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THE THEIS EQUATION: EVALUATION, SENSITIVITY TO STORAGE AND TRANSMISSIVITY, AND AUTOMATED FIT OF PUMPTEST DATA

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ABSTRACT

Traditionally, the Theis equation has played an important role in groundwater hydrology since its introduction. Comparison of experimental pumptest data with this theoretical curve by graphical means has been a standard method of determining aquifer transmissivity and storage. The purpose of this paper is to present techniques and computer programs to evaluate the Theis equation, to evaluate the sensitivity with respect to transmissivity and storage, and to automatically fit experimental pumptest data to the Theis equation obtaining the "best" transmissivity and storage in the least squares sense. The automated fit for pumptest data developed in this work should be a useful tool for the groundwater hydrologist. It is simple to use, quick, and inexpensive. The automated fit has the advantage that it is always objective. As a measure of the error in fitting, the standard deviation in drawdown is calculated for the "best" transmissivity and storage.

INTRODUCTION

Traditionally, the Theis equation has played an important role in groundwater hydrology since its introduction (Theis, 1935). Comparison of experimental pumptest data with this theoretical curve by graphical means has been a standard method of determining aquifer transmissivity and storage (Jacob, 1940). The purpose of this paper is to present techniques and computer programs to evaluate the Theis equation, to evaluate the sensitivity with respect to transmissivity and storage, and to automatically fit experimental pumptest data to the Theis equation obtaining the "best" transmissivity and storage in the least squares sense. For a more detailed discussion of sensitivity coefficients and their uses see McElwee and Yukler (1977).

The Theis equation involves an integral whose upper limit is infinity. Evaluation of this integral is considered in the section on numerical approximation. After the Theis equation has been evaluated, the sensitivity coefficients can be obtained with little additional work. These sensitivity coefficients are used in the section on least squares fitting to develop an algorithm for fitting the Theis equation to experimental pumptest data. The automated method is simple, quick, and inexpensive. The automated method has the advantage of always being objective and always indicating it's error by calculating the standard deviation in drawdown.

THE THEIS EQUATION

The Theis equation (Theis, 1935) describes radial confined groundwater flow in a uniformly thick horizontal, homogeneous, isotropic aquifer of infinite areal extent.

$$s = \frac{Q}{4\pi T} \int_{\frac{r^2 S}{4Tt}}^{\infty} \frac{e^{-u}}{u} du \qquad (1)$$

The radius of the pumped well is assumed negligible (line source or sink approximation). The derivation and solution is documented many places and will not be discussed further here (Jacob, 1940). In the above equation s is drawdown (L), Q is the discharge (L^3/T), T is the transmissivity (L^2/T), t is the time (T), S is the dimensionless storage coefficient, and r is the radial observation distance from the pumped well (L).

Usually, the Theis equation is fitted graphically to experimental pump test data to obtain approximations for the storage coefficient (S) and the transmissivity (T). In this paper an algorithm will be presented for a computer automated least squares fit to the experimental data yielding approximations for S and T and giving the standard deviation for drawdown.

NUMERICAL APPROXIMATION

Many times the integral in equation (1) is symbolically represented by W(u). The drawdown can then be written as

$$s = \frac{Q}{4\pi T} W(u) = \frac{Q}{4\pi T} W\left(\frac{r^2 S}{4Tt}\right) \qquad (2)$$

W(u) is the exponential integral and is tabulated in many places (Abramowitz and Stegun, 1968). For specific values of u table interpolation may be used to obtain the drawdown.

In order to evaluate equation (2) easily in an algorithm one needs an explicit expression for W(u) involving only simple arithmetic operations. For $0 \leq u \leq 1$ (Abramowitz and Stegun, 1968)

$$W(u) = -\ln u + a_0 + a_1 u + a_2 u^2 + a_3 u^3 + a_4 u^4 + a_5 u^5 + E(u) \quad (3)$$

$$|E(u)| < 2 \times 10^{-7}$$

where $a_0 = -.57721566$ $\qquad a_3 = .05519968$

$a_1 = .99999193$ $\qquad a_4 = -.00976004$

$a_2 = -.24991055$ $\qquad a_5 = .00107857.$

E(u) is the error in the approximation.

For values of u larger than one we use a rational approximation (Abramowitz and Stegun, 1968).

$$W(u) = \frac{e^{-u}}{u}\left[\frac{u^2 + a_1 u + a_2}{u^2 + b_1 u + b_2} + E(u)\right] \quad (4)$$

$|E(u)| < 5 \times 10^{-5}$ for $1 \leq u < \infty$

$a_1 = 2.334733$ $\qquad b_1 = 3.330657$

$a_2 = .250621$ $\qquad b_2 = 1.681534$

The maximum error in W(u) occurs for u = 1.

$$|E(1)/e| < 1.839 \times 10^{-5}$$

Therefore, we should always have at least four significant digits with these approximations.

SENSITIVITY ANALYSIS

In the mathematical treatment of dynamic systems it is permissible to speak of the precise values of the physical parameters. However, in the practical simulation of real dynamic systems we are immediately faced with uncertainty as to the exact physical parameters. The investigator must establish tolerances within which the parameters of the physical system may vary without appreciably affecting the model results. These tolerances are often obtained by introducing parameter perturbations in the system and observing the changes in the system's performance. However, the application of sensitivity analysis makes it possible to obtain these tolerances more efficiently (Tomovic, 1962; Vemuri et al., 1969; McCuen, 1973; Yukler, 1976).

In studying the sensitivity of a groundwater flow system to parameter variations, the following mathematical model is used;

$$F\ (h_{xx}, h_{yy}, h_t;\ T,\ S,\ Q) = 0 \tag{5}$$

where $h_{xx} = \dfrac{\partial^2 h}{\partial x^2}$, $h_{yy} = \dfrac{\partial^2 h}{\partial y^2}$, $h_t = \dfrac{\partial h}{\partial t}$,

h = hydraulic head,

T = transmissivity,

S = storage coefficient, and

Q = discharge

The solution of equation (5) may be written in the form $h = h(x,y,t;T,S,Q)$. Consider the variation of one of the parameters, T for example. Varying this parameter by a small amount, ΔT, the equation becomes

$$F(h^*_{xx},\ h^*_{yy},\ h^*_t;\ T + \Delta T,\ S,\ Q) = 0, \tag{6}$$

where h^* is the perturbed head. The solution to equation (6) may be written in the form $h^* = h^*(x,y,t;\ T + \Delta T,S,Q)$. Comparing the solutions of equations (5) and (6), one immediately obtains an indication of the stability of the system, which is expressed by means of the fraction

$$\frac{\Delta h}{\Delta T} = \frac{h^*(x,y,t;T+\Delta T,S,Q)-h(x,y,t;T,S,Q)}{\Delta T} \quad (7)$$

If expression (7) has a limiting value as ΔT approaches zero, it may be written as

$$U_T(x,y,t;T,S,Q) = \frac{\partial h}{\partial T} = \lim_{\Delta T \to 0} \frac{\Delta h}{\Delta T} \quad (8)$$

The function U_T $(x,y,t;T,S,Q)$ will be called the sensitivity coefficient (Tomovic, 1962) for variations in the T value of a groundwater flow system. By applying similar arguments for a variation in storage coefficient (ΔS) one obtains,

$$\frac{\Delta h}{\Delta S} = \frac{h^*(x,y,t;T,S+\Delta S,Q)-h(x,y,t;T,S,Q)}{\Delta S} \quad (9)$$

and

$$U_S(x,y,t;T,S,Q) = \frac{\partial h}{\partial S} = \lim_{\Delta S \to 0} \frac{\Delta h}{\Delta S}\,. \quad (10)$$

U_S is the sensitivity coefficient for variations in the storage coefficient of a groundwater flow system.

It is assumed that the solution of the flow equation (5) depends analytically upon the parameters T and S; and, that T, S, and Q are independent of each other. Now consider a perturbation of the transmissivity, ΔT. Since it has been assumed that the solutions depend analytically on the parameters, the function $h^*(x,y,t;T+\Delta T,S,Q)$ may be expanded into a Taylor series (Tomovic, 1962). If ΔT is small the second and higher order terms may be neglected,

$$\begin{aligned} h^*(x,y,t;T+\Delta T,S,Q) &= h(x,y,t;T,S,Q) + \frac{\partial h}{\partial T}\Delta T \\ &= h(x,y,t;T,S,Q) + U_T\,\Delta T \quad (11) \end{aligned}$$

Thus, the new head produced by a perturbation in transmissivity (ΔT) may be calcualted from equation (11) if the sensitivity coefficient and the unperturbed head are known. Similarly, if a perturbation in storage coefficient (ΔS) occurs the perturbed head is given by

$$h^*(x,y,t;T,S+\Delta S,Q) = h(x,y,t;T,S,Q) + \frac{\partial h}{\partial S}\Delta S$$
$$\simeq h(x,y,t;T,S,Q) + U_S \Delta S \qquad (12)$$

to first order in ΔS.

Equations (11) and (12) show that it would be desirable to calculate U_T and U_S for a given model, if possible. Then the response of the model to various perturbations could be calculated simply from equation (11) or (12) without actually evaluating the model equations again.

The sensitivity coefficients may be obtained from equations (1) by applying the definitions given in equations (8) and (10). After applying Leibnitz's rule for differentiating an integral (Hildebrand, 1962) to equation (1) one obtains

$$U_T = \frac{\partial s}{\partial T} = -\frac{s}{T} + \frac{Q}{4\pi T^2} EXP\left[-\frac{r^2 S}{4Tt}\right] \qquad (13)$$

and

$$U_S = \frac{\partial s}{\partial S} = -\frac{Q}{4\pi TS} EXP\left[-\frac{r^2 S}{4Tt}\right] \qquad (14)$$

These equations for the sensitivity coefficients may be evaluated quite easily. U_T and U_S calculated from equations (13) and (14) may be used in equations (11) and (12) to calculate what the drawdown would be if S and T were changed by ΔS and ΔT respectively. Other work (McElwee and Yukler, 1977) indicates that equations (11) and (12) are valid for ΔS and ΔT less than or roughly equal to twenty percent of S or T respectively.

LEAST SQUARES FIT

The objective is to use the sensitivity formalism to obtain a least squares fit of experimental pump test data to the Theis equation and thus obtain the "best" estimate for S and T. For a review of the least squares technique the reader is referred to Carnahan et al. (1969). The new drawdown, after changing T and S by ΔT and ΔS respectively, is given by

$$s^* = s + U_T \Delta T + U_S \Delta S \tag{15}$$

Equation (15) is obtained from equations (11) and (12) by observing that $s = h_o - h$, where h_o is the original head before pumping starts and is a constant independent of T and S.

Let $s_e(t)$ represent the experimentally measured drawdowns. Suppose it is possible to guess a reasonable S and T and let s(t) denote the drawdowns calculated from the Theis equation with these parameters. One would like to change the original guess by ΔS and ΔT in such a way that a better fit of the experimental data results. This is done by minimizing the following error function.

$$\begin{aligned} ERROR &= \sum_i \left[s_e(t_i) - s^*(t_i) \right]^2 = \sum_i \left[s_e(t_i) - s(t_i) - U_T(t_i)\Delta T - U_S(t_i)\Delta S \right]^2 \\ &= \sum_i \left[s_e(t_i) - s(t_i) \right]^2 - 2\Delta T \sum_i U_T(t_i)\left[s_e(t_i) - s(t_i) \right] \\ &\quad - 2\Delta S \sum_i U_S(t_i)\left[s_e(t_i) - s(t_i) \right] \\ &\quad + \sum_i \left[U_S^2(t_i)\Delta S^2 + 2U_T(t_i)U_S(t_i)\Delta S\Delta T + U_T^2(t_i)\Delta T^2 \right] \end{aligned} \tag{16}$$

The t_i represents a discrete time at which an experimental measurement is made for the drawdown. The error is defined as the sum over all measurements of the squared difference in s_e and s. Notice that the sensitivity coefficients U_T and U_S depend upon the time t_i.

The error is minimized by taking the first derivatives with respect to ΔT and ΔS, setting them equal to zero, and finally by solving the resulting equations for ΔT and ΔS.

$$\frac{\partial(\text{ERROR})}{\partial \Delta T} = -2\sum_i U_T(t_i)[s_e(t_i)-s(t_i)] + 2\Delta S\sum_i U_S(t_i)U_T(t_i) + 2\Delta T\sum_i U_T^2(t_i) = 0 \qquad (17)$$

$$\frac{\partial(\text{ERROR})}{\partial \Delta S} = -2\sum_i U_S(t_i)[s_e(t_i)-s(t_i)] + 2\Delta S\sum_i U_S^2(t_i) + 2\Delta T\sum_i U_S(t_i)U_T(t_i) = 0 \qquad (18)$$

For ease of writing define the variables

$$SSUS = \sum_i U_S^2(t_i) \qquad (19)$$

$$SSUT = \sum_i U_T^2(t_i) \qquad (20)$$

$$SUTUS = \sum_i U_S(t_i)U_T(t_i) \qquad (21)$$

$$SUSDIF = \sum_i U_S(t_i)[s_e(t_i) - s(t_i)] \qquad (22)$$

$$SUTDIF = \sum_i U_T(t_i)[s_e(t_i) - s(t_i)] \qquad (23)$$

Notice that all quantities in equations (19) through (23) are known from experimental data or can be calculated from equations (1), (13), or (14). Solving equation (17) for ΔT yields

$$\Delta T = [SUTDIF - (SUTUS)\Delta S]/SSUT \qquad (24)$$

Substituting for ΔT in equation (18) and solving for ΔS results in the following equation.

$$\Delta S = \frac{(SSUT)(SUSDIF)-(SUTUS)(SUTDIF)}{(SSUS)(SSUT)-(SUTUS)^2} \qquad (25)$$

Thus the ΔS which results in the "best" fit can be found from equation (25) which involves only known quantities. This ΔS may be substituted into equation (24) to find the "best" fit value for ΔT.

The values for ΔT and ΔS can be used to update the first guess for T and S. This better estimate for T and S is then used in the least squares procedure again to obtain new values of ΔT and ΔS. In general this can be continued until ΔT and ΔS become so small as to be insignificant, at which time the iteration is terminated. The "best" fit after the i^{th} iteration is obtained by using the following equations.

$$T^{i+1} = T^{i} + \Delta T^{i} \qquad (26)$$

$$S^{i+1} = S^{i} + \Delta S^{i} \qquad (27)$$

The procedure may not converge if the initial guess for T and S is especially bad. However, numerical experiments indicate that good convergence may be obtained even if the initial guess is off considerably. These numerical experiments show that the initial guesses for T and S may be overestimated or underestimated by about two or three orders of magnitude while still obtaining convergence. These experiments covered the normal range of T and S encountered in groundwater work $(.1 \geq S \geq 10^{-5})$ $(10^{6}\ \text{gal/day/ft} \geq T \geq 10^{2}\ \text{gal/day/ft})$.

It is possible to obtain an initial guess for T and S from the data if reasonable values are not known. The Theis equation may be expanded as (Jacob, 1950)

$$s = \frac{Q}{4\pi T}\left[-.5772 - \ln\left(\frac{r^2S}{4Tt}\right) + \left(\frac{r^2S}{4Tt}\right) - \frac{1}{2\cdot 2!}\left(\frac{r^2S}{4Tt}\right)^2 + \frac{1}{3\cdot 3!}\left(\frac{r^2S}{4Tt}\right)^3 - \cdots\right] \quad (2$$

For large values of t and small values of r such that

$$\frac{r^2S}{4Tt} << 1$$

only the constant and ln terms need to be considered. Differentiating the truncated expansion for s with respect to lnt one obtains

$$\frac{ds}{d(\ln t)} \cong \frac{Q}{4\pi T} \quad (29)$$

Solving for T yields an estimate for this parameter.

$$T \cong \frac{Q}{4\pi \frac{ds}{d(\ln t)}} \quad (30)$$

Equation (29) indicates that there is a linear relationship between s and lnt when $\frac{r^2 S}{4Tt} << 1$.

$$s = \left[\frac{ds}{d(\ln t)}\right]\ln t + C \quad (31)$$

C and $\frac{ds}{d(\ln t)}$ must be determined from the data. At some time t_o the drawdown predicted by equation (31) will be zero.

$$0 = \left[\frac{ds}{d(\ln t)}\right]\ln t_o + C \quad (32)$$

Solving for $\ln t_o$ gives

$$\ln t_o = -\left[\frac{C}{\frac{ds}{d(\ln t)}}\right] \quad (33)$$

The definition of t_o implies that the first two terms of equation (28) must equal zero when evaluated at t_o if $\frac{r^2 S}{4Tt} << 1$.

$$0 = \frac{Q}{4\pi T}\left[-.5772 - \ln\left(\frac{r^2 S}{4Tt_o}\right)\right] \quad (34)$$

Solving this equation for S gives the following result.

$$S = \frac{4T}{r^2} \exp\left[\ln t_o - .5772\right]$$

$$S = \frac{4T}{r^2} \exp\left[-\frac{C}{\frac{ds}{d(\ln t)}} - .5772\right] \quad (35)$$

Equations (30) and (35) show that one can estimate T and S by fitting equation (31) to the data. In fitting equation (31) to the data one attempts to find the "best" value for $\frac{ds}{d(\ln t)}$ and C. The method of least squares is ideally suited to this problem. Obviously, at least two drawdown-time pairs are needed to define a straight line. If more than two pairs are given the least squares technique finds the "best" fit. In this work the last four drawdown-time pairs are used to make an estimate of T and S if reasonable values are not known. It is assumed that r is small enough and t is large enough so the $\frac{r^2 S}{4Tt} << 1$ for these last four pairs. If this condition is not met then this procedure will probably not provide an acceptable guess for T and S.

Let $s_e(t)$ represent the experimental data. The squared error in fitting the last four points is

$$ERROR = \sum_{i=N-3}^{N} \left[s_e(t_i) - \frac{ds}{d(\ln t)} \ln t_i - C \right]^2$$

$$= \sum_{i=N-3}^{N} \left[s_e^2(t_i) + \left(\frac{ds}{d(\ln t)}\right)^2 (\ln t_i)^2 + C^2 - 2 s_e(t_i) \frac{ds}{d(\ln t)} \ln t_i - 2 s_e(t_i) C + 2 \frac{ds}{d(\ln t)} \ln t_i C \right] \qquad (36)$$

A necessary condition for the error to be minimized is that:

$$\frac{\partial(ERROR)}{\partial C} = \sum_{i=N-3}^{N} \left[2C - 2 s_e(t_i) + 2 \frac{ds}{d(\ln t)} \ln t_i \right] = 0 \qquad (37)$$

and

$$\frac{\partial(ERROR)}{\partial\left(\frac{ds}{d(\ln t)}\right)} = \sum_{i=N-3}^{N} \left[2 \frac{ds}{d(\ln t)} (\ln t_i)^2 - 2 s_e(t_i) \ln t_i + 2 \ln(t_i) C \right] = 0 \qquad (38)$$

Solving these two equations simultaneously gives

$$\frac{ds}{d(\ln t)} = \frac{4 \sum_{i=N-3}^{N} s_e(t_i) \ln t_i - \sum_{i=N-3}^{N} s_e(t_i) \sum_{i=N-3}^{N} \ln t_i}{4 \sum_{i=N-3}^{N} (\ln t_i)^2 - \left(\sum_{i=N-3}^{N} \ln t_i \right)^2} \qquad (39)$$

$$C = -\frac{1}{4} \frac{ds}{d(\ln t)} \sum_{i=N-3}^{N} \ln t_i + \frac{1}{4} \sum_{i=N-3}^{N} s_e(t_i) \qquad (40)$$

The results expressed by equations (39) and (40) can now be used in equations (30) and (35) to calculate an initial guess for T and S when needed. This procedure works well if the restrictions on r and t are observed.

PROGRAM THEIS

Appendix I contains a listing of program THEIS. It is a time sharing fortran program for evaluation of equation (1). In addition to drawdown (s) one may have the quantity $u = r^2S/4Tt$, the well function W(u), and the sensitivity coefficients given by equations (13) and (14) printed out. The user may utilize the gal-day-foot system or any consistent set of units.

Figure 1 contains a printout of a typical run. The user's response is underlined. The program initiates a series of questions after the RUN command is typed and a carriage return is given. A carriage return is required after each response. The first question asks if the user wants u, W, and the sensitivity coefficients printed. Any response other than YES with no leading or imbedded blanks is interpreted as NO. All other questions requiring a yes or no answer are similar. In figure 1 the extra printout was requested. The second question defines the system of units. The user can use the gal-day-foot system or any consistent set of units. A YES response, as in figure 1, means the gal-day-foot system is being used.

The units for each parameter the user must specify are stated as the program asks for the user to type in the value. L is any arbitrary length unit and T is any arbitrary time unit. A storage coefficient of .001 which is unitless has been used in figure 1. Transmissivity in units of gal/day/ft or L^2/T must be specified. A value of 24,000 gal/day/ft has been used in the example. A constant pumpage of 240,000 gal/day has been used in figure 1. In consistent units pumpage must be specified in units of L^3/T.

```
DO YOU WANT U, W, AND SENSITIVITY VALUES PRINTED ?
=YES
DO YOU WANT TO USE THE GAL, DAY, FT SYSTEM ?
=YES
STORAGE COEFFICIENT (UNITLESS)
=.001
TRANSMISSIVITY (GAL/DAY/FT) OR (L**2/T)
=24000
CONSTANT PUMPAGE (GAL/DAY) OR (L**3/T)
=240000
CONSTANT OBSERVATION POINT?
=YES
CONSTANT OBSERVATION TIME?
=NO
OBSERVATION POINT (FT) OR (L)
=100
OBSERVATION TIME (DAYS) OR (T)
=.001

THE DRAWDOWN IS            0.25669954
U =         0.77916666E 00
W =         0.32257789E 00
SENSITIVITY WITH RESPECT TO TRANSMISSIVITY =       0.45163665E-05
SENSITIVITY WITH RESPECT TO STORAGE =       -0.36509233E 03


OBSERVATION TIME (DAYS) OR (T)
=.01

THE DRAWDOWN IS            1.63239339
U =         0.77916667E-01
W =         0.20513243E 01
SENSITIVITY WITH RESPECT TO TRANSMISSIVITY =      -0.37344505E-04
SENSITIVITY WITH RESPECT TO STORAGE =       -0.73612525E 03


OBSERVATION TIME (DAYS) OR (T)
=.1

THE DRAWDOWN IS            3.41010541
U =         0.77916666E-02
W =         0.42852612E 01
SENSITIVITY WITH RESPECT TO TRANSMISSIVITY =      -0.10918776E-03
SENSITIVITY WITH RESPECT TO STORAGE =       -0.78959905E 03
```

Figure 1. Typical run of program THEIS.

At this point two more yes-no questions are asked. The first asks if the user wants a constant observation point. In other words, r in equation (1) will be constant for this run. This is the normal situation when one observation well is used to measure water levels as a function of time. The next question concerns time. Is t in equation (1) to be held constant for this run? This would be the situation if one measured the drawdown at the same time in a number of observation wells. If the answer to both of these questions is yes the program accepts only one value of r and t, calculates the desired quantities, and then terminates. If only one of the questions is answered yes the program continues to ask for updated values of the parameter that is not constant. In figure 1 time is not constant so the program continually asks for new times. To terminate the program simply hit the BREAK button. If both questions are not YES then the program asks for updated values of both r and t until the BREAK button is pushed. In figure 1 a constant r of 100 feet has been specified while several times have been given ranging from .001 days to .1 days.

SUBROUTINE THEIS

Appendix II contains a listing of subroutine THEIS. It is a fortran IV subroutine for the evaluation of equations (1), (13), and (14) that can be incorporated into any user deck and called by the mainline program. To utilize subroutine THEIS the user simply includes the following call statement at the appropriate place in the mainline program.

```
CALL THEIS(SC, KB, Q, R, T, S, DSDT, DSDSC, UNIT)
```

The parameters SC, KB, Q, R, T, and UNIT must be assigned a value or character designation prior to calling THEIS. SC is the storage coefficient which is unitless. UNIT must be declared a character type of variable in the mainline program. If the user wishes to use the gal-day-ft system, UNIT must be set to 3HYES in the mainline. Any other character string is interpreted as NO and the subroutine assumes a consistent set of units. KB is the transmissivity (gal/day/ft or L^2/T), Q is the constant pumpage (gal/day or L^3/T), R is the distance of the observation well from the pumped well (feet or L), and T is the elapsed time since pumping started (day or T). The transmissivity KB should be declared REAL in the mainline since it would be implicitly typed INTEGER.

Upon returning to the mainline, parameters S, DSDT, and DSDSC have been assigned values by subroutine THEIS. These values represent the evaluation of equations (1), (13) and (14) respectively. S is the drawdown in units of feet or L. DSDT is the sensitivity coefficient with respect to transmissivity in units of ft^2 day/gal or T/L. DSDSC is the sensitivity coefficient with respect to storage in units of feet or L. Upon returning to the mainline these three parameters are available to the user for printout or further computation. This subroutine is used in the next program to be discussed; so, the reader is referred there for an example of the usage of subroutine THEIS.

PROGRAM THEISFIT

This program fits the Theis equation to experimental pumptest data to obtain the "best" values for the storage coefficient and the transmissivity by using a least squares procedure discussed earlier in this work. The program exists in two forms: a time sharing fortran version and a fortran IV batch version. The time sharing version is listed in Appendix III. Appendix IV contains a listing of the batch version. The two programs are basically identical except for data input.

The printout of a typical time sharing run is contained in figure 2. The user's response is underlined. As with program THEIS the program initiates a series of questions after the RUN command is given with a carriage return. The first question defines the system of units. YES allows one to use the gal-day-foot system; any other response is interpreted as NO. In figure 2 NO was the response so a consistent set of units is assumed. The second question asks if the user wishes to make an initial guess for the storage and transmissivity. In figure 2 NO was given so no input for these quantities was required. If the response had been YES the program would have requested the user to type in the guesses for storage and transmissivity in the two following questions. In figure 2 the pumpage rate is given as 66.07 ft^3/min. The observation well was located 545 feet from the pumped well. The next question asks how many drawdown-time pairs are to be read into the program. In this case it is eighteen. At this point the program echo prints all data typed in thus far. This allows for error checking. Since guesses for storage and transmissivity were not given they are printed as zero. SC and KB stand for storage coefficient and transmissivity respectively.

The program is now ready to accept drawdown-time pairs. They should be read in order of increasing time since the last four are used to

```
*RUN
DO YOU WANT TO USE GAL, DAY, FT SYSTEM ?
=NO
GUESS FOR STORAGE AND TRANSMISSIVITY ?
=NO
CONSTANT PUMPAGE RATE ? GAL/DAY OR L**3/T
=66.07
OBSERVATION DISTANCE FROM PUMPING WELL ? FT OR L
=545
NUMBER OF DRAWDOWN-TIME PAIRS TO BE READ ?
=18
THE INITIAL DATA WAS
SC = 0.                 KB = 0.
Q = 0.66070000E 02 R = 0.54500000E 03 N =    18
TYPE IN DRAWDOWN-TIME PAIRS IN ORDER OF INCREASING TIME.
=.02,50
=.05,60
=.08,70
=.13,80
=.18,90
=.22,100
=.33,120
=.43,140
=.54,160
=.64,180
=.74,200
=.94,240
=1.12,280
=1.30,320
=1.47,360
=1.66,400
=1.92,460
=2.17,535
```

Figure 2. Typical run of program THEISFIT (Time Sharing Version).

```
THE PUMP TEST DATA IN DRAWDOWN-TIME PAIRS IS
      0.20000000E-01        0.50000000E 02
      0.50000000E-01        0.60000000E 02
      0.80000000E-01        0.70000000E 02
      0.13000000E 00        0.80000000E 02
      0.18000000E 00        0.90000000E 02
      0.22000000E 00        0.10000000E 03
      0.33000000E 00        0.12000000E 03
      0.43000000E 00        0.14000000E 03
      0.54000000E 00        0.16000000E 03
      0.64000000E 00        0.18000000E 03
      0.74000000E 00        0.20000000E 03
      0.94000000E 00        0.24000000E 03
      0.11200000E 01        0.28000000E 03
      0.13000000E 01        0.32000000E 03
      0.14700000E 01        0.36000000E 03
      0.16600000E 01        0.40000000E 03
      0.19200000E 01        0.46000000E 03
      0.21700000E 01        0.53500000E 03
THE CALCULATED GUESS FOR KB AND SC IS    0.29628059E 01  0.35149625E-02
BEST FIT KB AND SC THIS ITERATION ARE    0.25232340E 01  0.46495635E-02
BEST FIT KB AND SC THIS ITERATION ARE    0.22588631E 01  0.47946684E-02
BEST FIT KB AND SC THIS ITERATION ARE    0.22523235E 01  0.47765157E-02
BEST FIT KB AND SC THIS ITERATION ARE    0.22523888E 01  0.47765840E-02
THE BEST FIT DRAWDOWN-TIME PAIRS ARE
      0.25206928E-01        0.50000000E 02
      0.49396171E-01        0.60000000E 02
      0.81189803E-01        0.70000000E 02
      0.11926181E 00        0.80000000E 02
      0.16227960E 00        0.90000000E 02
      0.20906690E 00        0.10000000E 03
      0.31022453E 00        0.12000000E 03
      0.41701533E 00        0.14000000E 03
      0.52587939E 00        0.16000000E 03
      0.63457878E 00        0.18000000E 03
      0.74181843E 00        0.20000000E 03
      0.94917237E 00        0.24000000E 03
      0.11451357E 01        0.28000000E 03
      0.13292893E 01        0.32000000E 03
      0.15021422E 01        0.36000000E 03
      0.16645316E 01        0.40000000E 03
      0.18904877E 01        0.46000000E 03
      0.21471107E 01        0.53500000E 03
THE RMS ERROR FOR DRAWDOWN IS        0.17307440E-01
```

Figure 2. (Continued)

calculate an initial guess for storage and transmissivity. The guess calculating routine assumes these four are at large values of time. If the user supplies an initial estimate for storage and transmissivity, the drawdown-time pairs may be read in any order. Notice that the drawdown must be typed first and the time second with a separating comma. The values may be typed with or without a decimal point and may be in scientific notation (for example 1.3×10^5 would be typed 1.3E5). After the eighteen pairs have been typed the program echo prints them for error checking.

From this point on the user may not interact with the program. One of two things should now happen: the program converges to the "best" solution or the program does not converge. If it does not converge after twenty iterations the program terminates. However, if the initial guess for storage and transmissivity was bad or if the data is rather poor, unphysical values for storage and transmissivity or error messages may be generated in the iteration process. If this occurs the program may be terminated by hitting the BREAK key. In general, the storage and transmissivity guesses may be overestimated or underestimated by two or three orders of magnitude and still achieve convergence.

In the example shown in figure 2 the calculated guess is printed first then a series of iterations is started. The current "best" fit is printed for each iteration. Convergence is achieved in four iterations in this example. The convergence criteria requires the change in storage and transmissivity since the last iteration to be less than or equal to .1%. The program proceeds to print the "best" fit drawdown-time pairs and calculates the rms error in the drawdown. The rms error is a measure of the absolute error at an "average" data point. In this example one would expect the "average" difference between measured and calculated drawdown to be about .017 feet.

The data set for a typical run of the batch version of THEISFIT is shown in figure 3. The first card must contain values for the two character variables GUESS and UNIT. YES or NO are the appropriate responses. The first variable is GUESS. Its value must start in column one. YES means that the user is going to supply the first guess for storage and transmissivity. The second variable, UNIT, must start in column seven. YES means the user wants to use the gal-day-foot system. Any other response indicates a consistent set of units is being used. In this particular example an initial guess for SC and KB is given; and, the gal-day-foot system is used.

The next card contains five variables: storage (SC), transmissivity (KB), pumpage (Q), observation distance (R), and the number of drawdown-time pairs to be read (N). These variables are read under a (4F10.0, I10) format. Each variable field is ten columns wide. The first four variables may be punched with or without a decimal point; however, if no decimal is punched it will be assumed to be at the extreme right of the field. If no decimal is punched the value should be right justified. The last variable, N, must be right justified (ending in column 50) and punched without a decimal point. If GUESS is given as NO the program ignores any values given for SC and KB on the second card. In this example SC is .00001, KB is 2,000 gal/day/ft, Q is 316,800 gal/day, R is 824 feet, and N is 22 pairs.

```
YES    YES
    .00001      2000    316800       824        22
        .3   .002083        .7   .003472       1.3   .005556       2.1   .008333
       3.2   .013889       3.6   .016667       4.1   .020833       4.7   .026389
       5.1   .032639       5.3   .034722       5.7   .041667       6.1   .048611
       6.3   .055556       6.7   .062500       7.0   .069444       7.5   .090278
       8.3   .111111       8.5   .138889       9.2   .180556       9.7   .222222
      10.2   .263889      10.9   .347222
```

Figure 3. Typical data set for batch version of THEISFIT.

The drawdown-time pairs are punched on the third and following cards at a maximum of four pairs per card. They are read under an (8F10.0) format. Each data field is ten columns wide. Decimal consideration is the same as for SC, KB, Q, and R. They should be punched in order of increasing time if a guess for SC and KB is to be calculated by the program. In this example drawdowns are given in feet and time in days.

The output for the data set of figure 3 is shown in figure 4. The input data is printed out for error checking. Since GUESS was given as YES, no guess was calculated for SC and KB. The program converged in six iterations. The convergence criteria is the same as for the time sharing version. Comments on the convergence properties of the time sharing version also apply to the batch version. The best fit drawdown-time pairs are printed if convergence is obtained. The rms error for the drawdown is .091 feet for this example. Therefore, the "average" error in drawdown is .091 feet.

DISCUSSION AND SUMMARY

The automated fit for pumptest data developed in this work should be a useful tool for the groundwater hydrologist. We have used it on many more pumptests than the two examples included here. It is simple to use, quick, and inexpensive. Typically the computer costs for running a pumptest fit is less than two dollars. The automated fit has the advantage that it is always objective. As a measure of the error in fitting, the rms error in drawdown is calculated for the "best"

```
THE INITIAL DATA WAS
SC = 0.10000000E-04 KB = 0.20000000E 04
Q = 0.31680000E 06 R = 0.82400000E 03 N =    22
THE PUMP TEST DATA IN DRAWDOWN-TIME PAIRS IS
     0.30000000E 00      0.20830000E-02
     0.70000000E 00      0.34720000E-02
     0.13000000E 01      0.55560000E-02
     0.21000000E 01      0.83330000E-02
     0.32000000E 01      0.13889000E-01
     0.36000000E 01      0.16667000E-01
     0.41000000E 01      0.20833000E-01
     0.47000000E 01      0.26389000E-01
     0.51000000E 01      0.32639000E-01
     0.53000000E 01      0.34722000E-01
     0.57000000E 01      0.41667000E-01
     0.61000000E 01      0.48611000E-01
     0.63000000E 01      0.55556000E-01
     0.67000000E 01      0.62500000E-01
     0.70000000E 01      0.69444000E-01
     0.75000000E 01      0.90278000E-01
     0.83000000E 01      0.11111100E 00
     0.85000000E 01      0.13888900E 00
     0.92000001E 01      0.18055600E 00
     0.97000001E 01      0.22222200E 00
     0.10200000E 02      0.26388900E 00
     0.10900000E 02      0.34722200E 00
BEST FIT KB AND SC THIS ITERATION ARE   0.36231568E 04  0.15993002E-04
BEST FIT KB AND SC THIS ITERATION ARE   0.59841841E 04  0.21295657E-04
BEST FIT KB AND SC THIS ITERATION ARE   0.84381630E 04  0.22418721E-04
BEST FIT KB AND SC THIS ITERATION ARE   0.97266890E 04  0.21174726E-04
BEST FIT KB AND SC THIS ITERATION ARE   0.99078571E 04  0.20944681E-04
BEST FIT KB AND SC THIS ITERATION ARE   0.99086274E 04  0.20949939E-04
THE BEST FIT DRAWDOWN-TIME PAIRS ARE
     0.35065781E 00      0.20830000E-02
     0.82974025E 00      0.34720000E-02
     0.14774877E 01      0.55560000E-02
     0.21714488E 01      0.83330000E-02
     0.31821451E 01      0.13889000E-01
     0.35709338E 01      0.16667000E-01
     0.40622920E 01      0.20833000E-01
     0.45985823E 01      0.26389000E-01
     0.50920417E 01      0.32639000E-01
     0.52373781E 01      0.34722000E-01
     0.56696366E 01      0.41667000E-01
     0.60390812E 01      0.48611000E-01
     0.63617290E 01      0.55556000E-01
     0.66480276E 01      0.62500000E-01
     0.69053687E 01      0.69444000E-01
     0.75506012E 01      0.90278000E-01
     0.80648858E 01      0.11111100E 00
     0.86204650E 01      0.13888900E 00
     0.92767411E 01      0.18055600E 00
     0.97979767E 01      0.22222200E 00
     0.10230386E 02      0.26388900E 00
     0.10922440E 02      0.34722200E 00
THE RMS ERROR FOR DRAWDOWN IS       0.91011392E-01
```

Figure 4. Output for typical run of batch version of THEISFIT.

transmissivity and storage. For the cases we have run the rms error in drawdown is no more than a few tenths of a foot. If it is much larger than this one has either poor data or a hydrologic situation which can not be represented by the Theis equation.

The algorithm for fitting has good convergence properties. Convergence is generally achieved even if the initial guess is too large or too small by two or three orders of magnitude. The procedure has been tested over a wide range of transmissivity and storage.

This work deals only with the Theis equation. However, sensitivity analysis and least squares fitting could be applied to more hydrologically complicated situations. Automated fitting routines could be developed for anisotropic flow, partial penetration, leaky aquifers, delayed yield, and hydrologic boundaries to name some of the more common situations.

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Appendix I. Listing of program THEIS.

```
C      PROGRAM: THEIS
C      PURPOSE: CALCULATES THE DRAWDOWN FOR A WELL PUMPING AT
C          CONSTANT DISCHARGE FROM AN INFINITE AQUIFER BY THE
C          THEIS EQUATION
C
C      ARGUMENTS (L IS ARBITRARY LENGTH, T IS ARBITRARY TIME )
C               RS   CONSTANT OBSERVATION SWITCH; YES OR NO
C               TS   CONSTANT OBSERVATION TIME SWITCH; YES OR NO
C               US   UNIT SWITCH, USE GAL, DAYS, FT; YES OR NO
C            PRTSW   PRINT SWITCH FOR U, W, AND SENSITIVITY; YES OR NO
C               SC   STORAGE COEFFICIENT FOR AQUIFER (UNITLESS)
C               KB   TRANSMISSIVITY OF AQUIFER (GAL/DAY/FT) OR (L**2/T)
C                Q   CONSTANT PUMPAGE OF WELL (GAL/DAY) OR (L**3/T)
C                R   OBSERVATION DISTANCE FROM WELL (FT) OR (L)
C                T   OBSERVATION TIME (DAYS) OR (T)
C                S   DRAWDOWN (FT) OR (L)
C             DSDT   SENSITIVITY W.R.T. TRANSMISSIVITY (FT**2*DAY/GAL) OR (T/L)
C            DSDSC   SENSITIVITY W.R.T. STORAGE (FT) OR (L)
C -----------------------------------------------------------------------------
C
C READ IN ARGUMENTS
       CHARACTER RS, TS, US, PRTSW
         REAL KB
       ICOUNT =0
       PRINT 1
       PRINT 15
    15 FORMAT(' DO YOU WANT U, W, AND SENSITIVITY VALUES PRINTED ? ')
       READ:PRTSW
     1 FORMAT(1H0)
        PRINT 14
   14    FORMAT(' DO YOU WANT TO USE THE GAL, DAY, FT SYSTEM ?')
        READ:US
       PRINT 2
     2 FORMAT(' STORAGE COEFFICIENT (UNITLESS)')
       READ:SC
       PRINT 3
     3 FORMAT(' TRANSMISSIVITY (GAL/DAY/FT) OR (L**2/T)')
       READ:KB
       PRINT 4
     4 FORMAT(' CONSTANT PUMPAGE (GAL/DAY) OR (L**3/T)')
       READ:Q
       PRINT 10
    10 FORMAT (' CONSTANT OBSERVATION POINT? ' )
       READ:RS
       PRINT 11
    11 FORMAT (' CONSTANT OBSERVATION TIME? ')
       READ:TS
    80 IF (ICOUNT .GT. 0 .AND. RS .EQ. 3HYES) GO TO 70
       PRINT 5
     5 FORMAT(' OBSERVATION POINT (FT) OR (L)')
       READ:R
    70 IF (ICOUNT .GT. 0 .AND. TS .EQ. 3HYES) GO TO 95
       PRINT 6
     6 FORMAT(' OBSERVATION TIME (DAYS) OR (T)')
       READ:T
```

```
C CALCULATE THEIS SOLUTION
C THEIS EQUATION FROM 'INTRO TO HYDROLOGY' BY VIESSMAN PAGE 257
C RATIONAL APPROXIMATION FROM 'HANDBOOK OF MATH FUNCTIONS'
C   BY ABRAMOWITZ AND STEGUN PAGE 231
   95 CONTINUE
      U =  R*R*SC/(4.0*KB*T)
       IF (US .EQ. 3HYES ) U = 7.48*U
      IF (U .LE. 0.0) GO TO 96
      IF (U .GT. 1.0) GO TO 86
      W= -ALOG(U)-.57721566+.99999193*U-.24991055*U*U+
&     .05519968*U*U*U-.00976004*U**4+.00107857*U**5
      GO TO 87
   86 W = (EXP(-U)/U)*(U*U+2.334733*U+.250621)/
&     (U*U+3.330657*U + 1.681534)
   87 S = (Q/(4.0*3.14159*KB))*W
      DSDT = (Q/(4.0*3.14159*KB**2))*(-W + EXP(-U))
      DSDSC=-(Q/(4.0*3.14159*KB*SC))*EXP(-U)
C OUTPUT RESULTS
   90 PRINT 7, S
    7 FORMAT(1H0, 'THE DRAWDOWN IS ', F20.8)
      IF (PRTSW .EQ. 3HYES ) PRINT 8,U
    8 FORMAT (' U = ', E20.8)
      IF (PRTSW .EQ. 3HYES ) PRINT 9,W
    9 FORMAT (' W = ', E20.8 )
      IF (PRTSW .EQ. 3HYES ) PRINT 12,DSDT
   12 FORMAT ( ' SENSITIVITY WITH RESPECT TO TRANSMISSIVITY = ' , E20.8
      IF (PRTSW .EQ. 3HYES ) PRINT 21,DSDSC
   21 FORMAT(' SENSITIVITY WITH RESPECT TO STORAGE = ', E20.8 )
      GO TO 97
   96 PRINT 13
   13 FORMAT ( ' DRAWDOWN UNDEFINED U TOO SMALL ' )
   97 PRINT 1
      ICOUNT = ICOUNT +1
      IF (RS .EQ. 3HYES .AND. TS .EQ. 3HYES ) GO TO 99
      GO TO 80
   99 STOP
      END
```

Appendix II. Listing of subroutine THEIS.

```
      SUBROUTINE THEIS(SC,KB,Q,R,T,S,DSDT,DSDSC,UNIT)
C     PURPOSE   CALCULATES THE DRAWDOWN FOR A WELL PUMPING AT
C         CONSTANT DISCHARGE FROM AN INFINITE AQUIFER BY THE
C         THEIS EQUATION
C
C      ARGUMENTS (L IS ARBITRARY LENGTH, T IS ARBITRARY TIME)
C         SC     STORAGE COEFFICIENT FOR AQUIFER (UNITLESS)
C         KB     TRANSMISSIVITY OF AQUIFER (GAL/DAY/FT) OF (L**2/T)
C          Q     CONSTANT PUMPAGE OF WELL (GAL/DAY) OR (L**3/T)
C          R     OBSERVATION DISTANCE FROM WELL (FT) OR (L)
C          T     OBSERVATION TIME (DAYS) OR (T)
C          S     DRAWDOWN (FT) OR (L)
C       DSDT     SENSITIVITY W.R.T. TRANSMISSIVITY (FT**2*DAY/GAL) OR (T/L)
C      DSDSC     SENSITIVITY W.R.T. STORAGE (FT) OR (L)
C       UNIT     SYSTEM OF UNITS; YES FOR GAL, DAY, FT; OTHERWISE
C                   CONSISTENT UNITS ARE ASSUMED
C -------------------------------------------------------------
C
C CALCULATE THEIS SOLUTION
C THEIS EQUATION FROM 'INTRO TO HYDROLOGY' BY VIESSMAN PAGE 257
C RATIONAL APPROXIMATION FROM 'HANDBOOK OF MATH FUNCTIONS'
C   BY ABRAMOWITZ AND STEGUN PAGE 231
      REAL KB
      CHARACTER UNIT
      U =  R*R*SC/(4.0*KB*T)
      IF (UNIT .EQ. 3HYES      ) U = 7.48*U
      IF (U .LE. 0.0) GO TO 96
      IF (U .GT. 1.0) GO TO 86
      W= -ALOG(U)-.57721566+.99999193*U-.24991055*U*U+
&       .05519968*U*U*U-.00976004*U**4+.00107857*U**5
      GO TO 87
   86 W = (EXP(-U)/U)*(U*U+2.334733*U+.250621)/
&       (U*U+3.330657*U + 1.681534)
   87 S = (Q/(4.0*3.14159*KB))*W
      DSDT = (Q/(4.0*3.14159*KB**2))*(-W + EXP(-U))
      DSDSC=-(Q/(4.0*3.14159*KB*SC))*EXP(-U)
      RETURN
   96 PRINT 13
   13 FORMAT ( ' DRAWDOWN UNDEFINED U TOO SMALL ' )
   99 STOP
      END
```

Appendix III. Listing of program THEISFIT (Time Sharing Version)

```
C       PROGRAM THEISFIT (TIME SHARING VERSION)
C       PURPOSE:  TO CALCULATE THE BEST FIT STORAGE AND TRANSMISSIVITY
C           BY FITING THE THEIS EQUATION TO EXPERIMENTAL PUMPTEST DATA IN
C           A LEAST SQUARES SENSE.
C
C       IMPORTANT VARIABLES: (L IS ARBITRARY LENGTH, T IS ARBITRARY TIME)
C           UNIT     SYSTEM OF UNITS; YES FOR GAL, DAY, FT; OTHERWISE
C                        CONSISTENT UNITS ARE ASSUMED.
C          GUESS     DO YOU WANT TO ENTER AN INITIAL GUESS FOR SC AND KB?
C                         YES OR NO IS THE APPROPRIATE RESPONSE.
C                SC    STORAGE COEFFICIENT OF AQUIFER (UNITLESS)
C                KB    TRANSMISSIVITY OF AQUIFER (GAL/DAY/FT) OR (L**2/T)
C                 Q    CONSTANT PUMPAGE OF WELL (GAL/DAY) OR (L**3/T)
C                 R    OBSERVATION DISTANCE FROM WELL (FT) OR (L)
C                 N    NUMBER OF DRAWDOWN-TIME PAIRS TO BE READ
C              S(I)    EXPERIMENTAL DRAWDOWN AT TIME I (FT) OR (L)
C              T(I)    THE ITH TIME AT WHICH AN EXPERIMENTAL MEASUREMENT
C                         FOR THE DRAWDOWN IS MADE (DAYS) OR (T)
C           SIGMA      THE RMS ERROR IN DRAWDOWN AFTER THE BEST
C                         FIT HAS BEEN OBTAINED
C-----------------------------------------------------------------------
        DIMENSION S(100),T(100),SP(100),DSDT(100),DSDSC(100)
        REAL KB
        CHARACTER GUESS, UNIT
C READ IN THE INITIAL DATA
        PRINT 801
  801   FORMAT (' DO YOU WANT TO USE GAL, DAY, FT SYSTEM ? ')
        READ:UNIT
        PRINT 105
  105   FORMAT(' GUESS FOR STORAGE AND TRANSMISSIVITY ?')
        READ: GUESS
        IF (GUESS .NE. 3HYES ) GO TO 114
        PRINT 112
  112   FORMAT(' ESTIMATE FOR STORAGE ? ')
        READ: SC
        PRINT 113
  113   FORMAT(' ESTIMATE FOR TRANSMISSIVITY ? GAL/DAY/FT OR L**2/T ')
        READ: KB
  114   PRINT 115
  115   FORMAT(' CONSTANT PUMPAGE RATE ? GAL/DAY OR L**3/T ')
        READ: Q
        PRINT 116
  116   FORMAT(' OBSERVATION DISTANCE FROM PUMPING WELL ? FT OR L ')
        READ:R
        PRINT 117
  117   FORMAT(' NUMBER OF DRAWDOWN-TIME PAIRS TO BE READ ? ')
        READ: N
C ECHO PRINT THE INITIAL DATA
        WRITE (6, 106 ) SC, KB, Q, R, N
  106   FORMAT ( ' THE INITIAL DATA WAS ' / 5H SC =, E15.8, 5H KB =, E15.
```

```
&        - /4H Q =,E15.8, 4H R =,E15.8, 4H N =, I5 )
C TYPE IN THE DRAWDOWN-TIME PAIRS IN ORDER OF INCREASING TIME
         PRINT 118
     118 FORMAT(' TYPE IN DRAWDOWN-TIME PAIRS IN ORDER OF INCREASING TIME. '
         DO 120  I = 1,N
     120 READ: S(I),T(I)
C ECHO PRINT THE DRAWDOWN-TIME PAIRS
         WRITE (6, 107) (S(I),T(I), I = 1, N )
     107 FORMAT (' THE PUMP TEST DATA IN DRAWDOWN-TIME PAIRS IS '/(2E20.8))
     101 FORMAT ( 8F10.0 )
     100 FORMAT ( 4F10.0, I10 )
C CALCULATE THE INITIAL GUESS FOR KB AND SC IF NOT GIVEN
         NUM = 4
         IF (GUESS .EQ. 6HYES     ) GO TO 1
         SUMLNT = 0.0
         SMLNT2 = 0.0
         SUMSE = 0.0
         SSELNT = 0.0
         DO 50 I = 1,NUM
         II = N +1-I
         ALOGT = ALOG(T(II))
         SUMLNT = SUMLNT + ALOGT
         SMLNT2 = SMLNT2 + ALOGT**2
         SUMSE = SUMSE + S(II)
      50 SSELNT = SSELNT + S(II)*ALOGT
         SLOPE = (NUM*SSELNT-SUMSE*SUMLNT)/(NUM*SMLNT2-SUMLNT**2)
         CON =-(SLOPE*SUMLNT - SUMSE)/NUM
         KB =  Q/(SLOPE*4.0*3.14159)
         ALNTO = -CON/SLOPE
         SC = 4.0*KB/( R**2*EXP(.5772-ALNTO))
         IF (UNIT .EQ. 3HYES ) SC = SC/7.48
C PRINT THE CALCULATED GUESS FOR KB AND SC
         WRITE (6,110) KB, SC
     110 FORMAT (' THE CALCULATED GUESS FOR KB AND SC IS ', 2E16.8 )
       1 ICOUNT = 0
       5 TEMPKB = KB
         TEMPSC = SC
C USE SENSITIVITY ANALYSIS AND LEAST SQUARES TO FIND A BETTER KB AND SC
         DO 10 I = 1, N
      10 CALL THEIS(SC,KB,Q,R,T(I),SP(I),DSDT(I),DSDSC(I),UNIT)
         SSUS = 0.0
         SSUT = 0.0
         SUTUS=0.0
         SUSDIF  = 0.0
         SUTDIF = 0.0
         DO 15 I = 1, N
         SSUS = DSDSC(I)**2+SSUS
         SSUT = DSDT(I)**2+SSUT
         SUTUS = DSDSC(I)*DSDT(I) + SUTUS
         SUSDIF =  DSDSC(I)*(S(I)-SP(I))  + SUSDIF
      15 SUTDIF = DSDT(I)*(S(I)-SP(I)) + SUTDIF
         DELTSC = (SSUT*SUSDIF-SUTUS*SUTDIF)/(SSUS*SSUT-SUTUS**2)
         IF (DELTSC .LT. -.95*SC ) DELTSC = -.95*SC
         IF (DELTSC .GT. 2.0*SC ) DELTSC = 2.0*SC
         SC = SC + DELTSC
         IF (SC .GT. 1.0 ) SC = 1.0
         DELTKB = (SUTDIF-DELTSC*SUTUS)/SSUT
         IF (DELTKB .LT. -.95*KB ) DELTKB = -.95*KB
         IF (DELTKB .GT. 2.0*KB ) DELTKB = 2.0*KB
         KB = KB + DELTKB
```

```
      WRITE (6,104) KB, SC
  104 FORMAT( ' BEST FIT KB AND SC THIS ITERATION ARE ', 2E16.8 )
      ICOUNT = ICOUNT + 1
C IF IT DID NOT CONVERGE PRINT MESSAGE
      IF ( ICOUNT .GT. 20) GO TO 40
C DO ANOTHER ITERATION IF IT HASNT CONVERGED AND ITERATION LIMIT NOT
C    EXCEEDED.
      IF(ABS((TEMPKB-KB)/KB).GT..001.OR.ABS((TEMPSC-SC)/SC).GT..001)
&        GO TO 5
C PRINT BEST FIT DRAWDOWN-TIME PAIRS IF CONVERGENCE OBTAINED
  108 FORMAT (' THE BEST FIT DRAWDOWN-TIME PAIRS ARE ' )
      WRITE (6,108)
      DO 20 I = 1, N
      CALL THEIS(SC,KB,Q,R,T(I),SP(I),DSDT(I),DSDSC(I),UNIT)
      WRITE (6,109) SP(I), T(I)
  109 FORMAT(2E20.8)
   20 CONTINUE
C CALCULATE THE RMS ERROR IN DRAWDOWN AFTER BEST FIT
      SUM = 0.0
      DO 30 I = 1, N
   30 SUM = SUM + (SP(I)-S(I))**2
      SIGMA = SQRT(SUM/N)
      WRITE(6,111) SIGMA
  111 FORMAT(' THE RMS ERROR FOR DRAWDOWN IS ', E20.8 )
      STOP
   40 WRITE (6,125)
  125 FORMAT(' DID NOT CONVERGE IN 20 ITERATIONS ')
      STOP
      END
      SUBROUTINE THEIS(SC,KB,Q,R,T,S,DSDT,DSDSC,UNIT)
C     PURPOSE   CALCULATES THE DRAWDOWN FOR A WELL PUMPING AT
C         CONSTANT DISCHARGE FROM AN INFINITE AQUIFER BY THE
C         THEIS EQUATION
C
C      ARGUMENTS (L IS ARBITRARY LENGTH, T IS ARBITRARY TIME)
C         SC    STORAGE COEFFICIENT FOR AQUIFER (UNITLESS)
C         KB    TRANSMISSIVITY OF AQUIFER (GAL/DAY/FT) OF (L**2/T)
C          Q    CONSTANT PUMPAGE OF WELL (GAL/DAY) OR (L**3/T)
C          R    OBSERVATION DISTANCE FROM WELL (FT) OR (L)
C          T    OBSERVATION TIME (DAYS) OR (T)
C          S    DRAWDOWN (FT) OR (L)
C       DSDT    SENSITIVITY W.R.T. TRANSMISSIVITY (FT**2*DAY/GAL) OR (T/L
C      DSDSC    SENSITIVITY W.R.T. STORAGE (FT) OR (L)
C       UNIT    SYSTEM OF UNITS; YES FOR GAL, DAY, FT; OTHERWISE
C                  CONSISTENT UNITS ARE ASSUMED
C ----------------------------------------------------------------------
C
C CALCULATE THEIS SOLUTION
C THEIS EQUATION FROM 'INTRO TO HYDROLOGY' BY VIESSMAN PAGE 257
C RATIONAL APPROXIMATION FROM 'HANDBOOK OF MATH FUNCTIONS'
C   BY ABRAMOWITZ AND STEGUN PAGE 231
      REAL KB
      CHARACTER UNIT
      U =  R*R*SC/(4.0*KB*T)
      IF (UNIT .EQ. 3HYES      ) U = 7.48*U
```

```
      IF (U .LE. 0.0) GO TO 96
      IF (U .GT. 1.0) GO TO 86
      W= -ALOG(U)-.57721566+.99999193*U-.24991055*U*U+
&      .05519968*U*U*U-.00976004*U**4+.00107857*U**5
      GO TO 87
   86 W = (EXP(-U)/U)*(U*U+2.334733*U+.250621)/
&      (U*U+3.330657*U + 1.681534)
   87 S = (Q/(4.0*3.14159*KB))*W
      DSDT = (Q/(4.0*3.14159*KB**2))*(-W + EXP(-U))
      DSDSC=-(Q/(4.0*3.14159*KB*SC))*EXP(-U)
      RETURN
   96 PRINT 13
   13 FORMAT ( ' DRAWDOWN UNDEFINED U TOO SMALL ' )
   99 STOP
      END
```

Appendix IV. Listing of program THEISFIT (BATCH VERSION).

```
C       PROGRAM THEISFIT (FORTRAN IV BATCH VERSION)
C       PURPOSE:  TO CALCULATE THE BEST FIT STORAGE AND TRANSMISSIVITY
C           BY FITTING THE THEIS EQUATION TO EXPERIMENTAL PUMPTEST DATA
C           IN A LEAST SQUARES SENSE.
C
C       IMPORTANT VARIABLES: (L IS ARBITRARY LENGTH, T IS ARBITRARY TIME)
C            UNIT    SYSTEM OF UNITS; YES FOR GAL, DAY, FT; OTHERWISE
C                       CONSISTENT UNITS ARE ASSUMED.
C           GUESS    DO YOU WANT TO ENTER AN INITIAL GUESS FOR SC AND KB?
C                       YES OR NO IS THE APPROPRIATE RESPONSE.
C              SC    STORAGE COEFFICIENT OF AQUIFER (UNITLESS)
C              KB    TRANSMISSIVITY OF AQUIFER (GAL/DAY/FT) OR (L**2/T)
C               Q    CONSTANT PUMPAGE OF WELL (GAL/DAY) OR (L**3/T)
C               R    OBSWRVATION DISTANCE FROM WELL (FT) OR (L)
C               N    NUMBER OF DRAWDOWN-TIME PAIRS TO BE READ
C            S(I)    EXPERIMENTAL DRAWDOWN AT TIME I (FT) OR (L)
C            T(I)    THE ITH TIME AT WHICH AN EXPERIMENTAL MEASUREMENT
C                       FOR THE DRAWDOWN IS MADE (DAYS) OR (T)
C           SIGMA    THE RMS ERROR IN DRAWDOWN AFTER THE BEST
C                       FIT HAS BEEN OBTAINED
C-----------------------------------------------------------------------
      DIMENSION S(100), T(100),SP(100),DSDT(100),DSDSC(100)
      REAL KB
      CHARACTER GUESS, UNIT
C READ IN INITIAL DATA
      READ (5,105) GUESS, UNIT
 105  FORMAT ( 2A6 )
      READ (5,100) SC, KB, Q, R, N
C ECHO PRINT THE INITIAL DATA
      WRITE (6, 106 ) SC, KB, Q, R, N
 106  FORMAT ( ' THE INITIAL DATA WAS ' / 5H SC =, E15.8, 5H KB =, E15.8
     + /4H Q =,E15.8, 4H R =,E15.8, 4H N =, I5 )
C  READ IN DRAWDOWN-TIME PAIRS IN ORDER OF INCREASING TIME
      READ (5, 101) (S(I),T(I), I = 1, N)
C ECHO PRINT THE DRAWDOWN-TIME PAIRS
      WRITE (6, 107) (S(I),T(I), I = 1, N )
 107  FORMAT (' THE PUMP TEST DATA IN DRAWDOWN-TIME PAIRS IS '/(2E20.8))
 101  FORMAT ( 8F10.0 )
 100  FORMAT ( 4F10.0, I10 )
C CALCULATE THE INITIAL GUESS FOR KB AND SC IF NOT GIVEN
      NUM = 4
      IF (GUESS .EQ. 6HYES    ) GO TO 1
      SUMLNT = 0.0
      SMLNT2 = 0.0
      SUMSE = 0.0
      SSELNT = 0.0
      DO 50 I = 1,NUM
      II = N + 1 -I
      ALOGT = ALOG(T(II))
      SUMLNT = SUMLNT + ALOGT
      SMLNT2 = SMLNT2 + ALOGT**2
      SUMSE = SUMSE + S(II)
```

```
   50 SSELNT = SSELNT + S(II)*ALOGT
      SLOPE = (NUM*SSELNT-SUMSE*SUMLNT)/(NUM*SMLNT2-SUMLNT**2)
      CON = -(SLOPE*SUMLNT - SUMSE)/NUM
      KB =   Q/(SLOPE*4.0*3.14159)
      ALNTO = -CON/SLOPE
      SC = 4.0*KB/( R**2*EXP(.5772-ALNTO))
      IF (UNIT .EQ. 3HYES ) SC = SC/7.48
C PRINT THE CALCULATED GUESS FOR KB AND SC
      WRITE (6,110) KB, SC
  110 FORMAT (' THE CALCULATED GUESS FOR KB AND SC IS ', 2E16.8 )
    1 ICOUNT = 0
    5 TEMPKB = KB
      TEMPSC = SC
C USE SENSITIVITY ANALYSIS AND LEAST SQUATES TO FIND A BETTER KB AND SC
      DO 10 I = 1, N
   10 CALL THEIS(SC,KB,Q,R,T(I),SP(I),DSDT(I),DSDSC(I),UNIT)
      SSUS = 0.0
      SSUT = 0.0
      SUTUS=0.0
      SUSDIF  = 0.0
      SUTDIF = 0.0
      DO 15 I = 1, N
      SSUS = DSDSC(I)**2+SSUS
      SSUT = DSDT(I)**2+SSUT
      SUTUS = DSDSC(I)*DSDT(I) + SUTUS
      SUSDIF =  DSDSC(I)*(S(I)-SP(I))  + SUSDIF
   15 SUTDIF = DSDT(I)*(S(I)-SP(I)) + SUTDIF
      DELTSC = (SSUT*SUSDIF-SUTUS*SUTDIF)/(SSUS*SSUT-SUTUS**2)
      IF (DELTSC .LT. -.95*SC ) DELTSC = -.95*SC
      IF (DELTSC .GT. 2.0*SC ) DELTSC = 2.0*SC
      SC = SC + DELTSC
      IF (SC .GT. 1.0 ) SC = 1.0
      DELTKB = (SUTDIF-DELTSC*SUTUS)/SSUT
      IF (DELTKB .LT. -.95*KB ) DELTKB = -.95*KB
      IF (DELTKB .GT. 2.0*KB ) DELTKB = 2.0*KB
      KB = KB + DELTKB
      WRITE (6,104) KB, SC
  104 FORMAT( ' BEST FIT KB AND SC THIS ITERATION ARE ', 2E16.8 )
      ICOUNT = ICOUNT + 1
C IF IT DID NOT CONVERGE PRINT MESSAGE
      IF ( ICOUNT .GT. 20) GO TO 40
C DO ANOTHER ITERATION IF IT HASNT CONVERGED AND ITERATION LIMIT NOT
C   EXCEEDED.
      IF(ABS((TEMPKB-KB)/KB).GT..001.OR.ABS((TEMPSC-SC)/SC).GT..001)
     U  GO TO 5
C PRINT BEST FIT DRAWDOWN-TIME PAIRS IF CONVERGENCE OBTAINED
  108 FORMAT (' THE BEST FIT DRAWDOWN-TIME PAIRS ARE ' )
      WRITE (6,108)
      DO 20 I = 1, N
       CALL THEIS(SC,KB,Q,R,T(I),SP(I),DSDT(I),DSDSC(I),UNIT)
       WRITE (6,109) SP(I), T(I)
  109 FORMAT(2E20.8)
   20 CONTINUE
C CALCULATE THE RMS ERROR IN DRAWDOWN AFTER BEST FIT
       SUM = 0.0
       DO 30 I = 1, N
```

```
   30 SUM = SUM + (SP(I)-S(I))**2
      SIGMA = SQRT(SUM/N)
      WRITE(6,111) SIGMA
  111 FORMAT(' THE RMS ERROR FOR DRAWDOWN IS ', E20.8 )
      STOP
   40 WRITE (6,112)
  112 FORMAT(' DID NOT CONVERGE IN 20 ITERATIONS ')
      STOP
      END

      SUBROUTINE THEIS(SC,KB,Q,R,T,S,DSDT,DSDSC,UNIT)
C     PURPOSE   CALCULATES THE DRAWDOWN FOR A WELL PUMPING AT
C         CONSTANT DISCHARGE FROM AN INFINITE AQUIFER BY THE
C         THEIS EQUATION
C
C      ARGUMENTS (L IS ARBITRARY LENGTH, T IS ARBITRARY TIME)
C           SC     STORAGE COEFFICIENT FOR AQUIFER (UNITLESS)
C           KB     TRANSMISSIVITY OF AQUIFER (GAL/DAY/FT) OR (L**2/T)
C            Q     CONSTANT PUMPAGE OF WELL (GAL/DAY) OR (L**3/T)
C            R     OBSERVATION DISTANCE FROM WELL (FT) OR (L)
C            T     OBSERVATION TIME (DAYS) OR (T)
C            S     DRAWDOWN (FT) OR (L)
C         DSDT     SENSITIVITY W.R.T. TRANSMISSIVITY (FT**2*DAY/GAL) OR (T/L
C        DSDSC     SENSITIVITY W.R.T. STORAGE (FT) OR (L)
C         UNIT     SYSTEM OF UNITS; YES FOR GAL, DAY, FT; OTHERWISE
C                    CONSISTENT UNITS ARE ASSUMED
C ------------------------------------------------------------------
C
C CALCULATE THEIS SOLUTION
C THEIS EQUATION FROM 'INTRO TO HYDROLOGY' BY VIESSMAN PAGE 257
C RATIONAL APPROXIMATION FROM 'HANDBOOK OF MATH FUNCTIONS'
C    BY ABRAMOWITZ AND STEGUN PAGE 231
      REAL KB
      CHARACTER UNIT
      U =  R*R*SC/(4.0*KB*T)
      IF (UNIT .EQ. 6HYES     ) U = 7.48*U
      IF (U .LE. 0.0) GO TO 96
      IF (U .GT. 1.0) GO TO 86
      W= -ALOG(U)-.57721566+.99999193*U-.24991055*U*U+
     1.05519968*U*U*U-.00976004*U**4+.00107857*U**5
      GO TO 87
   86 W = (EXP(-U)/U)*(U*U+2.334733*U+.250621)/
     1(U*U+3.330657*U + 1.681534)
   87 S = (Q/(4.0*3.14159*KB))*W
      DSDT = (Q/(4.0*3.14159*KB**2))*(-W + EXP(-U))
      DSDSC=-(Q/(4.0*3.14159*KB*SC))*EXP(-U)
      RETURN
   96 PRINT 13
   13 FORMAT ( ' DRAWDOWN UNDEFINED U TOO SMALL ' )
   99 STOP
      END
```