of model layers that will be specified for defining parameter zones.
CONTACT is a flag that indicates vertical discretization will be defined by *nlay+1* contacts. The top of layer k is coincident with the bottom of layer k-1 if vertical discretization is defined with contacts.

Card 4B is read *nlay+1* times to define the thicknesses and elevations of all layers.

4B.DATA work
TYPE: Matrix reader

work is a *ncol* by *nrow* array. Either 1 or *ncol* x *nrow* values are read by the matrix reader. A uniform elevation is assigned to all cells if 1 value is read. Otherwise each elevation is assigned individually. If the number of values read is not equal to 1 or *ncol* x *nrow*, MODOPTIM will halt and the error will be reported. Data entry to the matrix reader is terminated with a ‘<end>’ flag on the line that follows the last value read.

DATA GROUP 5 -- Tops and Bottoms of layers

5A.DATA nlay (izpls) (q3dthk) **TOPandBOTTOM**
TYPE: Alphanumeric header card

nlay is the number of model layers in the Z-coordinate. Nlay can be specified as 0 and will be counted by MODOPTIM.
(izpls) is the number of layers in excess of model layers that will be specified for defining parameter zones.
(q3dthk) is the gap between layers that must be exceeded before water-level and subsidence observations are interpolated with a quasi-3D interpretation of vertical leakances.
TOPandBOTTOM is a flag that indicates vertical discretization will be defined with a top and bottom surface for each layer.

Cards 5B and 5C are read *nlay* times to define the top and bottom elevations of all layers.

5B.DATA top
TYPE: Matrix reader

top is a *ncol* by *nrow* by *nlay* array of layer top elevations. Either 1 or *ncol* x *nrow* values are read by the matrix reader for each layer. A uniform top elevation is assigned to all cells in a layer if 1 value is read. Otherwise each top elevation is assigned individually. If the number of values read is not equal to 1 or *ncol* x *nrow*, MODOPTIM will halt and the error will be reported. Data entry to the matrix reader is terminated with a ‘<end>’ flag on the line that follows the last value read.

5C.DATA bottom
TYPE: Matrix reader

bottom is a *ncol* by *nrow* by *nlay* array of layer bottom elevations. Either 1 or *ncol* x *nrow* values are read by the matrix reader for each layer. A uniform bottom elevation is assigned to all cells in a layer if 1 value is read. Otherwise each bottom elevation is assigned individually. If the number of values read is not equal to 1 or *ncol* x *nrow*, MODOPTIM will halt and the error will be reported. Data entry to the matrix reader is terminated with a ‘<end>’ flag on the line that follows the last value read.