DETERMINATION OF HYDRAULIC PARAMETERS OF SEMI-INFINITE AQUIFERS USING MARQUARDT ALGORITHM

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ABSTRACT

DETERMINATION OF HYDRAULIC PARAMETERS OF SEMI-INFINITE AQUIFERS USING MARQUARDT ALGORITHM

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In this study, transmissivity and storage coefficient of a semi-infinite, confined, homogeneous and isotropic aquifer, where the flow is one-dimensional and linear, are determined using Marquardt algorithm, considering two independent cases: constant drawdown in the adjacent stream; or constant discharge from the aquifer due to pumping at a constant rate. In the first case piezometric head and discharge measurements are utilized. Hydraulic diffusivity, which is the ratio of transmissivity to storage coefficient, is determined from piezometric head measurements; whereas their product is determined from discharge measurements. Then, the two parameters are calculated easily. In the second case piezometric head observations are utilized only and transmissivity and storage coefficient are determined simultaneously. Convergence to true values is very fast for both cases even for poor initial estimates.

Three examples, two using synthetic data for both cases and one using actual field data for the second case, are presented. Conventional type-curve matching method is used for comparison of the results. It is observed that the results of Marquardt algorithm are in a reasonable agreement with those of type-curve matching method.

Keywords: Stream-Aquifer Interaction, Inverse Problem, Identification Problem, Aquifer Parameters, Marquardt Algorithm, One-dimensional Flow.

ÖZ

YARI-SONSUZ AKİFERLERİN HİDROLİK PARAMETRELERİNİN MARQUARDT ALGORİTMASI İLE BELİRLENMESİ

TAŞKAN, Cüneyt
Yüksek Lisans, İnşaat Mühendisliği Bölümü
Tez Danışmanı: Prof. Dr. Halil ÖNDER

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Bu çalışmada, akımın bir boyutlu ve lineer olduğu, yarı-sonsuz, basınçlı, homojen ve izotrop bir akiferin iletim ve depolama katsayıları; Marquardt algoritması kullanılarak iki bağımsız durum için belirlenmiştir: bitişik olan akarsunun su seviyesindeki sabit düşme; veya sabit pompajdan kaynaklanan akiferden sabit debi. İlk durumda piyezometrik seviye ve debi ölçümlerinden faydalanılmıştır. Piyezometrik seviye ölçümlerinden hidrolik difüzivite, yani iletim katsayısının depolama katsayısına oranı saptanırken, debi ölçümlerinden bu iki parametrenin çarpımı saptanmıştır. Bu sayede her iki parametre de kolaylıkla hesaplanmıştır. İkinci durumda ise sadece piyezometrik seviye ölçümleri kullanılarak iletim ve depolama katsayıları eşzamanlı olarak saptanabilmiştir. Her iki durumda zayıf başlangıç değerleri için bile çok hızlı bir biçimde gerçek değerlere ulaşılmıştır.

Her iki durum için sentetik verinin kullanıldığı birer örnek, ayrıca ikinci durum için gerçek verinin kullanıldığı bir örnek olmak üzere toplam üç örnek sunulmuştur. Sonuçların karşılaştırılması amacıyla geleneksel tip eğri yöntemi kullanılmıştır. Marquardt algoritmasının sonuçlarıyla tip eğri yönteminin sonuçlarının makul bir uyumluluk içerisinde olduğu gözlenmiştir.

Anahtar Kelimeler: Akarsu-Akifer Etkileşimi, Ters Problem, Tanımlama Problemi, Akifer Parametreleri, Marquardt Algoritması, Bir Boyutlu Akım.

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To my family

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b	Saturated thickness of the aquifer
d	Displacement direction vector
f(**p**)	Difference between observed and calculated drawdown (cases 1 and 2) and squares of discharge (case 1) values using parameter vector **p**
f	Vector containing differences between observed and calculated values
g	Gradient vector
h(x,t)	Piezometric head within the aquifer
h_0	Initial water stage in the stream
i	Hydraulic gradient
k	Subscript denoting the iteration index
m	time step for measurements
p	Optimization parameter
p^*	True optimization parameter
p	Parameter vector containing optimization parameters
$\mathbf{p}^*$	True parameter vector containing true optimization parameters
$\mathbf{p}_{OPT}$	Optimized parameter vector that minimizes the residual squares
$\hat{\mathbf{p}}$	Parameter vector that makes gradient **g** equal to zero
s(x,t)	Drawdown within the aquifer
s	Step size along displacement direction vector **d**
$s_m^c(\alpha)$	Drawdown computed for time m using α

$s_m^c(\mathbf{p})$	Drawdown computed for time m using parameter vector **p**
s_m^{obs}	Drawdown observed at time m
s_0	Constant drawdown in the stream
t	Time
u	$=\frac{x}{\sqrt{4\alpha t}}$ (Eq. 2.5)
x	Horizontal distance from the interface into the aquifer
A	Cross sectional area corresponding to flow in the aquifer
A	Matrix containing derivatives of parameters
$D(u)_h$	Dimensionless drain function for constant drawdown
$D(u)_q$	Dimensionless drain function for constant discharge
E(**p**)	Residual squares associated to parameter vector **p** (Eq. (3.1))
G	Hessian matrix
$H_m^c(\mathbf{p})$	Head computed at time m using parameter vector **p**
H_m^{obs}	Head observed at time m
I	Identity matrix
K	Hydraulic conductivity
L	Length of the stream or fracture
M	Total number of measurements
N	Number of parameters to be optimized
Q	Total discharge from one stream bank
$Q_m^c(\beta)$	Discharge computed for time m using β
Q_m^{obs}	Discharge observed at time m
Q_0	Constant discharge from both banks per unit stream length (case 2, Eq. (2.27))
Q_T	Total discharge from both stream banks (=2Q)
Q(t)	Time dependent discharge from both banks per unit stream length (case 1, Eq. 2.19)

S	Storage coefficient
S^*	True storage coefficient
S_0	Initial estimate of storage coefficient
S_{OPT}	Optimized storage coefficient
T	Transmissivity
T^*	True transmissivity
T_0	Initial estimate of transmissivity
T_{OPT}	Optimized transmissivity
V	$=\sqrt{\frac{t}{\pi S}}T^{-\frac{1}{2}}e^{-\frac{x^2ST^{-1}}{4t}}$ (section 3.4.2)
W	$=\frac{x}{2T}\left(\operatorname{erf}\sqrt{\frac{x^2S}{4Tt}}-1\right)$ (section 3.4.2)
W_m	Weight associated to measurement m
Y	$=\sqrt{\frac{t}{\pi}}T^{-\frac{1}{2}}S^{-\frac{1}{2}}e^{-\frac{x^2S}{4Tt}}$ (section 3.4.2)

α	Hydraulic diffusivity
α^*	True hydraulic diffusivity
α_0	Initial estimate of hydraulic diffusivity
α_{OPT}	Optimized hydraulic diffusivity
β	Product of transmissivity and storage coefficient
β^*	True value of product of transmissivity and storage coefficient
β_0	Initial estimate of product of transmissivity and storage coefficient
β_{OPT}	Optimized product of transmissivity and storage coefficient
ε	Prescribed convergence criteria
φ	Square of discharge value
$\varphi_m^c(\beta)$	Square of discharge calculated at time m using β
φ_m^{obs}	Square of discharge observed at time m

λ	Convergence factor
$\Delta\mathbf{p}$	Respective increment in parameter vector **p**
ΔT	Respective increment in transmissivity
ΔS	Respective increment in storage coefficient
$\Delta\alpha$	Respective increment in hydraulic diffusivity
$\Delta\beta$	Respective increment in product of transmissivity and storage coefficient

CHAPTER 1

INTRODUCTION

1.1 Problem Definition

The beginning of the human's effort on understanding and benefiting from the nature coincides with the beginning of mankind history. Being the most vital source of life, water has always had a priority upon other natural resources.

The necessity of utilizing and/or controlling every possible water resource arouse with the increasing population, on the other hand, developing technology and advanced engineering methods enabled people to apply the laws of nature in order to supply water by building structures and establishing large scale networks to control and distribute it, in a much more efficient way. Groundwater, and consequently aquifers, gains great importance at this point as water resources and risk control agent; considering stream-aquifer interaction.

Assumed as linear and time-invariant systems, aquifers behave uniquely depending on their hydraulic parameters. This states that when the response of an aquifer to a constant drawdown or a constant discharge is obtained, then the response of the particular aquifer to any pattern of excitation can be obtained. In case of a dam break, a sudden drop occurs in the reservoir, and this case illustrates a condition where there is a constant drawdown in the upstream water surface. Constant discharge, which is a more frequent case, occurs usually due to pumping from the stream or from a fracture within the aquifer. Fig. 1.1 shows a schematic view of this type of stream-aquifer interaction.

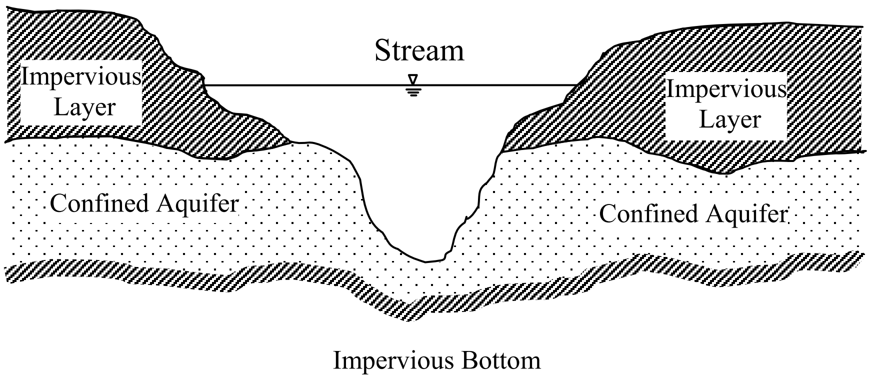

Figure 1.1 Definition sketch of stream-aquifer system

The purpose of this study is to bring an alternative solution to one of the three main problems that exist in groundwater systems: detection, identification and prediction. In detection problem, system (or aquifer) parameters and output are known while the input is to be “detected”. The term “input” refers to any excitation done to the aquifer, which may be a drop or a rise in the adjacent stream, or pumping. Similarly, the term “output” refers to the response of the aquifer, which may be the drawdown in the aquifer or the discharge to or from the aquifer. Identification problem (inverse problem) is the case when system parameters are unknown and they are to be “identified” using the known input (excitation) and corresponding output (response) of the aquifer. In a prediction problem input and system parameters are known and output needs to be “predicted”.

The case in question in the present work is the identification problem in a semi-infinite confined aquifer that is in a permanent hydraulic connection with a stream, as shown in Fig. 1.1. This is essentially a study of the interaction between the stream and the aquifer.

1.2 Literature Review

The literature contains a great amount of publications about determination of the aquifer parameters and most of them relate one or both of the aquifer parameters to pump test data. Stream-aquifer interaction was investigated by some authors by Laplace transform method but only one parameter was determined; transmissivity, storage coefficient or the division of these, namely aquifer diffusivity.

The mechanism of the interplay between groundwater recharge and depletion is examined in Venetis (1971), and simple practical methods are developed for the estimation of infiltration from groundwater level observations.

Morel-Seytoux (1988) suggests an approach to describe the various interactions between soil, aquifer and stream in a simplified but essentially physical and integrated manner considering multiple integration in time and space, with emphasis on stream-aquifer interaction.

Morel-Seytoux et al. (1985) presented a procedure to predict the base flow component of streamflow in a watershed using the concept of convolution integral and discrete kernel generation.

Singh and Sagar (1977) presented an analytical method to determine aquifer diffusivity from the measurements at the boundary of interaction between a stream and an aquifer using the Boussinesq equation as a mathematical model to describe the response of a rising stream on the water level in the aquifer.

Chander et al. (1981) used Marquardt algorithm for estimating aquifer parameters from pump test data in leaky and nonleaky aquifers for radial flow.

Mishra and Jain (1999), using both the Laplace transform approach and Marquardt's least-squares optimization technique, estimated hydraulic diffusivity of an aquifer. The measurements of stream stage during passage of a flood wave and the consequent water level fluctuations in a piezometer in the vicinity of the stream were used.

Singh (2001) proposed a derivative-based optimization method for the identification of aquifer parameters from the drawdowns observed at an observation well for radial flow.

Singh (2002) presented an optimization method for simultaneous estimation of aquifer parameters and well loss parameters for radial flow during a variable rate pumping or multiple step pumping test.

Swamee and Singh (2003) proposed a method for the estimation of aquifer hydraulic diffusivity from observed piezometric head variation in stream stage using the Fourier series representation for arbitrary stream stage variation.

Morel-Seytoux and Zhang (1990) developed a stream-aquifer model describing the system mathematically and treating the interaction between the stream and the aquifer as a time-dependent third type (Cauchy) boundary condition.

Johns et al. (1992) selected a conceptual aquifer model and estimated aquifer parameters by nonlinear least-squares analysis of pump test response.

Rowe (1960) applied the Laplace transform and derived an equation from which transmissibility and coefficient of storage of an aquifer can be estimated, assuming a linear change with time of a nearby surface body of water.

Jenkins and Prentice (1982) investigated linear groundwater flow in some fractured rocks, and presented various field data to verify the concept of linear flow in fractured rocks.

Tomasko (1987) used the linear flow model of Jenkins and Prentice (1982) to determine the orientation of a vertical fracture or a linear feature in fractured rock aquifer, and emphasized linear flow rather than radial flow in the aquifer in the vicinity of the fracture.

A mathematical description of groundwater flow toward vertical fractures is presented by Şen (1986). Type curves and recovery type curves are also given with the application of the method for available data in the literature.

A springflow model has been developed, which can simulate springflow for time variant recharge by Bhar and Mishra (1997). The inverse problem, which contains linear recharge terms and nonlinear depletion terms, has also been solved using Newton-Raphson method for solving a set of nonlinear equations.

Venetis (1968), using the Laplace transform, gives the impulse response and the response to a unit step function of the one-directional semi-infinite aquifer, derived from the approximate partial differential equation of the groundwater flow.

The development of computational techniques for the linear synthesis of monotone hydrologic systems from coincident discrete-time records of the input and output variables is presented by Eagleson et al. (1966). Unit hydrograph analogy is examined and linear programming methods are used to obtain physically realizable unit hydrographs.

Venetis (1970) examined the response to characteristic piezometric height inputs of aquifers of finite dimensions via the linear differential equation of groundwater flow and the Laplace transform.

Önder (1994) gives a type–curve matching method, for the determination of aquifer parameters from water level observations in a finite confined aquifer and discharge measurements at a line sink where there is a constant drawdown.

Lohman (1972) described two drain functions and type-curves for nonsteady flow in a semi-infinite nonleaky aquifer under constant drawdown and constant discharge conditions. Type–curve matching method is used as a quick reference for comparison of validity of the output in this thesis.

Although a number of works related to the parameter estimation in radial flow exist in the literature, the estimation of transmissivity and the storage coefficient independently for linear (nonradial) flow have been given less attention. This thesis aims to fill this gap using Marquardt algorithm for constant drawdown and constant discharge separately.

1.3 Objectives of the Thesis

The objective of this study is to device an optimization methodology, based on Marquardt algorithm, for the identification of hydraulic parameters of a semi-infinite confined aquifer for two boundary conditions: constant drawdown in the adjacent stream, and constant discharge due to pumping. Conventional type curve matching method will be used for comparison of the results.

1.4 Description of the Thesis

This thesis is composed of five chapters. In Chapter 2, theoretical background of the problem is given. Mathematical models and the analytical solutions are presented, and the basic equations to be used in the algorithm are derived.

Chapter 3 is dedicated to the formulation of Marquardt algorithm for the determination of aquifer parameters. The procedure to introduce collected data into the algorithm is given.

In Chapter 4, the application of the proposed method is presented, and the corresponding results are discussed.

The study is finalized in Chapter 5 by summarizing the work. A certain number of conclusions and recommendations for future studies are given.

Appendix contains some important iteration tables.

CHAPTER 2

THEORETICAL BACKGROUND

2.1 General

The problem that will be investigated is the determination of transmissivity and storage coefficient of a semi-infinite confined aquifer subject to a permanent hydraulic connection with a stream, using measurements of drawdown in an observation well in the aquifer and discharge into or from the aquifer. Two cases will be considered: in the first case, the flow results from a sudden drop in the stream stage; while it is induced by a constant pumping in the second case. The aquifer is of semi-infinite horizontal extent. The interface between the stream and the aquifer is vertical. The aquifer is homogeneous and isotropic and has unchanging properties (hydraulic conductivity, K, and storage coefficient, S). Initially it is assumed that the aquifer and the stream are in equilibrium with each other, and the drawdown is zero everywhere.

2.2 Constant Drawdown Case

When there occurs a constant drop as in the present study, the stream stage drops a finite amount instantaneously, and stays at this level indefinitely thereafter. The aquifer responds by lowering its head and discharging into the stream. As time proceeds the piezometric head in the aquifer approaches the water level in the stream. Water continues to flow into the stream until the piezometric level in the aquifer equals the water stage in the stream.

It is assumed that the stream, which is perfectly straight of uniform rectangular cross section, exerts control over the aquifer. In other words the stream's prescribed stage is an imposed boundary condition on the groundwater. This very special type of step drawdown can be observed in case of a dam break. The idealized form of this case is shown in Fig. 2.1:

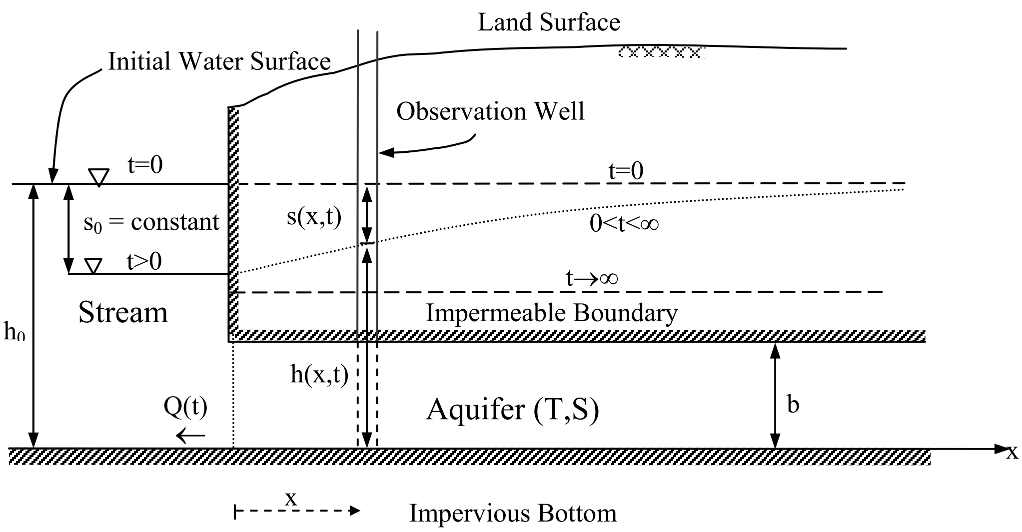

Figure 2.1 Constant drawdown case

The horizontal distance from the interface into the aquifer is denoted by x and the initial water stage in the stream is denoted by h_o. Time, t, is measured since the onset of change in stream stage. The sudden drop in the stream is constant with an amount of s_0, while the drawdown within the aquifer is a function of x and t and is denoted by s(x,t). The piezometric head within the aquifer is h(x,t) and the discharge per unit stream length from the aquifer into the stream is Q(t). It can be inferred from the figure that the sum of s(x,t) and h(x,t) always yields h_o. L is the stream length measured perpendicular to the figure plane and b is the aquifer thickness.

2.2.1 Mathematical Model

To investigate a groundwater flow problem, its mathematical statement must be developed. A complete mathematical statement consists of five parts (Bear, 1979). These are,

i)	Flow region:	$0 \le x \le \infty$	(2.1)
ii)	The dependent variable:	s(x,t)	
iii)	Governing partial differential equation:	$\alpha \frac{\partial^2 s}{\partial x^2} = \frac{\partial s}{\partial t}$	(2.2)
	where α=T/S (hydraulic diffusivity)		
iv)	Initial condition:	$s(x,0) = 0$	(2.3)
v)	Boundary conditions:	$s(0,t) = s_0$	(2.4a)
		$s(\infty,t) = 0$	(2.4b)

The governing partial differential equation (GDE) in Eq. (2.2) is the one-dimensional linearized Boussinesq equation and is used to describe unsteady flows.

2.2.2 Analytical Solution

The solution to this special boundary value problem of constant drawdown is obtained by defining a new variable

$$u = \frac{x}{\sqrt{4\alpha t}} \qquad (2.5)$$

which permits Eq. (2.2) to be written as the ordinary differential equation

$$\frac{d^2s}{du^2}+2u\frac{ds}{du}=0 \quad (2.6)$$

subject to the conditions that $s=s_0$, $u=0$, and $s=0$, $u=\infty$. In this form the groundwater equation has the same structure as the heat conduction equation (Carslaw and Jaeger, 1959). Integration of Eq. (2.6) is given as

$$s(x,t)=s_0[1-\mathrm{erf}(u)] \quad (2.7)$$

where erf(u) is known as "error function" defined by

$$\mathrm{erf}(u)=\frac{2}{\sqrt{\pi}}\int_0^u e^{-y^2}dy \quad (2.8)$$

Eq. (2.7) may be written using the "complementary error function" which is

$$\mathrm{erfc}(u) = 1-\mathrm{erf}(u) \quad (2.9)$$

The drawdown equation becomes

$$s(x,t)=s_0\mathrm{erfc}(u)=s_0\mathrm{erfc}\left(\frac{x}{\sqrt{4\alpha t}}\right) \quad (2.10)$$

For argument zero (at $t=\infty$ in Eq. (2.5)) the complementary error function takes the value 1, and for an infinite value of the argument (at $t=0$ in Eq. (2.5)) it takes the value 0; behaving as expected when compared with the actual physical response of an aquifer.

The discharge from the aquifer to the channel is obtained by applying Darcy's law, as follows:

$$Q = A.K.i \quad (2.11)$$

where Q is the total volume of water flowing from one stream bank into the stream per unit time, A is the cross sectional area corresponding to the flow, namely Lb, where L is the reach length in the stream direction and b is the thickness, K is the hydraulic conductivity and i is the hydraulic gradient, namely $-\partial s/\partial x$. Since the concern is the discharge at the interfaces from both banks into the stream, x must be assigned a value of zero and Eq. (2.11) must be multiplied by a factor of two. Combining the above expansions, Eq. (2.11) takes the form:

$$Q_T = -2LbK\frac{\partial s}{\partial x}\bigg|_{x=0} \tag{2.12}$$

where Q_T is the total discharge from both stream banks. A true return flow is positive while a negative return flow means a stream loss. For a step drawdown, $\partial s/\partial x$ is negative and Q_T is positive, which means the flow is from the aquifer to the stream. In order to calculate $\partial s/\partial x$ from Eq. (2.10) the chain rule of differentiation is applied. The derivative of Eq. (2.10) is taken with respect to the argument of the complementary error function, and then the derivative of the argument is taken with respect to x.

$$\frac{\partial s}{\partial x} = \frac{\partial s}{\partial u}\frac{\partial u}{\partial x} \tag{2.13}$$

The derivative of s with respect to u, considering Eqs. (2.8) and (2.10) is

$$\frac{\partial s}{\partial u} = -s_0\frac{2}{\sqrt{\pi}}e^{-u^2} = -\frac{2s_0}{\sqrt{\pi}}e^{-\frac{x^2}{4\alpha t}} \tag{2.14}$$

The derivative of u with respect to x, considering Eq. (2.5) is

$$\frac{\partial u}{\partial x} = \frac{1}{\sqrt{4\alpha t}} \tag{2.15}$$

The product of Eqs. (2.14) and (2.15) yields

$$\frac{\partial s}{\partial x} = \frac{-s_0 e^{-\frac{x^2}{4\alpha t}}}{\sqrt{\alpha\pi t}} \tag{2.16}$$

Evaluation of Eq. (2.16) at the interface gives

$$\frac{\partial s}{\partial x}\bigg|_{x=0} = -\frac{s_0}{\sqrt{\alpha\pi t}} \tag{2.17}$$

Substituting Eq. (2.17) into Eq. (2.12) knowing the fact that bK=T, the total discharge becomes

$$Q_T = \frac{2s_0LT}{\sqrt{\alpha\pi t}} \tag{2.18}$$

The flow rate per unit length of the stream from both banks, which is denoted by Q(t), is

$$Q(t) = \frac{Q_T}{L} = \frac{2s_0 T}{\sqrt{\alpha \pi t}} \qquad (2.19)$$

Letting $\beta = T.S$,

$$Q(t) = \frac{2s_0\sqrt{\beta}}{\sqrt{\pi t}} \qquad (2.20)$$

Eqs. (2.10) and (2.20), which are obtained by analytical solution of the mathematical model (Eqs. 2.1 - 2.4), are conventionally known as analytical model, and they will be used for simulation for constant drawdown case.

2.3 Constant Discharge Case

A conceptual model of the particular case is shown in Fig. 2.2. Constant discharge occurs mainly due to pumping from the stream directly as shown in Fig. 2.2, or from a well that penetrates a fracture having permeability many orders of magnitude greater than the permeability of the surrounding aquifer, as in Fig. 2.3.

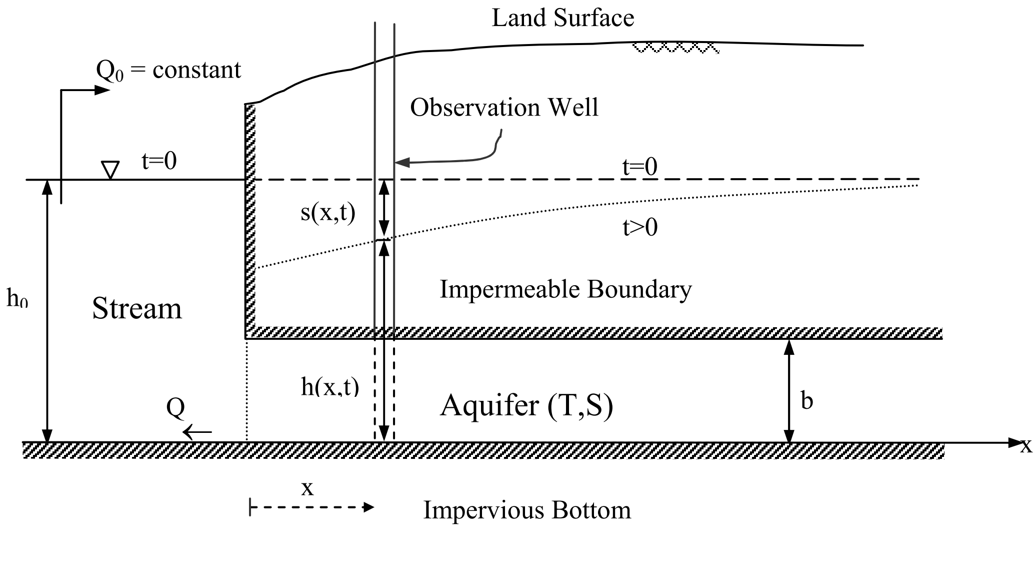

Figure 2.2 Constant discharge case

The terminology is the same as in the previous case except that there is a constant total pumping rate Q_T having dimensions of L^3/T, instead of a constant drawdown in the stream. Consequently, the total flow from one bank, Q, and the flux (or pumping rate), Q_0, from the aquifer per unit length are also constant. The drop in the stream stage occurs as a result of extraction of water during pumping period. It is assumed in this case that the discharge is an imposed boundary condition on the groundwater.

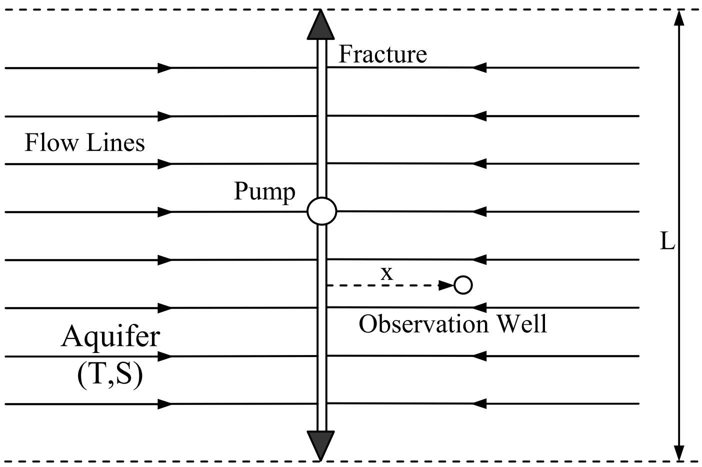

Figure 2.3 Flow in fractured rock aquifer

The flow of groundwater in fractured rock aquifer under constant pumping rate is shown in Fig. 2.3. Jenkins and Prentice (1982) and Şen (1986) stated that the flow from a semi-infinite confined aquifer to such a fracture exhibits linear flow characteristics rather than radial flow. The aquifer is isotropic, homogeneous and bisected by a highly permeable, vertical fracture of length L, which has been fully penetrated by a well. When the well is pumped, the water level in the fracture declines, inducing flow into the fracture from the aquifer. The open fracture is a planar production surface that is an extension of the well itself. The well and its hydraulically connected production surface are here called an extended well (Jenkins and Prentice (1982)). The flow lines in the aquifer is linear and laminar toward the extended well; and the fracture is assumed to have no significant storage capacity. Drawdown is a function of the perpendicular distance, x, from the well, and the time, t.

2.3.1 Mathematical Model

The mathematical model for constant discharge case is given by Jenkins and Prentice (1982) as:

i) Flow region: $0 \le x \le \infty$ (2.21)

ii) The dependent variable: $s(x,t)$

iii) Governing partial differential equation: $\alpha \frac{\partial^2 s}{\partial x^2} = \frac{\partial s}{\partial t}$ (2.22)

iv) Initial condition: $s(x,0) = 0$ (2.23)

v) Boundary conditions: $-LT \frac{\partial s(0,t)}{\partial x} = \frac{Q_T}{2}$ (2.24a)

$s(\infty,t) = 0$ (2.24b)

The boundary condition stated in Eq. (2.24a) is the application of Darcy's law for one bank of the stream (or one side of the fracture), evaluated at x=0.

2.3.2 Analytical Solution

Analytical solution of Eq. (2.22) subject to initial and boundary conditions defined in Eqs. (2.23), (2.24a) and (2.24b) is given by Carslaw and Jaeger (1959) using the method of Laplace transforms as:

$$s(x,t) = \frac{Q_T}{2LT}\left\{\sqrt{\frac{4Tt}{\pi S}}e^{-u^2} + x\left[\mathrm{erf}(u) - 1\right]\right\} \quad (2.25)$$

Drawdown at the stream-aquifer interface (or just at the fracture) can be obtained by equating x=0 (which also makes u=0) in the equation above:

$$s(0,t) = \frac{Q_T \sqrt{t}}{L\sqrt{\pi TS}} \qquad (2.26)$$

Discharge from both banks per unit length has already been defined above as

$$Q_0 = \frac{Q_T}{L} \qquad (2.27)$$

Drawdown for constant discharge is then

$$s(x,t) = \frac{Q_0}{2T}\left\{\sqrt{\frac{4Tt}{\pi S}}e^{-u^2} + x\left[\mathrm{erf}(u) - 1\right]\right\} \qquad (2.28)$$

or

$$s(x,t) = \frac{Q_0}{2T}\left[\sqrt{\frac{4Tt}{\pi S}}e^{-u^2} - x.\mathrm{erfc}(u)\right] \qquad (2.29)$$

Similar to Eqs. 2.10 and 2.20, in constant discharge case, Eqs. (2.26) and (2.29) represent the analytical model of the problem, and may be used for simulation.

CHAPTER 3

DETERMINATION OF AQUIFER PARAMETERS

3.1 General

To estimate transmissivity and storage coefficient of a semi-infinite confined aquifer, a least-squares optimization method developed by Marquardt (1963) is used. The Marquardt algorithm has been applied by several investigators to determine the aquifer parameters of a confined aquifer from pumping test data (Chander et al., 1981; Johns et al., 1992).

3.2 General Description of Optimization Algorithm

Basic materials presented in this section, in section 3.3 and in section 3.4 up to section 3.4.1, where Marquardt algorithm is formulated for the general case, are taken from the electronic book by Karvonen (2002). The formulation is explained thoroughly in order to give the reader a general perspective.

An inverse problem cannot be solved unless the corresponding direct (or forward) problem has been solved a priori. This involves simulation of the system using initial estimates and comparing the output with the observed values. This comparison is performed usually by minimizing the squares of the difference between observed and computed parameters. The main criterion in optimization algorithms for parameter estimation is the Output Least Squares (OLS) defined by

$$E(\mathbf{p}) = \sum_{m=1}^{M} W_m^2 \left[H_m^c(\mathbf{p}) - H_m^{obs}\right]^2 \tag{3.1}$$

where $H_m^c(\mathbf{p})$ is the calculated head, H_m^{obs} is the observed head, M is total number of measurements, W_m is a weight associated to measurement m, and $\mathbf{p}$ is the parameter vector defined as

$$\mathbf{p} = \begin{bmatrix} p_1 \\ p_2 \\ \vdots \\ p_N \end{bmatrix} \tag{3.2}$$

and components p_1, p_2, … p_N need to be estimated. $E(\mathbf{p})$ is the sum of squares of the difference between calculated and observed head (residual square error) associated to parameter vector $\mathbf{p}$ and N is the number of parameters to be optimized. If $E(\mathbf{p}_2) < E(\mathbf{p}_1)$, then parameter vector $\mathbf{p}_2$ is a better estimate than $\mathbf{p}_1$.

The general optimization procedure consists of the steps below (Karvonen, 2002):

1. Input observation data H^{obs}
2. Give initial values for parameters, $\mathbf{p}_0$
3. Solve the forward problem (i.e. simulation with the given parameters). Get $H^c(\mathbf{p}_0)$
4. Calculate $E(\mathbf{p}_0)$
5. If $E(\mathbf{p}_0) < \varepsilon$ then end; if not, then modify $\mathbf{p}_0$ by the optimization algorithm to obtain new estimate $\mathbf{p}_1$ and return to step 3.

The symbol ε in the last step stands for the prescribed convergence criteria. The aim is to find a specific set of parameters $\mathbf{p}_{OPT}$ such that

$$E(\mathbf{p}_{OPT}) = \min E(\mathbf{p}) \tag{3.3}$$

To reach a convergence, the forward problem is solved several times. In other words, the inverse problem is solved indirectly through the solution of the forward problem until the true parameter vector **p*** is reached or approached with a reasonable error. True parameter vector contains the true aquifer parameters p_1^*, p_2^*, ... p_N^* to be reached:

$$\mathbf{p}^* = \begin{bmatrix} p_1^* \\ p_2^* \\ \vdots \\ p_N^* \end{bmatrix} \tag{3.4}$$

The percentage error of the estimated parameter p at the end of the optimization process is defined conventionally by the following equation:

$$\text{Error}(p) = \frac{p_{OPT} - p^*}{p^*} \times 100 \tag{3.5}$$

Since the optimization problem involves nonlinear equations, the next section is devoted to formulation of the nonlinear optimization problem.

3.3 Formulation of the Nonlinear Optimization Problem

For the general formulation, an N-dimensional optimization problem is considered, where the objective function E(**p**) is given in Eq. (3.1). If function E(**p**) is second-order differentiable, the following are necessary conditions for $\hat{\mathbf{p}}$ being a local minimum of E(**p**) (Karvonen, 2002):

- First derivative of E with respect to $\mathbf{p}$ (gradient $\mathbf{g}$) vanishes at $\hat{\mathbf{p}}$:

$$\left.\frac{\partial E}{\partial \mathbf{p}_n}\right|_{\hat{\mathbf{p}}} = 0 \qquad (n=1,\ldots,N) \tag{3.6}$$

- Second derivative of E with respect to $\mathbf{p}$ (Hessian matrix $\mathbf{G}$) is a positive semi-definite matrix.

The first derivative is gradient $\mathbf{g}$:

$$\mathbf{g} = \nabla E(\mathbf{p}) = \begin{bmatrix} \dfrac{\partial E}{\partial p_1} \\ \dfrac{\partial E}{\partial p_2} \\ \vdots \\ \dfrac{\partial E}{\partial p_N} \end{bmatrix} \tag{3.7}$$

The second derivative is Hessian matrix $\mathbf{G}$:

$$\mathbf{G} = \nabla^2 E(\mathbf{p}) = \begin{bmatrix} \dfrac{\partial^2 E}{\partial p_1^2} & \dfrac{\partial^2 E}{\partial p_1 \partial p_2} & \cdots & \dfrac{\partial^2 E}{\partial p_1 \partial p_N} \\ \dfrac{\partial^2 E}{\partial p_1 \partial p_2} & \dfrac{\partial^2 E}{\partial p_2^2} & \cdots & \dfrac{\partial^2 E}{\partial p_2 \partial p_N} \\ \vdots & \vdots & & \vdots \\ \dfrac{\partial^2 E}{\partial p_1 \partial p_N} & \dfrac{\partial^2 E}{\partial p_2 \partial p_N} & \cdots & \dfrac{\partial^2 E}{\partial p_N^2} \end{bmatrix} \tag{3.8}$$

In the identification of model parameters, objective function $E(\mathbf{p})$ defined in Eq. (3.1) depends on model output; therefore, an explicit expression for $\nabla E(\mathbf{p})$ may not be obtained and Eq. (3.6) may not be solved directly. For practical optimization problems, $\nabla E(\mathbf{p})$ has to be obtained numerically and the solution of the problem is iterative as follows:

1. Choose initial guess $\mathbf{p}_0$.
2. Designate a way to generate a search sequence:

$\mathbf{p}_0, \mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_k$

such that $E(\mathbf{p}_k) < E(\mathbf{p}_{k-1})$ for all iteration index k.

3. Check the convergence and if it is satisfied, then end the search procedure, and a local minimum is approximately achieved.

Search sequence has a general form:

$$\mathbf{p}_k = \mathbf{p}_{k-1} + s_k \mathbf{d}_k \quad (3.9)$$

where $\mathbf{p}_k$ is the new parameter vector computed using the previous parameter vector $\mathbf{p}_{k-1}$, s_k is a step size along a direction that is called displacement direction $\mathbf{d}_k$. The key problem of the parameter optimization procedure is how to determine s_k and $\mathbf{d}_k$. Marquardt algorithm uses Newton's method for the evaluation of s_k and $\mathbf{d}_k$, which uses the Hessian matrix multiplied by the negative gradient as the search direction, and selects a unit amount of step size. This makes

$$\mathbf{d}_k = -\mathbf{G}_k^{-1} \mathbf{g}_k \quad (3.10)$$

and

$$s_k = 1 \quad (3.11)$$

Then Eq. (3.9) becomes

$$\mathbf{p}_k = \mathbf{p}_{k-1} - \mathbf{G}_k^{-1} \mathbf{g}_k \quad (3.12)$$

3.4 Formulation of Marquardt Algorithm

The algorithm was developed by Marquardt (1963). Derivation of the algorithm begins with modifying the OLS equation given in Eq. (3.1). The equation in question can be rewritten in an alternative form:

$$E(\mathbf{p}) = \sum_{m=1}^{M} f_m^2(\mathbf{p}) \quad (3.13)$$

where

$$f_m(\mathbf{p}) = W_m\left[H_m^c(\mathbf{p}) - H_m^{obs}\right] \qquad (3.14)$$

The first order derivatives of E(**p**) are

$$\frac{\partial E}{\partial p_i} = 2\sum_{m=1}^{M} f_m \frac{\partial f_m}{\partial p_i} \qquad (i=1,\ldots,N) \qquad (3.15)$$

In an expanded form, Eq. (3.15) can be written as:

$$\frac{\partial E}{\partial p_i} = 2\left[f_1 \frac{\partial f_1}{\partial p_i} + f_2 \frac{\partial f_2}{\partial p_i} + \cdots + f_M \frac{\partial f_M}{\partial p_i} \right] \qquad (3.16)$$

The set of equations for the first order derivatives are obtained by writing Eq. (3.16) explicitly:

$$\frac{\partial E}{\partial p_1} = 2\left[f_1 \frac{\partial f_1}{\partial p_1} + f_2 \frac{\partial f_2}{\partial p_1} + \cdots + f_M \frac{\partial f_M}{\partial p_1} \right] \qquad (3.17a)$$

$$\frac{\partial E}{\partial p_2} = 2\left[f_1 \frac{\partial f_1}{\partial p_2} + f_2 \frac{\partial f_2}{\partial p_2} + \cdots + f_M \frac{\partial f_M}{\partial p_2} \right] \qquad (3.17b)$$

$$\vdots$$

$$\frac{\partial E}{\partial p_N} = 2\left[f_1 \frac{\partial f_1}{\partial p_N} + f_2 \frac{\partial f_2}{\partial p_N} + \cdots + f_M \frac{\partial f_M}{\partial p_N} \right] \qquad (3.17c)$$

The second derivatives are

$$\frac{\partial^2 E}{\partial p_i \partial p_j} = 2\sum_{m=1}^{M}\left[\frac{\partial f_m}{\partial p_i}\frac{\partial f_m}{\partial p_j} + f_m \frac{\partial^2 f_m}{\partial p_i \partial p_j} \right] \quad (i=1,\ldots,N;\ j=1,\ldots,N) \qquad (3.18)$$

In Eq. (3.18) $f_m(\mathbf{p})$ is a residual. When **p** is not too far from the optimum value, it can be assumed that the value of $f_m(\mathbf{p})$ is small and the second order terms of the right-hand side of Eq. (3.18) can be ignored. Thus

$$\frac{\partial^2 E}{\partial p_i \partial p_j} = 2\sum_{m=1}^{M}\left[\frac{\partial^2 f_m}{\partial p_i \partial p_j}\right] \qquad (i=1,\ldots,N;\ j=1,\ldots,N) \tag{3.19}$$

Rewritten in expanded form:

$$\frac{\partial^2 E}{\partial p_i \partial p_j} = 2\sum_{m=1}^{M}\left[\frac{\partial^2 f_1}{\partial p_i \partial p_j} + \frac{\partial^2 f_2}{\partial p_i \partial p_j} + \cdots + \frac{\partial^2 f_M}{\partial p_i \partial p_j}\right] \tag{3.20}$$

If Eq. (3.19) is rewritten in an explicit form:

$$\frac{\partial^2 E}{\partial p_1 \partial p_1} = 2\sum_{m=1}^{M}\left[\frac{\partial^2 f_1}{\partial p_1^2} + \frac{\partial^2 f_2}{\partial p_1^2} + \cdots + \frac{\partial^2 f_M}{\partial p_1^2}\right] \tag{3.21a}$$

$$\frac{\partial^2 E}{\partial p_1 \partial p_2} = 2\sum_{m=1}^{M}\left[\frac{\partial^2 f_1}{\partial p_1 \partial p_2} + \frac{\partial^2 f_2}{\partial p_1 \partial p_2} + \cdots + \frac{\partial^2 f_M}{\partial p_1 \partial p_2}\right] \tag{3.21b}$$

$$\vdots$$

$$\frac{\partial^2 E}{\partial p_N \partial p_N} = 2\sum_{m=1}^{M}\left[\frac{\partial^2 f_1}{\partial p_N^2} + \frac{\partial^2 f_2}{\partial p_N^2} + \cdots + \frac{\partial^2 f_M}{\partial p_N^2}\right] \tag{3.21c}$$

It is possible to define a new matrix

$$\mathbf{A} = \begin{bmatrix} \frac{\partial f_1}{\partial p_1} & \frac{\partial f_1}{\partial p_2} & \cdots & \frac{\partial f_1}{\partial p_N} \\ \frac{\partial f_2}{\partial p_1} & \frac{\partial f_2}{\partial p_2} & \cdots & \frac{\partial f_2}{\partial p_N} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_M}{\partial p_1} & \frac{\partial f_M}{\partial p_2} & \cdots & \frac{\partial f_M}{\partial p_N} \end{bmatrix} \tag{3.22}$$

which consists of derivatives of functions $f_1(\mathbf{p})$, $f_2(\mathbf{p})$,…, $f_M(\mathbf{p})$ with respect to the variation of each parameter components p_1, p_2, …, p_N. Usually M is much larger than N, therefore **A** is not a square matrix. If we take the transpose of **A** and multiply with **f**, where

$$\mathbf{A}^T = \begin{bmatrix} \frac{\partial f_1}{\partial p_1} & \frac{\partial f_2}{\partial p_1} & \cdots & \frac{\partial f_M}{\partial p_1} \\ \frac{\partial f_1}{\partial p_2} & \frac{\partial f_2}{\partial p_2} & \cdots & \frac{\partial f_M}{\partial p_2} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_1}{\partial p_N} & \frac{\partial f_2}{\partial p_N} & \cdots & \frac{\partial f_M}{\partial p_N} \end{bmatrix} \quad \text{and} \quad \mathbf{f} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_M \end{bmatrix}$$

Then the product of the two matrices above results in

$$\mathbf{A}^T\mathbf{f} = \begin{bmatrix} \left\{ f_1 \frac{\partial f_1}{\partial p_1} + f_2 \frac{\partial f_2}{\partial p_1} + \cdots + f_M \frac{\partial f_M}{\partial p_1} \right\} \\ \left\{ f_1 \frac{\partial f_1}{\partial p_2} + f_2 \frac{\partial f_2}{\partial p_2} + \cdots + f_M \frac{\partial f_M}{\partial p_2} \right\} \\ \vdots \\ \left\{ f_1 \frac{\partial f_1}{\partial p_N} + f_2 \frac{\partial f_2}{\partial p_N} + \cdots + f_M \frac{\partial f_M}{\partial p_N} \right\} \end{bmatrix} \tag{3.23}$$

which is an Nx1 column matrix. When the members of the above matrix are examined, it can be observed that each row is equal to half of the first order derivatives, $\frac{1}{2}\frac{\partial E}{\partial p_i}$. That is

$$\mathbf{A}^T\mathbf{f} = \frac{1}{2}\begin{bmatrix} \frac{\partial E}{\partial p_1} \\ \frac{\partial E}{\partial p_2} \\ \vdots \\ \frac{\partial E}{\partial p_N} \end{bmatrix} \tag{3.24}$$

This means that gradient $\nabla E(\mathbf{p})$ can now be represented in matrix form

$$\mathbf{g} = \nabla E(\mathbf{p}) = 2\mathbf{A}^T\mathbf{f} \tag{3.25}$$

The product of matrix **A** and its transpose in explicit form is:

$$\mathbf{A}^T\mathbf{A} = \begin{bmatrix} \left\{\frac{\partial^2 f_1}{\partial p_1^2} + \cdots + \frac{\partial^2 f_M}{\partial p_1^2}\right\} & \cdots & \left\{\frac{\partial^2 f_1}{\partial p_1 \partial p_N} + \cdots + \frac{\partial^2 f_M}{\partial p_1 \partial p_N}\right\} \\ \left\{\frac{\partial^2 f_1}{\partial p_1 \partial p_2} + \cdots + \frac{\partial^2 f_M}{\partial p_1 \partial p_2}\right\} & \cdots & \left\{\frac{\partial^2 f_1}{\partial p_2 \partial p_N} + \cdots + \frac{\partial^2 f_M}{\partial p_2 \partial p_N}\right\} \\ \vdots & & \vdots \\ \left\{\frac{\partial^2 f_1}{\partial p_1 \partial p_N} + \cdots + \frac{\partial^2 f_M}{\partial p_1 \partial p_N}\right\} & \cdots & \left\{\frac{\partial^2 f_1}{\partial p_N^2} + \cdots + \frac{\partial^2 f_M}{\partial p_N^2}\right\} \end{bmatrix} \quad (3.26)$$

The matrix above is an NxN square matrix, and its members are the half of second order derivatives. Therefore the product in Eq. (3.26) can also be written as

$$\mathbf{A}^T\mathbf{A} = \frac{1}{2}\begin{bmatrix} \frac{\partial^2 E}{\partial p_1^2} & \frac{\partial^2 E}{\partial p_1 \partial p_2} & \cdots & \frac{\partial^2 E}{\partial p_1 \partial p_N} \\ \frac{\partial^2 E}{\partial p_1 \partial p_2} & \frac{\partial^2 E}{\partial p_2^2} & \cdots & \frac{\partial^2 E}{\partial p_2 \partial p_N} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 E}{\partial p_1 \partial p_N} & \frac{\partial^2 E}{\partial p_2 \partial p_N} & \cdots & \frac{\partial^2 E}{\partial p_N^2} \end{bmatrix} \quad (3.27)$$

which allows us to replace the Hessian matrix **G** approximately by

$$\mathbf{G} \approx 2\mathbf{A}^T\mathbf{A} \quad (3.28)$$

Substituting Eqs. (3.25) and (3.28) into Newton's equation given in Eq. (3.12),

$$\mathbf{p}_k = \mathbf{p}_{k\text{-}1} - (\mathbf{A}_k^T\mathbf{A}_k)^{-1}\mathbf{A}_k^T\mathbf{f}_k \quad (3.29)$$

or

$$\Delta\mathbf{p}_k = -(\mathbf{A}_k^T\mathbf{A}_k)^{-1}\mathbf{A}_k^T\mathbf{f}_k \quad (3.30)$$

where $\Delta\mathbf{p}_k = \mathbf{p}_k - \mathbf{p}_{k\text{-}1}$ and the subscript k in the equation above indicates that $\mathbf{A}_k$ and $\mathbf{f}_k$ are evaluated at $\mathbf{p}_k$. Multiplying both sides of Eq. (3.30) by $(\mathbf{A}_k^T\mathbf{A}_k)$, Eq. (3.30) can be written as

$$(\mathbf{A}_k^T\mathbf{A}_k)\Delta\mathbf{p}_k = -\mathbf{A}_k^T\mathbf{f}_k \quad (3.31)$$

which is a linear system of equations where $\mathbf{A}_k^T \mathbf{A}_k$ is N by N square matrix and $\mathbf{A}_k^T \mathbf{f}_k$ is an N-dimensional vector. $\Delta \mathbf{p}_k$ is the unknown vector to be determined from the product of $\mathbf{A}_k^T \mathbf{f}_k$ and inverse of $\mathbf{A}_k^T \mathbf{A}_k$. This requires that $\mathbf{A}_k^T \mathbf{A}_k$ is invertible. The magnitude of $\mathbf{A}_k^T \mathbf{A}_k$ may become so small for some k that it can be rounded to zero, which makes it singular. In order to avoid singularity and ensure convergence with relatively poor initial estimates, an additional term is added to $\mathbf{A}_k^T \mathbf{A}_k$:

$$(\mathbf{A}_k^T \mathbf{A}_k + \lambda_k \mathbf{I}) \Delta \mathbf{p}_k = -\mathbf{A}_k^T \mathbf{f}_k \tag{3.32}$$

where λ_k is a coefficient and **I** is the identity matrix. Initial values of λ_k are large and decrease towards zero as convergence is reached (Karvonen, 2002). The unknown vector $\Delta \mathbf{p}_k$ is determined from the following equation:

$$\Delta \mathbf{p}_k = -(\mathbf{A}_k^T \mathbf{A}_k + \lambda_k \mathbf{I})^{-1} \mathbf{A}_k^T \mathbf{f}_k \tag{3.33}$$

and finally parameter $\mathbf{p}_{k-1}$ is updated to the improved estimate $\mathbf{p}_k$ as

$$\mathbf{p}_k = \mathbf{p}_{k-1} + \Delta \mathbf{p}_k \tag{3.34}$$

The forward problem is then solved using the new estimate $\mathbf{p}_k$, and the procedure is repeated until convergence criterion is reached.

3.4.1 Marquardt Solution for Constant Drawdown

General formulation includes terms such as H, head, and f, introduced in Eq. (3.14), whereas the particular case involves drawdown and discharge measurements. The equations in the previous section therefore need to be adapted to the present problem.

Total number of measurements for both drawdown and discharge is taken as 20, that is M=20. Assigning a unit value for each weight, W_m is automatically omitted from Eq. (3.1), since $W_m=1$. The number of parameters to be optimized in both cases are 1, which makes N=1. In section 3.4.1.1, drawdown measurements are utilized and the ratio of transmissivity to storage coefficient is determined. The parameter to be optimized is α in Eq. (2.10), which means $\mathbf{p} = [\alpha]$. In section 3.4.1.2, discharge measurements are utilized and the product of transmissivity and storage coefficient is determined. The parameter to be optimized is β in Eq. (2.20), that is $\mathbf{p} = [\beta]$.

3.4.1.1 Determination of Ratio of Transmissivity to Storage Coefficient From Drawdown Measurements

The iteration parameter for utilization of drawdown values is α, which is the hydraulic diffusivity, T/S. Assigning a unit value for each weight; W_m is automatically omitted from Eq. (3.14), which is modified for drawdown as

$$f_m(\alpha) = \left[s_m^c(\alpha) - s_m^{obs} \right] \quad (3.35)$$

where $s_m^c(\alpha)$ is the drawdown at time m computed using α, and s_m^{obs} is the observed drawdown at time m. Then the residual square error defined in Eq. (3.1) becomes

$$E(\alpha) = \sum_{m=1}^{20} \left[s_m^c(\alpha) - s_m^{obs} \right]^2 \quad (3.36)$$

The difference between observed and calculated values written in matrix form is

$$\mathbf{f} = \begin{bmatrix} f_1(\alpha) \\ f_2(\alpha) \\ \vdots \\ f_{20}(\alpha) \end{bmatrix} = \begin{bmatrix} s_1^c(\alpha) - s_1^{obs} \\ s_2^c(\alpha) - s_2^{obs} \\ \vdots \\ s_{20}^c(\alpha) - s_{20}^{obs} \end{bmatrix} \quad (3.37)$$

The respective increment to yield the improved estimate α at the end of each trial is denoted by $\Delta\alpha$, which replaces $\Delta\mathbf{p}$ in Eqs. (3.31) through (3.34). Rewriting Eq. (3.30) for drawdown to obtain the iteration cycle,

$$\Delta\alpha_k = -(\mathbf{A}_k^T\mathbf{A}_k + \lambda_k\mathbf{I})^{-1}\mathbf{A}_k^T\mathbf{f}_k \tag{3.38a}$$

or

$$\Delta\alpha_k = (\mathbf{A}_k^T\mathbf{A}_k + \lambda_k\mathbf{I})^{-1}\mathbf{A}_k^T\left[s^{obs} - s^c(\alpha)\right]_k \tag{3.38b}$$

In order to calculate the hydraulic diffusivity T/S, members of matrix **A** have to be determined. Derivative of Eq. (3.35) with respect to α is

$$\frac{\partial f_m(\alpha)}{\partial\alpha} = \frac{\partial s_m^c(\alpha)}{\partial\alpha} \tag{3.39}$$

Thus modified form of **A** is:

$$\mathbf{A} = \begin{bmatrix} \dfrac{\partial s_1^c(\alpha)}{\partial\alpha} \\ \dfrac{\partial s_2^c(\alpha)}{\partial\alpha} \\ \vdots \\ \dfrac{\partial s_{20}^c(\alpha)}{\partial\alpha} \end{bmatrix} \tag{3.40}$$

In order to calculate $\partial s/\partial\alpha$ from Eq. (2.10) the chain rule of differentiation is applied as done in the previous chapter to calculate $\partial s/\partial x$. The derivative of Eq. (2.10) is taken with respect to the argument of the complementary error function, and then the derivative of the argument is taken with respect to α.

$$\frac{\partial s}{\partial\alpha} = \frac{\partial s}{\partial u}\frac{\partial u}{\partial\alpha} \tag{3.41}$$

The derivative of s with respect to u has already been taken in Eq. (2.14):

$$\frac{\partial s}{\partial u} = -s_0\frac{2}{\sqrt{\pi}}e^{-u^2} = -\frac{2s_0}{\sqrt{\pi}}e^{-\frac{x^2}{4\alpha t}}$$

The derivative of u with respect to α is

$$\frac{\partial u}{\partial \alpha} = -\frac{1}{2}\frac{x}{2\sqrt{t}}\alpha^{-\frac{3}{2}} \tag{3.42}$$

The product of Eqs. (2.14) and (3.42) gives

$$\frac{\partial s}{\partial \alpha} = \frac{s_0 x}{\sqrt{4\pi t}}\alpha^{-\frac{3}{2}} e^{-\frac{x^2}{4\alpha t}} \tag{3.43}$$

Eq. (3.43) enables us to generate matrix **A** and apply the Marquardt iteration cycle given in Eq. (3.38b). New estimate of α is computed from

$$\alpha_k = \alpha_{k-1} + \Delta\alpha_k \tag{3.44}$$

The iteration procedure is then repeated using the new estimate.

3.4.1.2 Determination of Product of Transmissivity and Storage Coefficient From Discharge Measurements

The iteration parameter for utilization of discharge values is β, the product of transmissivity and storage coefficient, that is $\beta = T.S$. Considering Eq. (2.20), it is observed that square roots of β are used to determine the discharge. Since this may cause divergence problems in case negative β values exist at any instant of iteration, the square of Eq. (2.20) is taken. Letting $Q^2 = \varphi$,

$$\varphi = \frac{4s_0^2\beta}{\pi t} \tag{3.45}$$

Derivative of this new parameter with respect to β is

$$\frac{\partial \varphi}{\partial \beta} = \frac{4s_0^2}{\pi t} \tag{3.46}$$

Eq. (3.14) can be rewritten for squares of discharge as

$$f_m(\beta) = \left[\varphi_m^c(\beta) - \varphi_m^{obs}\right] \tag{3.47}$$

where $\varphi_m^c(\beta)$ and φ_m^{obs} are the squares of $Q_m^c(\beta)$ and Q_m^{obs} respectively, $Q_m^c(\beta)$ being the discharge at time m computed using β and Q_m^{obs} being the observed discharge at time m. Similar to Eq. (3.36), E(**p**) in Eq. (3.1) becomes

$$E(\beta) = \sum_{m=1}^{20} \left[\varphi_m^c(\beta) - \varphi_m^{obs} \right]^2 \quad (3.48)$$

In matrix form, Eq. (3.47) can be written as

$$\mathbf{f} = \begin{bmatrix} f_1(\beta) \\ f_2(\beta) \\ \vdots \\ f_{20}(\beta) \end{bmatrix} = \begin{bmatrix} \varphi_1^c(\beta) - \varphi_1^{obs} \\ \varphi_2^c(\beta) - \varphi_2^{obs} \\ \vdots \\ \varphi_{20}^c(\beta) - \varphi_{20}^{obs} \end{bmatrix} \quad (3.49)$$

The iteration cycle obtained for discharge is similar to Eq. (3.38b):

$$\Delta\beta_k = (\mathbf{A}_k^T \mathbf{A}_k + \lambda_k \mathbf{I})^{-1} \mathbf{A}_k^T \left[\varphi^{obs} - \varphi^c(\beta) \right]_k \quad (3.50)$$

where Δβ is the respective increment in β. Derivative of φ with respect to β is required for determining members of matrix **A**.

$$\frac{\partial f_m(\beta)}{\partial \beta} = \frac{\partial \varphi_m^c(\beta)}{\partial \beta} \quad (3.51)$$

Matrix **A** then becomes

$$\mathbf{A} = \begin{bmatrix} \dfrac{\partial \varphi_1^c(\beta)}{\partial \beta} \\ \dfrac{\partial \varphi_2^c(\beta)}{\partial \beta} \\ \vdots \\ \dfrac{\partial \varphi_{20}^c(\beta)}{\partial \beta} \end{bmatrix} \quad (3.52)$$

The differential ∂φ / ∂β has already been determined in Eq. (3.46). Marquardt iteration can be applied hereafter using Eq. (3.50). New estimate of β is computed from

$$\beta_k = \beta_{k-1} + \Delta\beta_k \quad (3.53)$$

Using the improved estimate, the iteration procedure is repeated until the convergence criterion is satisfied.

3.4.2 Marquardt Solution for Constant Discharge

Drawdown measurements performed during pumping period are used for the determination of transmissivity and storage coefficient simultaneously. The discharge rate is constant throughout the measurements.

Total number of measurements is 20 and a unit value is assigned for each weight, as in the previous case. Since there are two parameters to be optimized simultaneously, $\mathbf{p} = \begin{bmatrix} T & S \end{bmatrix}^T$ and N=2. Eq. (3.14) can then be written, similar to Eq. (3.35), as

$$f_m(\mathbf{p}) = \left[s_m^c(\mathbf{p}) - s_m^{obs} \right] \tag{3.54}$$

where $\mathbf{p}$ in Eq. (3.54) involves the trial values for T and S, $s_m^c(\mathbf{p})$ is the drawdown at time m computed using T and S, and s_m^{obs} is the observed drawdown at time m. The residual square error for constant discharge case then becomes

$$E(\mathbf{p}) = \sum_{m=1}^{20} \left[s_m^c(\mathbf{p}) - s_m^{obs} \right]^2 \tag{3.55}$$

Matrix form of Eq. (3.54) is similar to the matrix in Eq. (3.37):

$$\mathbf{f} = \begin{bmatrix} f_1(\mathbf{p}) \\ f_2(\mathbf{p}) \\ \vdots \\ f_{20}(\mathbf{p}) \end{bmatrix} = \begin{bmatrix} s_1^c(\mathbf{p}) - s_1^{obs} \\ s_2^c(\mathbf{p}) - s_2^{obs} \\ \vdots \\ s_{20}^c(\mathbf{p}) - s_{20}^{obs} \end{bmatrix} \tag{3.56}$$

Derivative of Eq. (3.54) with respect to parameter vector **p** is:

$$\frac{\partial f_m(\mathbf{p})}{\partial \mathbf{p}} = \frac{\partial s_m^c(\mathbf{p})}{\partial \mathbf{p}} \tag{3.57}$$

The iteration cycle for constant discharge case is identical with Eq. (3.33):

$$\Delta \mathbf{p}_k = -(\mathbf{A}_k^T \mathbf{A}_k + \lambda_k \mathbf{I})^{-1} \mathbf{A}_k^T \mathbf{f}_k$$

where $\Delta\mathbf{p}$ stands for the respective increment in T and S to yield the improved estimates at the end of each trial, that is

$$\Delta \mathbf{p} = [\Delta T \quad \Delta S]^T \tag{3.58}$$

Matrix of respective increments can also be obtained from

$$\Delta \mathbf{p}_k = (\mathbf{A}_k^T \mathbf{A}_k + \lambda_k \mathbf{I})^{-1} \mathbf{A}_k^T \left[s^{obs} - s^c(\mathbf{p}) \right]_k \tag{3.59}$$

Considering Eq. (3.22), matrix **A** for constant discharge case becomes

$$\mathbf{A} = \begin{bmatrix} \frac{\partial s_1^c(\mathbf{p})}{\partial T} & \frac{\partial s_1^c(\mathbf{p})}{\partial S} \\ \frac{\partial s_2^c(\mathbf{p})}{\partial T} & \frac{\partial s_2^c(\mathbf{p})}{\partial S} \\ \vdots & \vdots \\ \frac{\partial s_{20}^c(\mathbf{p})}{\partial T} & \frac{\partial s_{20}^c(\mathbf{p})}{\partial S} \end{bmatrix} \tag{3.60}$$

Generation of matrix **A** requires computation of derivative of s with respect to T and S. The drawdown for constant discharge given by Carslaw and Jaeger (1959) has already been determined in Eq. (2.28):

$$s(x,t) = \frac{Q_0}{2T} \left\{ \sqrt{\frac{4Tt}{\pi S}} e^{-u^2} + x[\operatorname{erf}(u) - 1] \right\}$$

Derivation of $\frac{\partial s}{\partial T}$ begins with rewriting s(x,t):

$$s(x,t) = \frac{Q_0}{2T} \left[2\sqrt{\frac{t}{\pi S}} T^{\frac{1}{2}} e^{-\frac{x^2 S T^{-1}}{4t}} + x\left(\operatorname{erf}\sqrt{\frac{x^2 S}{4Tt}} - 1 \right) \right] \tag{3.61a}$$

$$s(x,t) = Q_0 \left[\sqrt{\frac{t}{\pi S}} T^{-\frac{1}{2}} e^{-\frac{x^2 S T^{-1}}{4t}} + \frac{x}{2T}\left(\operatorname{erf}\sqrt{\frac{x^2 S}{4Tt}} - 1 \right) \right] \tag{3.61b}$$

Let $V=\sqrt{\frac{t}{\pi S}}T^{-\frac{1}{2}}e^{-\frac{x^2ST^{-1}}{4t}}$ and $W=\frac{x}{2T}\left(\operatorname{erf}\sqrt{\frac{x^2S}{4Tt}}-1\right)$

Then Eq. (3.61b) becomes

$$s(x,t)=Q_0\left(V+W\right) \tag{3.62}$$

which yields

$$\frac{\partial s}{\partial T}=Q_0\left(\frac{\partial V}{\partial T}+\frac{\partial W}{\partial T}\right) \tag{3.63}$$

Derivative of V with respect to T is obtained as follows:

$$\frac{\partial V}{\partial T}=\sqrt{\frac{t}{\pi S}}\left[-\frac{1}{2}T^{-\frac{3}{2}}e^{-\frac{x^2S}{4Tt}}+T^{-\frac{1}{2}}\left(e^{-\frac{x^2S}{4Tt}}\frac{x^2S}{4t}T^{-2}\right)\right] \tag{3.64a}$$

$$\frac{\partial V}{\partial T}=\sqrt{\frac{t}{\pi S}}\left(-\frac{1}{2}T^{-\frac{3}{2}}e^{-\frac{x^2S}{4Tt}}+e^{-\frac{x^2S}{4Tt}}\frac{x^2S}{4t}T^{-\frac{5}{2}}\right) \tag{3.64b}$$

$$\frac{\partial V}{\partial T}=\sqrt{\frac{t}{\pi S}}T^{-\frac{3}{2}}e^{-\frac{x^2S}{4Tt}}\left(-\frac{1}{2}+\frac{x^2S}{4t}T^{-1}\right) \tag{3.64c}$$

Rearranging gives

$$\frac{\partial V}{\partial T}=\sqrt{\frac{t}{\pi S}}T^{-\frac{3}{2}}e^{-u^2}\left(u^2-\frac{1}{2}\right) \tag{3.64d}$$

Derivative of W with respect to T is obtained similarly:

$$\frac{\partial W}{\partial T}=-\frac{x}{2T^2}\left(\operatorname{erf}\sqrt{\frac{x^2S}{4Tt}}-1\right)+\frac{x}{2T}\left(-\frac{1}{\sqrt{\pi}}e^{-\frac{x^2S}{4Tt}}\sqrt{\frac{x^2S}{4t}}T^{-\frac{3}{2}}\right) \tag{3.65a}$$

$$\frac{\partial W}{\partial T}=\frac{x}{2T^2}\left[\left(1-\operatorname{erf}\sqrt{\frac{x^2S}{4Tt}}\right)+T\left(-\frac{1}{\sqrt{\pi}}e^{-\frac{x^2S}{4Tt}}\sqrt{\frac{x^2S}{4t}}T^{-\frac{3}{2}}\right)\right] \tag{3.65b}$$

$$\frac{\partial W}{\partial T}=\frac{x}{2T^2}\left(\operatorname{erfc}\sqrt{\frac{x^2S}{4Tt}}-\frac{1}{\sqrt{\pi}}e^{-\frac{x^2S}{4Tt}}\sqrt{\frac{x^2S}{4Tt}}\right) \tag{3.65c}$$

Rearranging gives

$$\frac{\partial W}{\partial T}=\frac{x}{2T^2}\left[\operatorname{erfc}(u)-\frac{ue^{-u^2}}{\sqrt{\pi}}\right] \tag{3.65d}$$

Considering Eq. (3.63), derivative of s(x,t) with respect to transmissivity is

$$\frac{\partial s}{\partial T}=Q_0\left\{\sqrt{\frac{t}{\pi S}}T^{-\frac{3}{2}}e^{-u^2}\left(u^2-\frac{1}{2}\right)+\frac{x}{2T^2}\left[\operatorname{erfc}(u)-\frac{ue^{-u^2}}{\sqrt{\pi}}\right]\right\} \tag{3.66}$$

In order to determine $\frac{\partial s}{\partial S}$, Eq. (2.28) is rearranged in terms of powers of S:

$$s(x,t)=Q_0\left[\sqrt{\frac{t}{\pi}}T^{-\frac{1}{2}}S^{-\frac{1}{2}}e^{-\frac{x^2S}{4Tt}}+\frac{x}{2T}\left(\operatorname{erf}\sqrt{\frac{x^2S}{4Tt}}-1\right)\right] \tag{3.67}$$

Let $Y=\sqrt{\frac{t}{\pi}}T^{-\frac{1}{2}}S^{-\frac{1}{2}}e^{-\frac{x^2S}{4Tt}}$

Then the equation of drawdown becomes similar to Eq. (3.62):

$$s(x,t)=Q_0(Y+W) \tag{3.68}$$

and the derivative is then

$$\frac{\partial s}{\partial S}=Q_0\left(\frac{\partial Y}{\partial S}+\frac{\partial W}{\partial S}\right) \tag{3.69}$$

Derivative of Y with respect to S is obtained below:

$$\frac{\partial Y}{\partial S}=\sqrt{\frac{t}{\pi}}T^{-\frac{1}{2}}\left(-\frac{1}{2}S^{-\frac{3}{2}}e^{-\frac{x^2S}{4Tt}}-S^{-\frac{3}{2}}e^{-\frac{x^2S}{4Tt}}\frac{x^2}{4Tt}\right) \tag{3.70a}$$

$$\frac{\partial Y}{\partial S}=\sqrt{\frac{t}{\pi}}T^{-\frac{1}{2}}e^{-\frac{x^2S}{4Tt}}\left(-\frac{1}{2}S^{-\frac{3}{2}}-S^{-\frac{1}{2}}\frac{x^2}{4Tt}\right) \tag{3.70b}$$

$$\frac{\partial Y}{\partial S}=-\sqrt{\frac{t}{\pi T}}e^{-\frac{x^2S}{4Tt}}S^{-\frac{1}{2}}\left(\frac{1}{2}S^{-1}+\frac{x^2}{4Tt}\right) \tag{3.70c}$$

Derivative of W with respect to S is

$$\frac{\partial W}{\partial S} = \frac{x}{2T}\left(\frac{1}{\sqrt{\pi}}\sqrt{\frac{x^2}{4Tt}}e^{-\frac{x^2S}{4Tt}}S^{-\frac{1}{2}}\right) \tag{3.71a}$$

$$\frac{\partial W}{\partial S} = \frac{x^2}{4T}\sqrt{\frac{1}{\pi Tt}}e^{-\frac{x^2S}{4Tt}}S^{-\frac{1}{2}} \tag{3.71b}$$

Derivative of s(x,t) with respect to storage coefficient is obtained considering Eq. (3.69):

$$\frac{\partial s}{\partial S} = Q_0\left[\frac{x^2T^{-\frac{3}{2}}}{4\sqrt{\pi t}}e^{-\frac{x^2S}{4Tt}}S^{-\frac{1}{2}} - \sqrt{\frac{t}{\pi T}}e^{-\frac{x^2S}{4Tt}}S^{-\frac{1}{2}}\left(\frac{1}{2S}+\frac{x^2}{4Tt}\right)\right] \tag{3.72a}$$

$$\frac{\partial s}{\partial S} = Q_0\left\{e^{-\frac{x^2S}{4Tt}}S^{-\frac{1}{2}}\left[\frac{x^2T^{-\frac{3}{2}}}{4\sqrt{\pi t}} - \frac{1}{S}\sqrt{\frac{t}{\pi T}}\left(\frac{1}{2}+\frac{x^2S}{4Tt}\right)\right]\right\} \tag{3.72b}$$

Finally, rearranging gives

$$\frac{\partial s}{\partial S} = Q_0\left\{e^{-u^2}S^{-\frac{1}{2}}\left[\frac{x^2T^{-\frac{3}{2}}}{4\sqrt{\pi t}} - \frac{1}{S}\sqrt{\frac{t}{\pi T}}\left(u^2+\frac{1}{2}\right)\right]\right\} \tag{3.72c}$$

Matrix **A** is generated using Eqs. (3.66) and (3.72c), and the algorithm is run within the iteration cycle given in Eq. (3.59). New estimates of transmissivity and storage coefficient are obtained respectively as:

$$T_k = T_{k-1} + \Delta T_k \tag{3.73}$$

$$S_k = S_{k-1} + \Delta S_k \tag{3.74}$$

CHAPTER 4

APPLICATION AND DISCUSSION

In this chapter, the procedure for optimization of the parameters is given through three examples, and the results are presented. In order to apply Marquardt algorithm to actual semi-infinite confined aquifers, observation at various time intervals has to be performed in the field, which consists of measuring the drawdown, s_m^{obs}, at a predefined distance, x, from the stream-aquifer interface, and the discharge, Q_m^{obs}, just at the interface.

Published papers have been surveyed in order to find field data representing constant drawdown in the stream, or constant discharge due to pumping. Unfortunately, only one set of data presented by Tomasko (1987) were appropriate for use in constant discharge case. The other two examples contain synthetic data generated using equations derived in the analytical solutions.

The algorithm is run using the spreadsheet software Microsoft Excel, so as to view each iteration table explicitly.

4.1 Constant Drawdown Case

As stated above, synthetic data are generated by simulation for this case due to lack of appropriate field data. A hypothetical aquifer is assumed, having a transmissivity of T^*=172.8 m^2/day (0.002 m^2/s) and a storage coefficient of S^*=0.0002; yielding $\alpha^*=10$ m^2/s and $\beta^*=4\times10^{-7}$ m^2/s. The fictitious observation well is assumed to be located at x=50 m from the interface through the aquifer. Magnitude of the constant drawdown is chosen as s_0=2.4 m. Time series start at t=30 seconds and end at t=259200 seconds (72 hours).

The next step is to calculate (i.e. simulate) drawdown and discharge values for an aquifer having the parameters assumed above. Drawdown values, which are going to replace observed drawdown series s_m^{obs}, are calculated for each time interval from Eq. (2.10) using $\alpha^*=10$ m^2/s. Discharge values, which are going to replace observed discharge series Q_m^{obs}, are calculated again for each time interval from Eq. (2.20) using $\beta^*=4\times10^{-7}$ m^2/s. Square of Q_m^{obs} gives φ_m^{obs}. The simulated drawdown and discharge values are presented in Table 4.1.

4.1.1 Results of Marquardt Solution

The procedure for optimization of α and β is explained below.

1. Initial values are assigned for α and β as α_0=0.1 m^2/s and β_0=0.001 m^2/s, and for the convergence factor λ=0.
2. Drawdown values s(x,t) for 20 values of time are computed from Eq. (2.10) using initial estimate α_0, and discharge values Q(t) are computed from Eq. (2.20) using initial estimate β_0. Computed drawdown values constitute $s^c(\alpha)$ and squares of computed discharge values constitute $\varphi^c(\beta)$.

3. $\frac{\partial s}{\partial \alpha}$ and $\frac{\partial \varphi}{\partial \beta}$ are calculated using Eqs. (3.43) and (3.46) respectively. Matrices $\mathbf{A}_k$ are determined for α and β.
4. Coefficient matrix $[\mathbf{A}_k^T\mathbf{A}_k+\lambda_k\mathbf{I}]$ and vectors $\mathbf{A}_k^T[s^{obs}-s^c(\alpha)]_k$ and $\mathbf{A}_k^T[\varphi^{obs}-\varphi^c(\beta)]_k$ are calculated separately for drawdown and discharge measurements.
5. Respective increments $\Delta\alpha$ in α and $\Delta\beta$ in β are calculated. New estimates for the parameters are computed using Eqs. (3.44) and (3.53); and the iteration procedure is repeated beginning from step 2, until convergence is reached.

Table 4.1 Simulation of observed values for constant drawdown

i	t_i [s]	u_i	SIMULATED VALUES		
			s_i^{obs} [m]	Q_i^{obs} [m^2/s]	$\psi_i^{obs} = (Q_i^{obs})^2$
1	30	1.44338	0.09894	0.0003127	9.77848E-08
2	60	1.02062	0.3574	0.0002211	4.88924E-08
3	120	0.72169	0.73784	0.0001564	2.44462E-08
4	300	0.45644	1.24465	9.889E-05	9.77848E-09
5	600	0.32275	1.55538	6.992E-05	4.88924E-09
6	900	0.26352	1.70253	5.709E-05	3.25949E-09
7	1200	0.22822	1.79253	4.944E-05	2.44462E-09
8	1500	0.20412	1.85479	4.422E-05	1.9557E-09
9	1800	0.18634	1.90115	4.037E-05	1.62975E-09
10	2400	0.16137	1.96674	3.496E-05	1.22231E-09
11	3600	0.13176	2.04523	2.855E-05	8.14873E-10
12	7200	0.09317	2.14841	2.019E-05	4.07437E-10
13	10800	0.07607	2.19438	1.648E-05	2.71624E-10
14	18000	0.05893	2.24061	1.277E-05	1.62975E-10
15	28800	0.04658	2.27393	1.009E-05	1.01859E-10
16	43200	0.03804	2.29704	8.241E-06	6.79061E-11
17	86400	0.0269	2.32718	5.827E-06	3.39531E-11
18	129600	0.02196	2.34054	4.758E-06	2.26354E-11
19	172800	0.01902	2.3485	4.12E-06	1.69765E-11
20	259200	0.01553	2.35795	3.364E-06	1.13177E-11

Even in case of extremely poor initial estimates of hydraulic diffusivity T/S and product of the two parameters TS, the iteration reached convergence very quickly. It must be noted that α_0 is 1% of the true (synthetic) value α^* and β_0 is 250000% of β^*. The true value of $\alpha^*=10\ m^2/s$ is reached after 7 iteration cycles with no error whereas only 1 iteration was enough to obtain $\beta^*=4\times10^{-7}\ m^2/s$ error free. The respective increment in α and consequently the residual squares completely vanish after 10 iterations, which makes the method robust. Note that percentage error is defined by Eq. (3.5) while Eq. (3.36) gives the residual square error.

Optimization of α and β are performed within one Microsoft Excel iteration table at a time, where a separate table is employed for each iteration index k. The first iteration table (k=1) is given in Appendix A, Table A.1; and the iteration table for k=10 is given in Table A.2.

The transmissivity and the storage coefficient can easily be computed once their ratio and product are determined. Aquifer parameters are calculated using α_{OPT} and β_{OPT} as $T_{OPT}=0.002\ m^2/s$ (172.8 m^2/day) and $S_{OPT}=0.0002$, which are identical with the parameters that are used to generate the synthetic data at the beginning ($T_{OPT}=T^*$; $S_{OPT}=S^*$). A table summarizing the iteration process is given in Table 4.2.

4.1.2 Results of Type Curve Method

Type curve for an aquifer with the assumed characteristics, which is adjacent to a stream where constant drawdown occurs, is generated with reference to Lohman (1972). The drawdown equation for constant drop in the stream has already been given in Eq. (2.10):

$s = s_0 \mathrm{erfc}(u)$

The part of the above equation that is dependent on (u) may be written $D(u)_h$, the drain function of (u) for constant drawdown; where the subscript h identifies the constant change of head in the stream. Eq. (2.10), therefore, may be written:

$$s = s_0 D(u)_h \tag{4.1}$$

where

$$D(u)_h = \text{erfc}(u) \tag{4.2}$$

The dimensionless quantity u^2 is

$$u^2 = \frac{x^2 S}{4Tt} \tag{4.3}$$

Table 4.2 Summary of optimization process for constant drawdown

k	λ_k	α_{k-1} **[m²/s]**	$\Delta\alpha_k$ **[m²/s]**	α_k **[m²/s]**	**Error (α)***	**E(α)****	β_{k-1} **[m²/s]**	$\Delta\beta_k$ **[m²/s]**	β_k **[m²/s]**	**Error (β)***	**E(β)*****
1	0	0.1****	0.2824	0.3824	-96.18%	34.7	0.001****	-1E-03	4E-07	0.00%	8E-08
2	0	0.382	0.9739	1.3563	-86.44%	19.9	4E-07	2E-19	4E-07	0.00%	3E-39
3	0	1.356	2.1817	3.538	-64.62%	7.06	4E-07	0	4E-07	0.00%	0
4	0	3.538	3.323	6.861	-31.39%	1.74	4E-07	0	4E-07	0.00%	0
5	0	6.861	2.5275	9.3884	-6.12%	0.22	4E-07	0	4E-07	0.00%	0
6	0	9.388	0.591	9.9794	-0.21%	0.01	4E-07	0	4E-07	0.00%	0
7	0	9.979	0.0206	10	0.00%	0	4E-07	0	4E-07	0.00%	0
8	0	10	2E-05	10	0.00%	0	4E-07	0	4E-07	0.00%	0
9	0	10	-3E-11	10	0.00%	0	4E-07	0	4E-07	0.00%	0
10	0	10	0	10	0.00%	0	4E-07	0	4E-07	0.00%	0

**Computed by Eq. (3.5)*
*** Computed by Eq. (3.36)*
**** Computed by Eq. (3.48)*
*****Initial estimates*

Type curve, for a semi-infinite confined aquifer adjacent to a stream where a constant drawdown occurs, is generated by plotting $D(u)_h$ against u^2 on logarithmic scale (Lohman, 1972). Values of $D(u)_h$ for corresponding values of (u) and u^2, computed from Eq. (4.2), are given in Table 4.3; and the type curve is given in Fig 4.1.

The time dependent discharge, Q, of the aquifer from both sides and per unit length of the stream resulting from the constant drawdown, s_0, in the stream has already been given in Eq. (2.20):

$$Q = \frac{2s_0\sqrt{\beta}}{\sqrt{\pi t}}$$

Solving for β (or TS),

$$\beta = TS = \frac{Q^2\pi t}{4{s_0}^2} \tag{4.4}$$

Solving Eq. (4.3) to obtain S,

$$S = \frac{4Ttu^2}{x^2} \tag{4.5}$$

Substituting Eq. (4.5) into Eq. (4.4) to eliminate S and replacing s_0 by $s/D(u)_h$,

$$T = \frac{QD(u)_h\,x}{4su}\sqrt{\pi} \tag{4.6}$$

Table 4.3 Values of $D(u)_h$, u and u^2 for constant drawdown

u	u^2	$D(u)_h$	u	u^2	$D(u)_h$
0.0316	0.0010	0.9643	0.5000	0.2500	0.4795
0.0400	0.0016	0.9549	0.6325	0.4001	0.3711
0.0500	0.0025	0.9436	0.7746	0.6000	0.2733
0.0633	0.0040	0.9287	0.8944	0.8000	0.2059
0.0775	0.0060	0.9128	1.0000	1.0000	0.1573
0.0894	0.0080	0.8993	1.1400	1.2996	0.1069
0.1000	0.0100	0.8875	1.2650	1.6002	0.0736
0.1265	0.0160	0.8580	1.3780	1.8989	0.0513
0.1581	0.0250	0.8231	1.4830	2.1993	0.0360
0.2000	0.0400	0.7773	1.5810	2.4996	0.0254
0.2449	0.0600	0.7291	1.6430	2.6994	0.0201
0.2828	0.0800	0.6892	1.7320	2.9998	0.0143
0.3162	0.1000	0.6547	1.7890	3.2005	0.0114
0.4000	0.1600	0.5716	1.8000	3.2400	0.0109

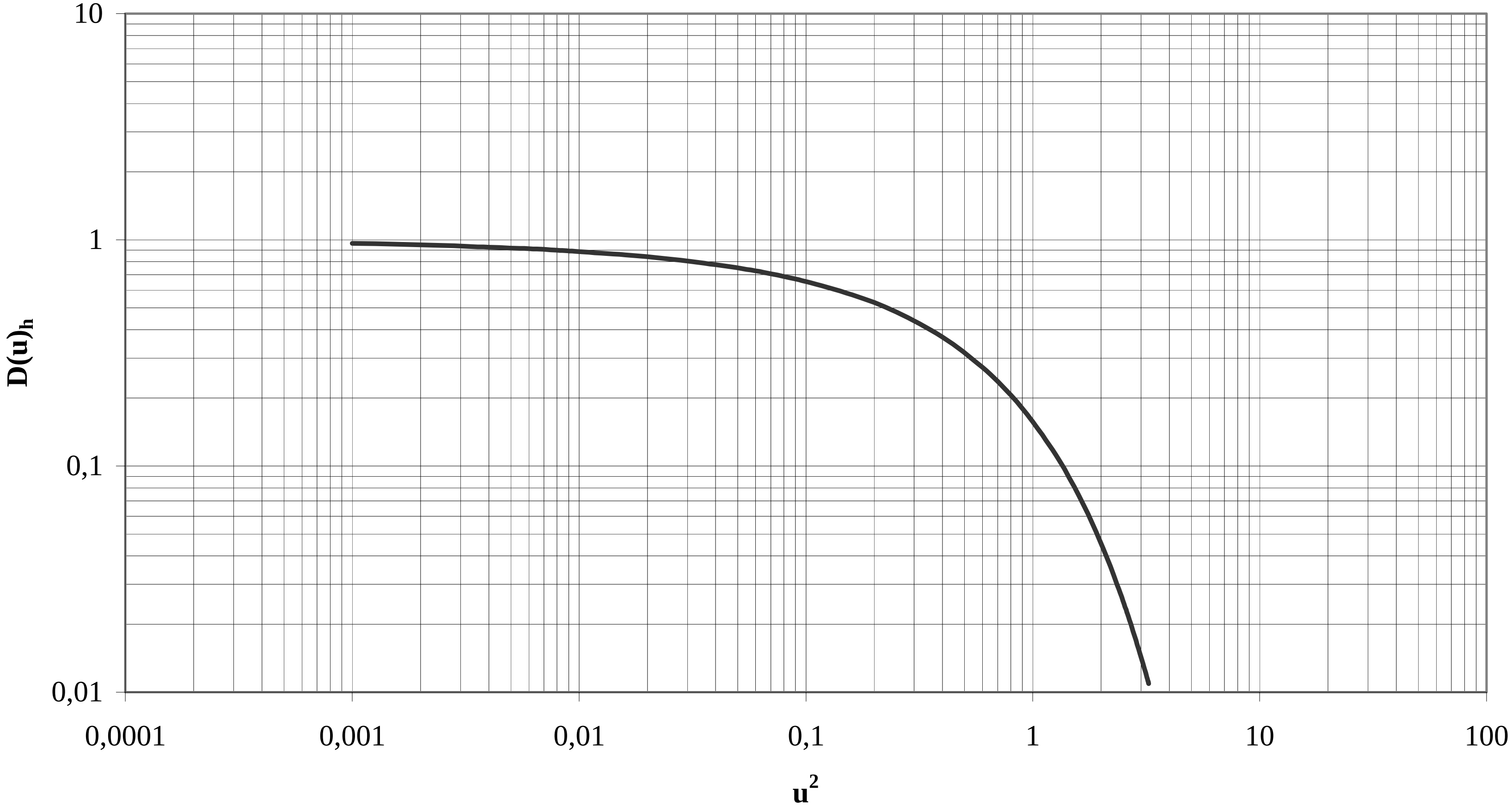

Fig. 4.1 Type curve for a semi-infinite aquifer-constant drawdown case

Observed values of s versus x^2/t are plotted on log-log paper of the same scale as the type curve, and fitted to it by the usual curve-matching procedure (Lohman, 1972). The values of s versus x^2/t (where x=50 m), which have already been determined via simulation using Eq. (2.10), are presented in Table 4.4; and the corresponding logarithmic plot is shown in Fig. 4.2. From the matching of the two curves, given in Fig. 4.3, a match point is selected, coordinates of which will provide values of u^2, $D(u)_h$, s and x^2/t.

Table 4.4 Values of t, x^2/t and s for constant drawdown

i	t (sec)	x^2/t (m^2/s)	s^{obs} (m)	i	t (sec)	x^2/t (m^2/s)	s^{obs} (m)
1	30	83.3333	0.0989	11	3600	0.6944	2.0452
2	60	41.6667	0.3574	12	7200	0.3472	2.1484
3	120	20.8333	0.7378	13	10800	0.2315	2.1944
4	300	8.3333	1.2447	14	18000	0.1389	2.2406
5	600	4.1667	1.5554	15	28800	0.0868	2.2739
6	900	2.7778	1.7025	16	43200	0.0579	2.2970
7	1200	2.0833	1.7925	17	86400	0.0289	2.3272
8	1500	1.6667	1.8548	18	129600	0.0193	2.3405
9	1800	1.3889	1.9012	19	172800	0.0145	2.3485
10	2400	1.0417	1.9667	20	259200	0.0096	2.3580

Calculation of the aquifer parameters follows these simple steps:

1. Value of time t is calculated from the value of x^2/t obtained from the curve match; since x is a known and constant value.
2. The discharge Q corresponding to the time t calculated above has already been measured and recorded. Using the predetermined values of x and Q, and the values read from the match point u^2, $D(u)_h$ and s, transmissivity is obtained using Eq. (4.6).
3. Storage coefficient is obtained from Eq. (4.5).

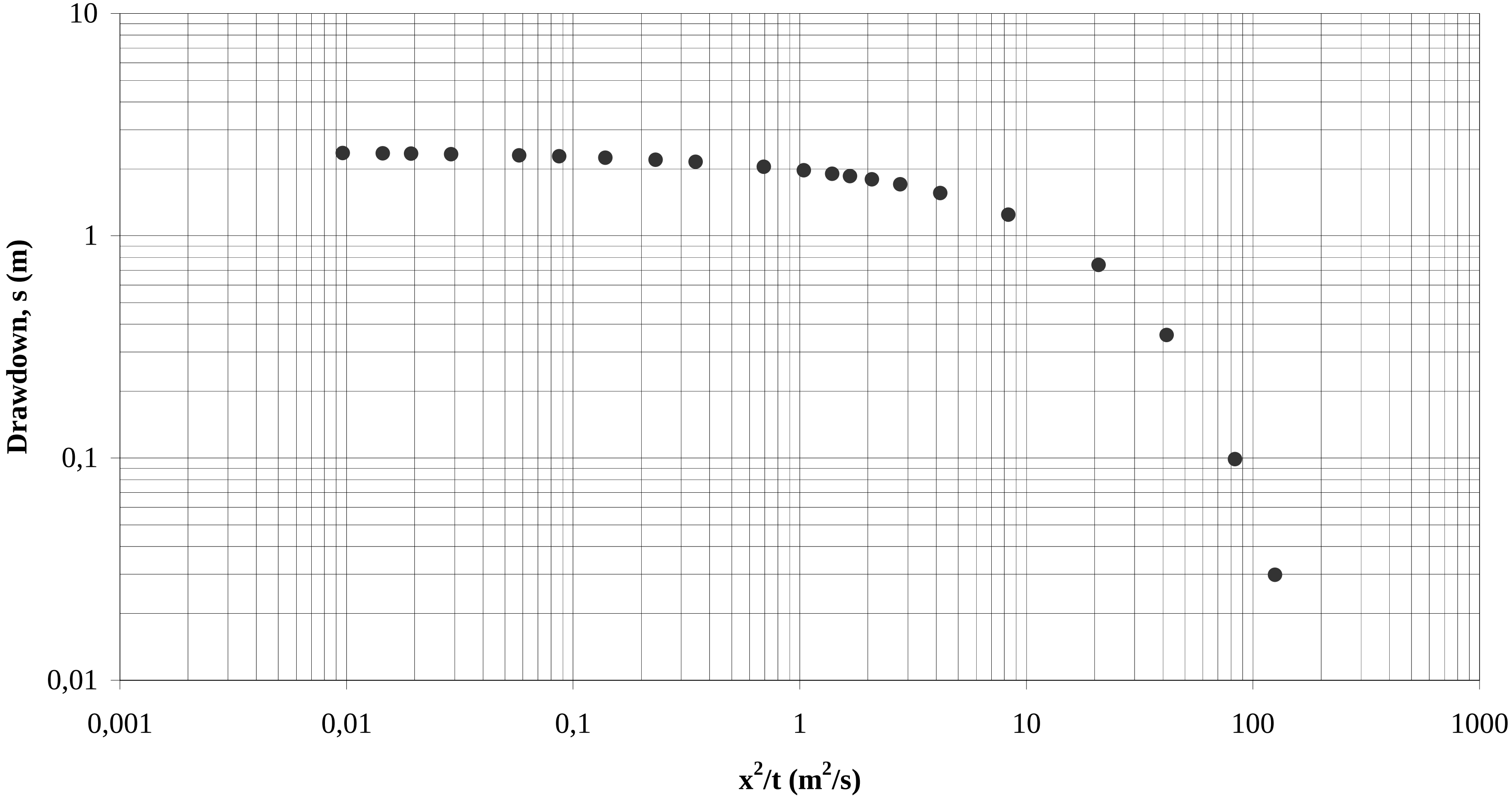

Fig. 4.2 Logarithmic plot of observed drawdown versus x^2/t for constant drawdown

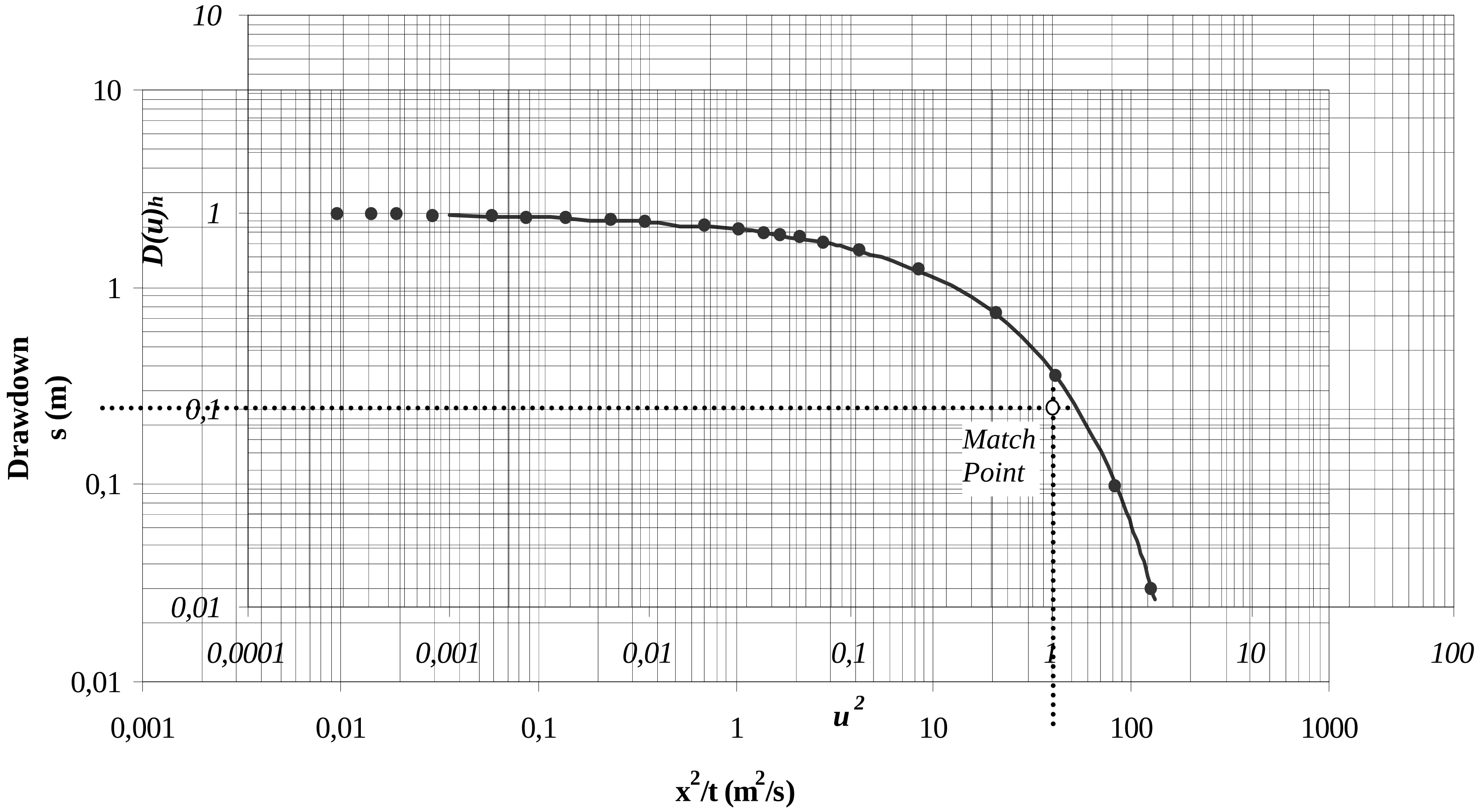

Fig. 4.3 Type curve matching to observed data for constant drawdown

From Fig. 4.3, match point coordinates are obtained as:

$u^2=1$

$D(u)_h=0.1$

$x^2/t=40\ m^2/s$

$s=0.24\ m$

Using the value of x^2/t, time t corresponding to the match point is calculated as:

$$t = \frac{x^2}{(x^2/t)} = \frac{50^2}{40} = 62.5 \text{ seconds.}$$

The discharge Q in Eq. (4.6) is time dependent and must be determined from the plot of observed values of Q versus t given in Table 4.1, corresponding to the time obtained from the match point coordinates. From the log-log plot of observed discharge versus time presented in Fig. 4.4, Q is obtained as:

$Q=2.2\times10^{-4}\ m^2/s$

Finally, transmissivity and storage coefficient are obtained using Eqs. (4.6) and (4.5), as:

$$T = \frac{QD(u)_h x}{4su}\sqrt{\pi} = \frac{2.2\times10^{-4}\times0.1\times50}{4\times0.24\times1}\sqrt{\pi} = 2.031\times10^{-3}\ m^2/s$$

$$S = \frac{4Ttu^2}{x^2} = \frac{4\times2.031\times10^{-3}\times62.5\times1}{50^2} = 2.031\times10^{-4}$$

4.1.3 Comparison of Results

Transmissivity and storage coefficient obtained by type curve method are almost the same as those assumed for the hypothetical aquifer, which means the two methods are consistent with each other. The results obtained by Marquardt algorithm and type curve are shown in Table 4.5.

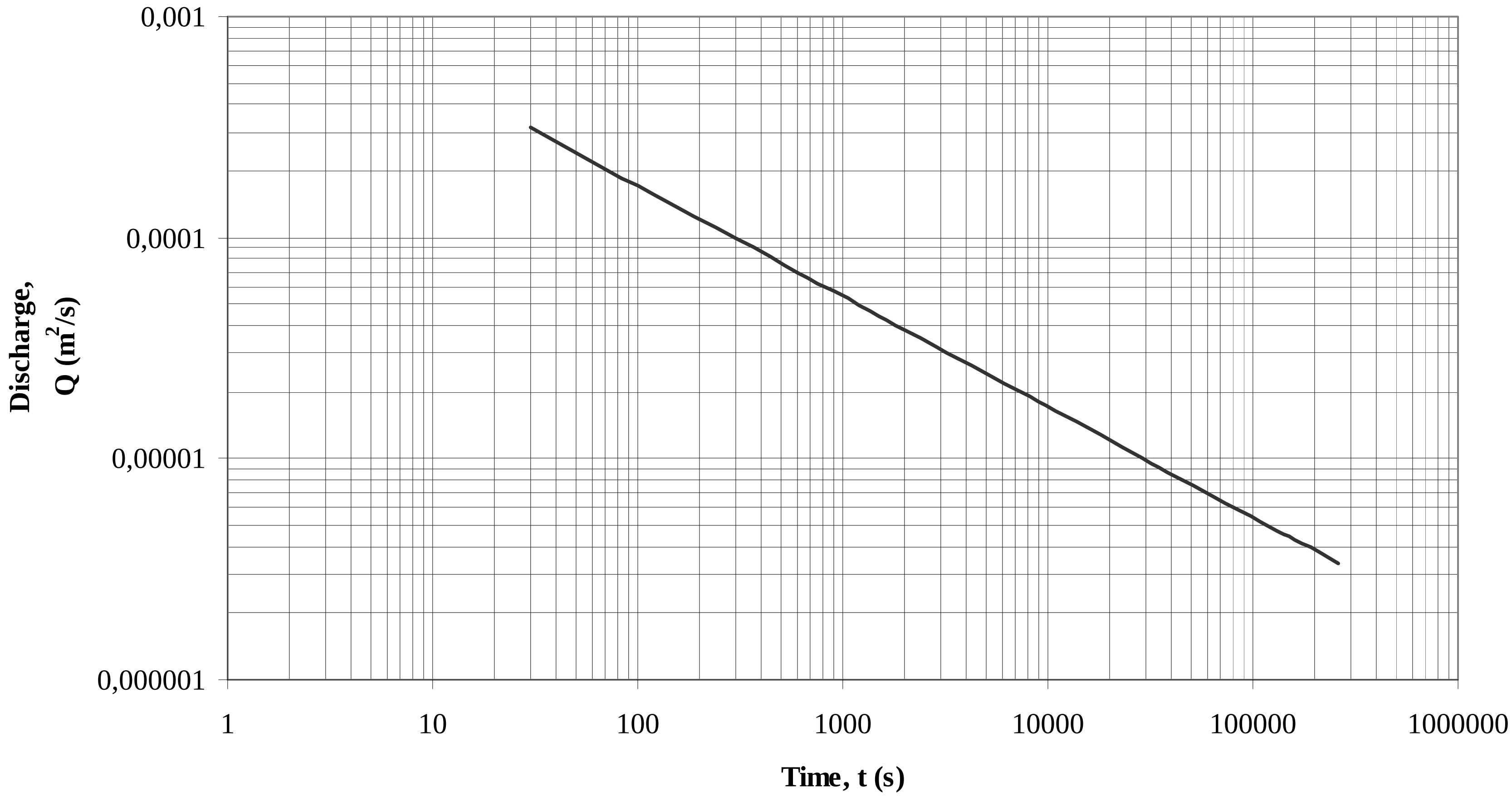

Fig. 4.4 Logarithmic plot of observed discharge versus time for constant drawdown

Table 4.5 Comparison of aquifer parameters using different methods for constant drawdown

Method of Analysis	Transmissivity $[m^2/s]$	Error (T)	Storage Coefficient	Error (S)
Marquardt algorithm	2.000×10^{-3}	0.00%	2.000×10^{-4}	0.00%
Type curve	2.031×10^{-3}	1.55%	2.031×10^{-4}	1.55%

It is obvious that the results of the present study are almost identical with those of conventional method of type curve.

4.2 Constant Discharge Case

Marquardt algorithm is applied first to synthetic data, then to published field data. The results are reasonable for both examples.

4.2.1 Synthetic Data Generation

Synthetic aquifer for this case is assumed to have the same basic shape and characteristics with the one in the previous case, except for the transmissivity and the storage coefficient, which are ten times of the values of the aquifer in the previous case, namely $T^*=1728\ m^2/day$ ($0.02\ m^2/s$) and $S^*=0.002$. Both time series and location of the fictitious observation well are identical with the case of constant drawdown. There is a constant pumping rate of $Q_0=50\ m^2/day$ ($5.787\times10^{-4}\ m^2/s$) instead of a constant drawdown in the stream. Drawdown values, which constitute the observed drawdown series s_m^{obs} for 20 time series, are computed (simulated) from Eq. (2.29). The simulated drawdown values are presented in Table 4.6.

Table 4.6 Simulation of observed values for constant discharge

i	t_i [s]	u_i	SIMULATED VALUES s_i^{obs} [m]
1	30	1.44338	0.00538457
2	60	1.02062	0.033381314
3	120	0.72169	0.113536725
4	300	0.45644	0.350847214
5	600	0.32275	0.670625173
6	900	0.26352	0.931661427
7	1200	0.22822	1.157267653
8	1500	0.20412	1.358741878
9	1800	0.18634	1.542451789
10	2400	0.16137	1.871243899
11	3600	0.13176	2.427677972
12	7200	0.09317	3.695028498
13	10800	0.07607	4.67255692
14	18000	0.05893	6.226736613
15	28800	0.04658	8.056502629
16	43200	0.03804	10.02197907
17	86400	0.0269	14.46187957
18	129600	0.02196	17.87020835
19	172800	0.01902	20.74405954
20	259200	0.01553	25.56558799

4.2.1.1 Results of Marquardt Solution

The optimization procedure to determine transmissivity and storage coefficient is similar to the procedure listed for the previous case. In this case the two parameters are optimized simultaneously using drawdown measurements.

1. Initial parameter values are assigned as T_0=0.1 m^2/s, S_0=0.1 and $\lambda=5\times10^6$. The high value of initial lambda is an indication of very poor initial estimates, which are 500% and 5000% of T^* and S^* respectively. However, the value of lambda first decreases then completely vanishes after a few iterations as the convergence is approached.
2. Drawdown values s(x,t) for 20 values of time, which constitute $s^c(\mathbf{p})$, are computed from Eq. (2.29) using initial estimates T_0 and S_0.
3. $\frac{\partial s}{\partial T}$ and $\frac{\partial s}{\partial S}$ are calculated using Eqs. (3.66) and (3.72c) respectively.
4. Coefficient matrix $[\mathbf{A}_k^T\mathbf{A}_k+\lambda_k\mathbf{I}]$ and vector $\mathbf{A}_k^T[s^{obs}-s^c(\mathbf{p})]_k$ are determined.
5. Respective increments ΔT and ΔS are calculated. New estimates for the parameters are computed using Eqs. (3.73) and (3.74); and the iteration procedure is repeated.

Table 4.7 Summary of optimization process for constant discharge

k	λ_k	T_{k-1} [m^2/s]	ΔT_k [m^2/s]	T_k [m^2/s]	Error (T)*	S_{k-1}	ΔS_k	S_k	Error (S)*	E(p)**
1	5E+06	0.1***	-9E-05	0.0999	399.56%	0.1***	-1E-04	0.0999	4894.24%	1660
2	5526	0.099	-0.075	0.0253	26.60%	0.0999	-0.0989	0.0010	-50.02%	1660
3	0	0.025	-0.006	0.0194	-3.17%	0.0010	0.0007	0.0017	-17.75%	145.4
4	0	0.019	0.0006	0.0199	-0.01%	0.0017	0.0003	0.0019	-2.73%	28.98
5	0	0.02	2E-06	0.02	0.00%	0.0019	5.4E-05	0.002	-0.06%	0.400
6	0	0.02	-6E-07	0.02	0.00%	0.002	1.2E-06	0.002	0.00%	2E-04
7	0	0.02	-3E-10	0.02	0.00%	0.002	5.4E-10	0.002	0.00%	3E-11
8	0	0.02	-9E-16	0.02	0.00%	0.002	1.8E-16	0.002	0.00%	1E-24
9	0	0.02	1E-19	0.02	0.00%	0.002	-9E-21	0.002	0.00%	1E-32

**Computed by Eq. (3.5)*
*** Computed by Eq. (3.55)*
****Initial estimates*

The first iteration table is given in Table A.3 and a summary of the iteration process for constant discharge case is presented in Table 4.7.

The true transmissivity T^* is reached after 5 iterations with no error and the true storage coefficient S^* is reached after 6 iteration cycles with no error as well ($T_{OPT}=T^*$; $S_{OPT}=S^*$). Residual squares, computed by Eq. (3.55), are minimized to 1×10^{-32} after a total of nine runs. The iteration table for k=9 is given in Table A.4.

4.2.1.2 Results of Type Curve Method

Lohman (1972) gives the method of type curve for an aquifer in the vicinity of a stream (or an aquifer having a fracture) where water is discharged at a constant rate. The drawdown for such a case has already been given in Eq. (2.28):

$$s(x,t) = \frac{Q_0}{2T}\left\{\sqrt{\frac{4Tt}{\pi S}}e^{-u^2} + x\left[\operatorname{erf}(u) - 1\right]\right\}$$

Solving Eq. (2.28) for T,

$$T = \frac{Q_0}{2s}\left\{\sqrt{\frac{4Tt}{\pi S}}e^{-u^2} + x\left[\operatorname{erf}(u) - 1\right]\right\} \tag{4.7a}$$

$$T = \frac{Q_0 x}{2s}\left[\sqrt{\frac{4Tt}{\pi x^2 S}}e^{-u^2} - \operatorname{erfc}(u)\right] \tag{4.7b}$$

$$T = \frac{Q_0 x}{2s}\left[\frac{e^{-u^2}}{u\sqrt{\pi}} - \operatorname{erfc}(u)\right] \tag{4.7c}$$

The bracketed part of the above equation, which is a function of (u) may be written $D(u)_q$, the drain function of (u) for constant discharge; where the subscript q identifies the constant discharge. Namely,

$$D(u)_q = \left[\frac{e^{-u^2}}{u\sqrt{\pi}} - \operatorname{erfc}(u)\right] \tag{4.8}$$

which lets us to write Eq. (4.7c) as

$$T = \frac{Q_0 x}{2s} D(u)_q \tag{4.9}$$

Equation for storage coefficient has already been derived in Eq. (4.5). Values of $D(u)_q$ for corresponding values of (u) and u^2, computed from Eq. (4.8), are given in Table 4.8. A logarithmic plot of $D(u)_q$ versus u^2, which is the type curve for this case, is given in Fig. 4.5.

Table 4.8 Values of $D(u)_q$, u and u^2 for constant discharge

u	u^2	$D(u)_q$	u	u^2	$D(u)_q$
0.0510	0.0026	10.0913	0.3000	0.0900	1.0474
0.0600	0.0036	8.4370	0.3317	0.1100	0.8847
0.0700	0.0049	7.0993	0.3605	0.1300	0.7641
0.0800	0.0064	6.0975	0.4000	0.1600	0.6303
0.0900	0.0081	5.3195	0.4359	0.1900	0.5327
0.1000	0.0100	4.6982	0.4796	0.2300	0.4370
0.1140	0.0130	4.0132	0.5291	0.2799	0.3516
0.1265	0.0160	3.5312	0.5745	0.3301	0.2895
0.1414	0.0200	3.0695	0.6164	0.3799	0.2426
0.1581	0.0250	2.6574	0.6633	0.4400	0.1996
0.1732	0.0300	2.3547	0.7071	0.5000	0.1666
0.1871	0.0350	2.1204	0.7616	0.5800	0.1333
0.2000	0.0400	1.9330	0.8124	0.6600	0.1083
0.2236	0.0500	1.6483	0.8718	0.7600	0.0850
0.2449	0.0600	1.4406	0.9487	0.9000	0.0621
0.2646	0.0700	1.2798	1.0000	1.0000	0.0503

The procedure is exactly the same as in the previous case. Observed values of s versus x^2/t are plotted on log-log paper of the same scale as the type curve, and fitted to it by the usual curve-matching procedure (Lohman, 1972). Drawdown values that have already been simulated using Eq. (2.29), are tabulated versus x^2/t in Table 4.9, where x=50 m. The corresponding logarithmic plot is shown in Fig. 4.6, and matching of the two curves is presented in Fig. 4.7.

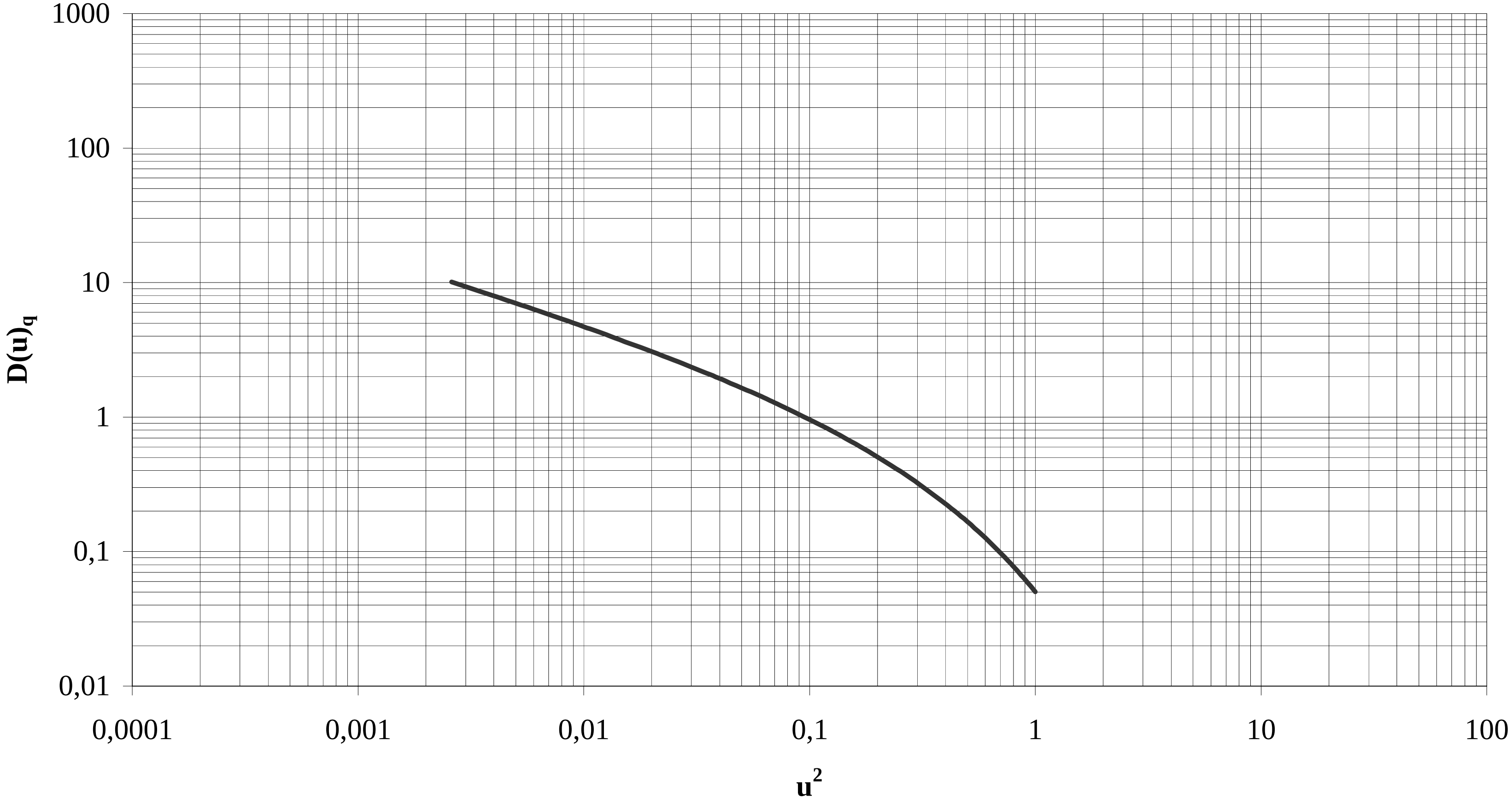

Fig. 4.5 Type curve for a semi-infinite aquifer-constant discharge case

Table 4.9 Values of t, x^2/t and s for constant discharge

i	t (sec)	x^2/t (m^2/s)	s^{obs} (m)	i	t (sec)	x^2/t (m^2/s)	s^{obs} (m)
1	30	83.3333	0.0054	11	3600	0.6944	2.4277
2	60	41.6667	0.0334	12	7200	0.3472	3.6950
3	120	20.8333	0.1135	13	10800	0.2315	4.6726
4	300	8.3333	0.3508	14	18000	0.1389	6.2267
5	600	4.1667	0.6706	15	28800	0.0868	8.0565
6	900	2.7778	0.9317	16	43200	0.0579	10.0220
7	1200	2.0833	1.1573	17	86400	0.0289	14.4619
8	1500	1.6667	1.3587	18	129600	0.0193	17.8702
9	1800	1.3889	1.5425	19	172800	0.0145	20.7441
10	2400	1.0417	1.8712	20	259200	0.0096	25.5656

The selected match points coordinates give:

$u^2=0.05$

$D(u)_q=0.7$

$x^2/t=2\ m^2/s$

$s=0.5\ m$

Value of time, t, is calculated from the value of x^2/t obtained from the curve match:

$$t=\frac{x^2}{(x^2/t)}=\frac{50^2}{2}=1250\ \text{seconds.}$$

Transmissivity is determined from Eq. (4.9):

$$T=\frac{Q_0 x}{2s}D(u)_q=\frac{5.787\times10^{-4}\times50}{2\times0.5}\times0.7=2.025\times10^{-2}\ m^2/s$$

Storage coefficient is determined from Eq. (4.5):

$$S=\frac{4Ttu^2}{x^2}=\frac{4\times2.025\times10^{-2}\times1250\times0.05}{50^2}=2.025\times10^{-3}$$

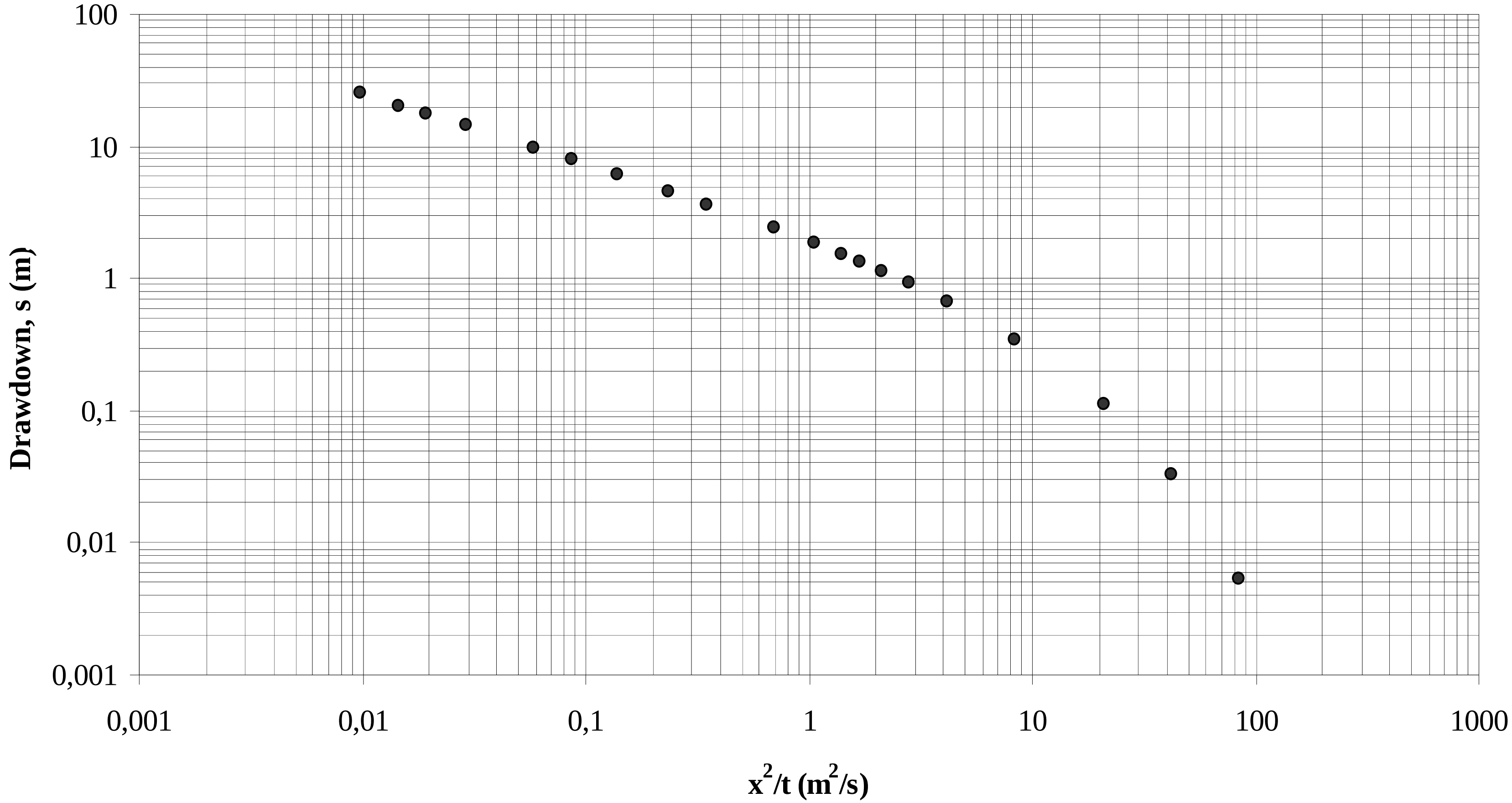

Fig. 4.6 Logarithmic plot of observed drawdown versus x^2/t for constant discharge

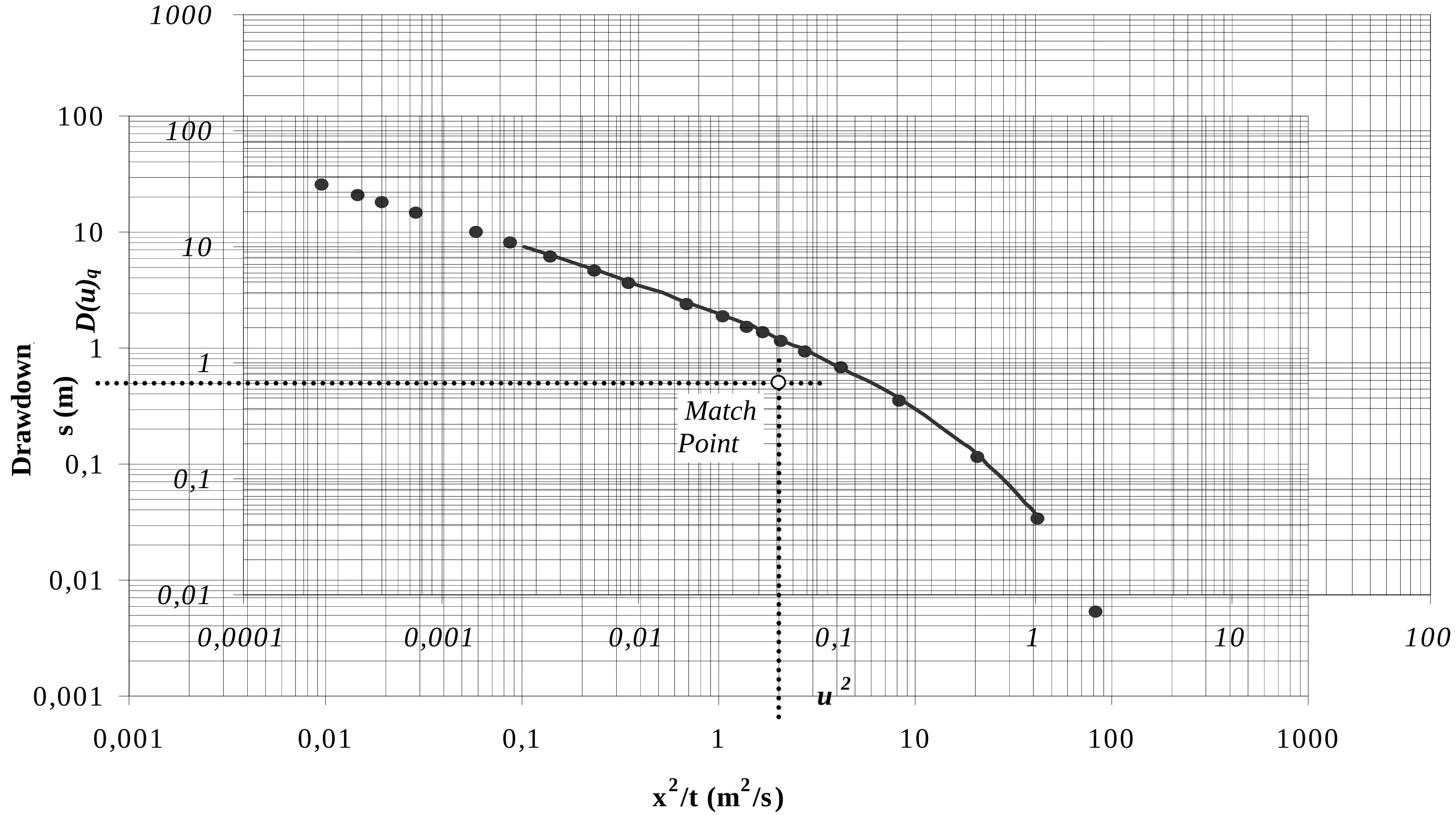

Fig. 4.7 Type curve matching to observed data for constant discharge

4.2.1.3 Comparison of Results

The aquifer parameters obtained by the two methods are presented in Table 4.10. It is clear that the parameters are in a close agreement. The slight error in type curve method may be due to reading errors.

Table 4.10 Comparison of aquifer parameters using different methods for constant discharge

Method of Analysis	**Transmissivity [m^2/s]**	**Error (T)**	**Storage Coefficient**	**Error (S)**
Marquardt algorithm	2.000×10^{-2}	0.00%	2.000×10^{-3}	0.00%
Type curve	2.025×10^{-2}	1.25%	2.025×10^{-3}	1.25%

4.2.2 Application to Field Data

The method is also demonstrated using field data, obtained from the H-3 multiwell pumping test performed in 1985 and early 1986 in the Culebra Dolomite member of the Rustler Formation located above the proposed Waste Isolation Pilot Plant (WIPP) in southeastern New Mexico, as reported by Tomasko (1987). The assumptions stated and the linear flow model utilized are referred to Jenkins and Prentice (1982) which makes it possible to use the data obtained in the test to determine the aquifer parameters.

Results of drawdown are plotted in Fig. 3 of Tomasko (1987) against square root of total time for observation wells located at various distances from the fracture ranging from x=0 m to x=4500 m where the pumping well intersects an 1800-meter long (L=1800 m) vertical fracture of infinite conductivity in a porous medium. The production well was pumped at an average rate, Q_T, of approximately 3.16×10^{-4} m^3/s for 1488 hours, which yields

$$Q_0 = \frac{3.16\times10^{-4}\,m^3/s}{1800\ m} = 1.756\times10^{-7}\,m^2/s$$

The example is identical to the one shown in Fig. 2.3. The perpendicular distance from the fracture to the observation well is selected as x=75 m. Four coordinates were available for use up to the recovery time of 1488 hours, which is tabulated in Table 4.11 below.

Table 4.11 Drawdown values from field data for constant discharge case (Tomasko, 1987)

Time		**Drawdown (m)**
[hr]	**[s]**	
30.02	108088	3.48
243.87	877943	13.44
677.43	2438732	24.00
1268.53	4566711	34.56

4.2.2.1 Results of Marquardt Solution

Application of Marquardt algorithm is identical with the procedure given for synthetic data in section 4.2.1.1, except that there exist 4 time values instead of 20. Initial estimates of both transmissivity and storage coefficient are $T_0=S_0=1\times10^{-10}$ where T_0 has a dimension of m^2/s. The first iteration table is given in Table A.5. The optimized transmissivity is obtained as $T_{OPT}=2.243\times10^{-6}$ m^2/s, and the optimized storage coefficient is obtained as $S_{OPT}=1.445\times10^{-5}$; which indicates that initial estimates for T and S are 0.004% and 0.0007% of the respective optimized values. After 21 iterations convergence was reached with residual squares of 0.23. The iteration table for k=21 and the summary table are given in Tables A.6 and 4.12 respectively.

Table 4.12 Summary of optimization process for field data

k	λ_k	T_{k-1} [m^2/s]	ΔT_k [m^2/s]	T_k [m^2/s]	S_{k-1}	ΔS_k	S_k	E(p)*
1	0	1E-10**	1E-10	2E-10	1E-10**	1E-10	2E-10	7,22E+12
2	0	2E-10	2E-10	4E-10	2E-10	2E-10	4E-10	1,8E+12
3	0	4E-10	4E-10	8E-10	4E-10	4E-10	8E-10	4,51E+11
4	0	8E-10	8E-10	1,6E-09	8E-10	8E-10	1,6E-09	1,13E+11
5	0	1,6E-09	2E-09	3,2E-09	1,6E-09	2E-09	3,2E-09	2,82E+10
6	0	3,2E-09	3E-09	6,39E-09	3,2E-09	3E-09	6,4E-09	7,05E+09
7	0	6,39E-09	6E-09	1,28E-08	6,4E-09	6E-09	1,28E-08	1,76E+09
8	0	1,28E-08	1E-08	2,55E-08	1,28E-08	1E-08	2,56E-08	4,4E+08
9	0	2,55E-08	3E-08	5,07E-08	2,56E-08	3E-08	5,13E-08	1,1E+08
10	0	5,07E-08	5E-08	1E-07	5,13E-08	5E-08	1,03E-07	27309788
11	0	1E-07	1E-07	1,96E-07	1,03E-07	1E-07	2,06E-07	6770196
12	0	1,96E-07	2E-07	3,77E-07	2,06E-07	2E-07	4,14E-07	1664340
13	0	3,77E-07	3E-07	6,95E-07	4,14E-07	4E-07	8,36E-07	402386
14	0	6,95E-07	5E-07	1,19E-06	8,36E-07	9E-07	1,69E-06	94132,34
15	0	1,19E-06	6E-07	1,79E-06	1,69E-06	2E-06	3,38E-06	20649,07
16	0	1,79E-06	4E-07	2,22E-06	3,38E-06	3E-06	6,42E-06	4005,792
17	0	2,22E-06	9E-08	2,31E-06	6,42E-06	4E-06	1,05E-05	618,1785
18	0	2,31E-06	-4E-08	2,26E-06	1,05E-05	3E-06	1,36E-05	60,69992
19	0	2,26E-06	-2E-08	2,25E-06	1,36E-05	8E-07	1,44E-05	2,154478
20	0	2,25E-06	-3E-09	2,24E-06	1,44E-05	5E-08	1,45E-05	0,233306
21	0	2,24E-06	-2E-10	2,24E-06	1,45E-05	1E-09	1,45E-05	0,229297

* *Computed by Eq. (3.55)*
***Initial estimates*

The summary table above contains no columns for percentage error since the field drawdown values of are not simulated using synthetic parameters but taken directly from a published paper. According to Tomasko (1987), the aquifer parameters are $T=2.7\times10^{-6}$ m^2/s and $S=2\times10^{-5}$, which yields that transmissivity and storage coefficient obtained by Marquardt algorithm are respectively 83.07% and 72.25% of the ones given in the paper. Drawdown values were also calculated from Eq. (2.29) using the aquifer parameters given in the paper to allow for comparison. Table 4.13 presents the drawdown values and sum of the residual squares computed from Eq. (3.55) using the aquifer parameters obtained from both Tomasko (1987) and present study.

Table 4.13 Comparison of drawdown and error values computed using aquifer parameters obtained from different sources

Time [s]	**Tomasko (1987)** ***$T=2.7\times10^{-6}$ m²/s*** ***$S=2\times10^{-5}$***				**Present study** ***$T=2.243\times10^{-6}$ m²/s*** ***$S=1.445\times10^{-5}$***		
	s^{obs} [m]	**s^{c} [m]***	**$s^{obs} - s^{c}$**	**E(p)**	**s^{c} [m]***	**$s^{obs} - s^{c}$**	**E(p)**
108088	3.480	2.413	1.067	104.915	3.257	0.223	0.229
877943	13.440	10.341	3.100		13.532	-0.092	
2438732	24.000	18.700	5.300		24.330	-0.330	
4566711	34.560	26.431	8.129		34.311	0.249	

**Obtained by post-simulation*

When compared to the observed values s^{obs}, which were given in Fig 3 of the paper, the drawdown values obtained by iteration in the present study deviate much less than those obtained by solution of Eq. (2.29) using the aquifer parameters given in the paper considered. In addition, E(**p**), which is computed by summing the squares of the difference between observed and calculated drawdown values, is negligible in the present study; while that obtained by simulation of published aquifer parameters is 104.915, which is an unacceptable value.

It can be concluded that the aquifer, on which the pump test was conducted, is much likely to have a transmissivity of 2.243×10^{-6} m²/s rather than 2.7×10^{-6} m²/s, and/or a storage coefficient of 1.445×10^{-5} rather than 2×10^{-5}.

4.2.2.2 Results of Type Curve Method

Type curve method is applied to the set of data obtained from the paper considered. The procedure of type curve method for constant discharge and the type curve itself has already been explained in section 4.2.1.2. Observed values of s versus x^2/t, where x=75 m, are presented in Table 4.14, and the plot of observed drawdown versus time is given in Fig. 4.8.

Table 4.14 Values of t, x^2/t and s for field data from Tomasko, 1987

i	t (sec)	x^2/t (m^2/s)	s^{obs} (m)
1	108088	3.48	0.0520
2	877943	13.44	0.0064
3	2438732	24.00	0.0023
4	4566711	34.56	0.0012

From the matching of the curves given in Fig. 4.9, the match point coordinates obtained are:

u^2=0.01

$D(u)_q$=3.8

x^2/t=0.0075 m^2/s

s=10 m

Values of the corresponding time, transmissivity, and storage coefficient are determined in a similar manner as done in section 4.2.1.2:

$$t = \frac{x^2}{(x^2/t)} = \frac{75^2}{0.0075} = 750000 \text{ seconds.}$$

$$T = \frac{Q_0 x}{2s} D(u)_q = \frac{1.756\times10^{-7}\times75}{2\times10}\times3.8 = 2.502\times10^{-6}\ m^2/s$$

$$S = \frac{4Ttu^2}{x^2} = \frac{4\times2.502\times10^{-6}\times750000\times0.01}{75^2} = 1.334\times10^{-5}$$

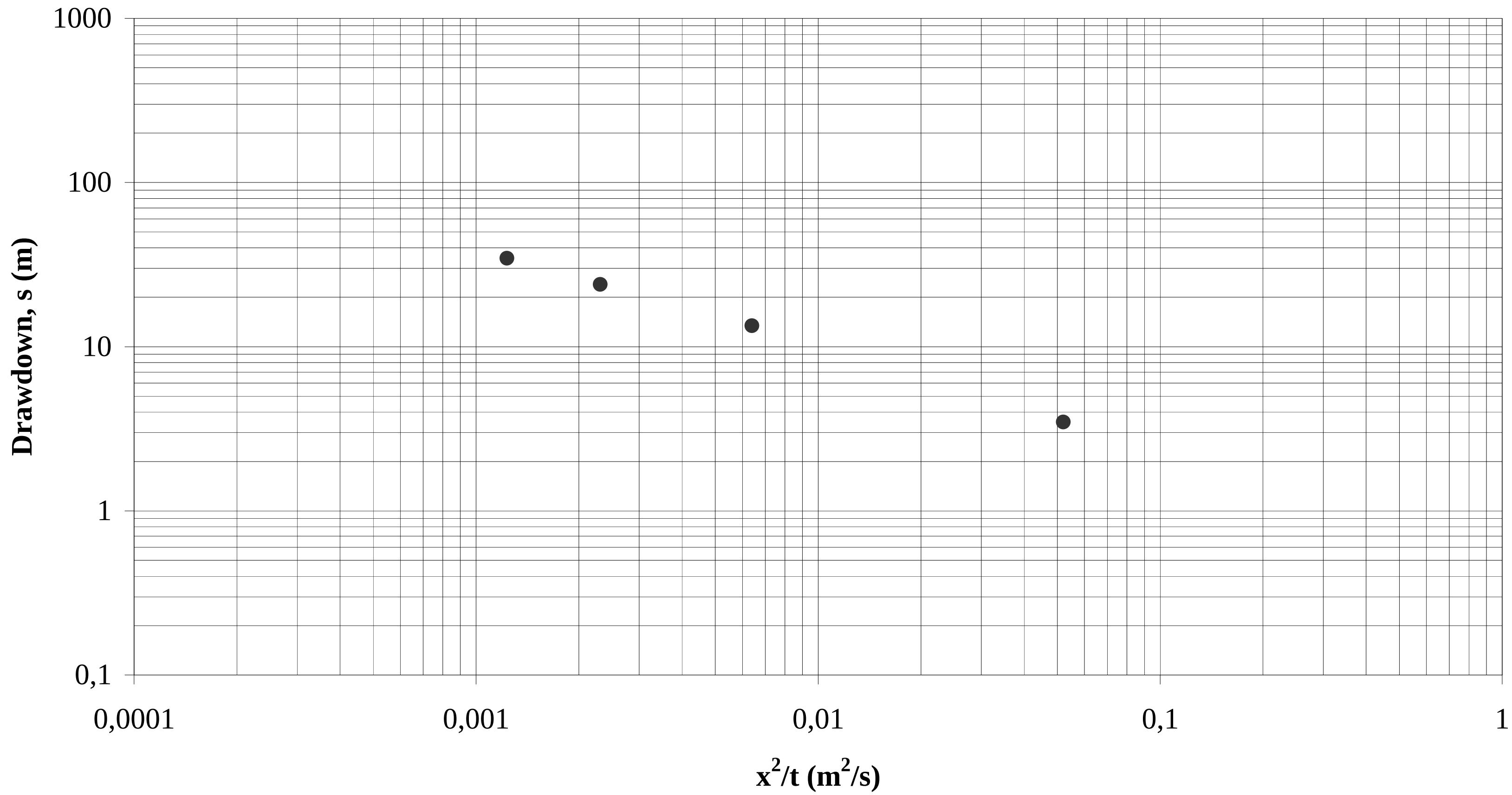

Fig. 4.8 Logarithmic plot of observed drawdown versus x^2/t for field data of Tomasko, 1987

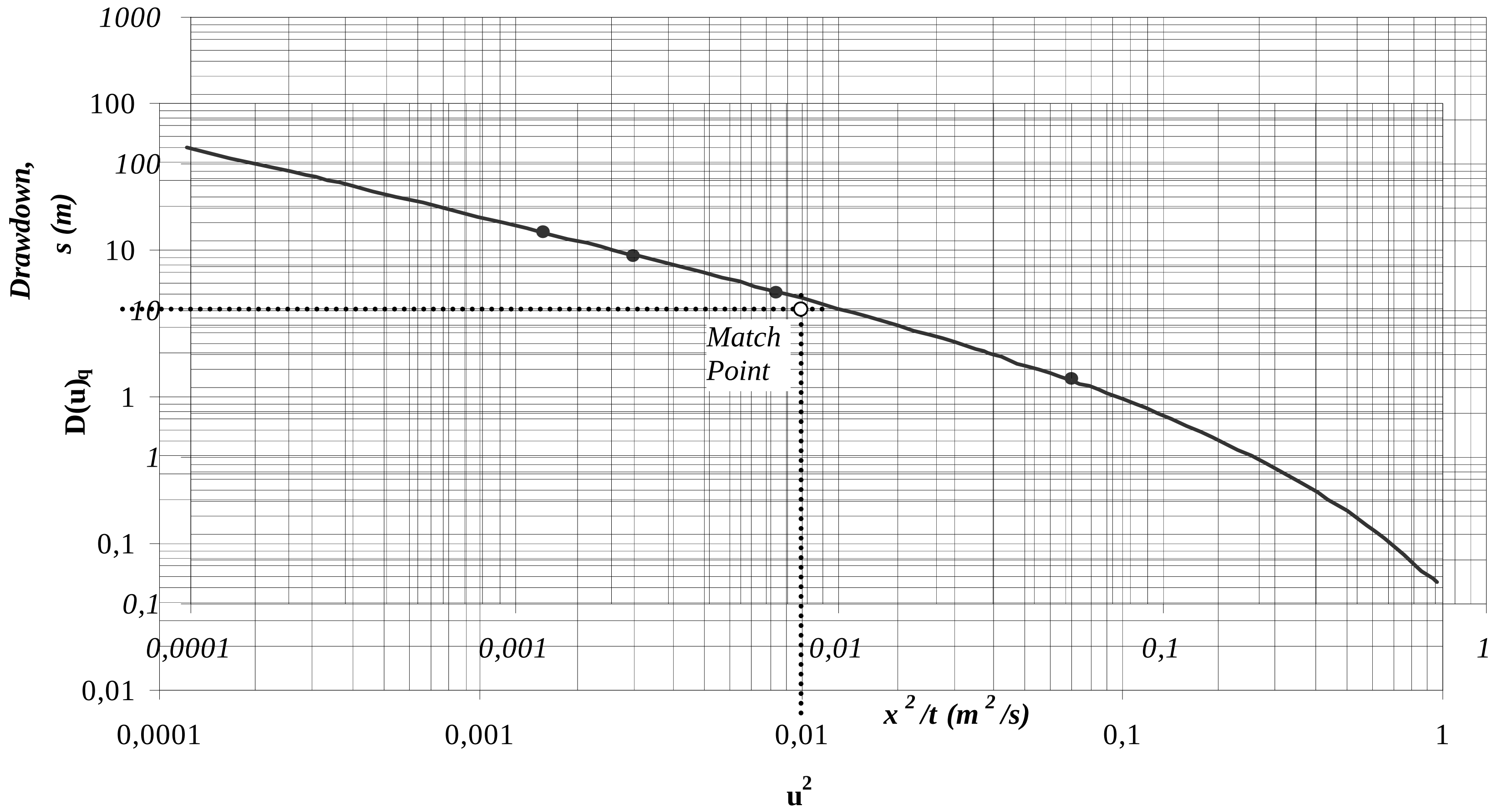

Fig. 4.9 Type curve matching to field data of Tomasko, 1987

4.2.2.3 Comparison of Results

The aquifer parameters obtained by Marquardt algorithm and type curve method; and those given by Tomasko (1987) are presented below in Table 4.15 for comparison:

Table 4.15 Comparison of aquifer parameters from different references for constant discharge

Reference	Transmissivity [m^2/s]	Storage Coefficient
Marquardt algorithm	2.243×10^{-6}	1.445×10^{-5}
Type curve	2.502×10^{-6}	1.334×10^{-5}
Tomasko (1987)	2.700×10^{-6}	2.000×10^{-5}

It can be inferred from Table 4.15 that the transmissivity obtained by type curve is close to the value obtained by both of the remaining methods, being approximately the arithmetic mean of them. This makes the transmissivity given by Tomasko (1987) acceptable. However, the value of storage coefficient given in the paper lies far from the values obtained by both Marquardt algorithm and type curve method, which means that the true value of storage coefficient of the aquifer considered may be accepted as the one obtained by Marquardt algorithm.

4.3 Discussion

Marquardt algorithm was applied at first for a sudden and constant drop in a stream adjacent to a semi-infinite and confined aquifer; then for a constant discharge in the stream or in a fractured rock. The algorithm converged quickly in the first case of constant drawdown, for poor initial estimates above or below the true value.

The case of constant discharge involves considerably complicated equations, which may yield negative values of the aquifer parameters in the first few iterations. This makes the coefficient matrix singular and prevents convergence. However, as explained in section 3.4, the role of lambda is to assure convergence. When lambda is given an appropriate value, convergence will be reached within a few iterations.

Tomasko's (1987) data of the pump test were used to check the performance of the proposed method. Four data points were appropriate to use for constant discharge case, which were in the form of plotted values of drawdown versus square root of time in an observation well 75 meters away from the pump.

The transmissivity and the storage coefficient were obtained by the proposed method with a corresponding sum of residual squares of 0.23. However, the parameters given by Tomasko (1987) differ from the ones obtained by the present study. This difference may be due to uncertainties in the field measurements, and deviations from idealized aquifer assumptions; for example, nonhomogeneity and/or anisotropy of the aquifer. In addition, the linear flow equations used for the field data assume that the fracture appears to be infinite during an aquifer test. Fractures die out, become clogged with clay, or terminate against other structures (Jenkins and Prentice, 1982). This violates the assumption of infinite fracture length. The number of data points is also too few from statistical point of view, which enhances the effect of observation errors and outliers.

The slight error introduced in the type curve matching method may be due to the subjectivity involved in visual inspection and matching of curves.

Nevertheless, the results obtained by the proposed method are in a reasonable agreement with the method of type curves and observed field data.

CHAPTER 5

SUMMARY AND CONCLUSIONS

5.1 Summary

An optimization method has been presented for the identification of semi-infinite confined aquifer parameters, transmissivity, T, and storage coefficient, S, using Marquardt algorithm for two boundary conditions. The imposed boundary conditions involve step drawdown in the stream stage and step discharge in the stream or in a fracture due to pumping. Piezometric head measurements in an observation well, and discharge measurements, with time, are required for the case of step drawdown, whereas only piezometric head observations with respect to time are required for the case of step discharge.

A spreadsheet software, Microsoft Excel, has been used to run the algorithm, in order to ease the visualization of the process and to enable the majority, who are familiar with Microsoft Office but have no programming background, to easily apply the proposed method.

Conventional type curve matching method has been used for comparison of results, and almost an exact agreement is observed. A complete summary of the whole work is given in Table 5.1. Note that T^* and S^* of example 3 in Table 5.1 are not used in optimization but given in the paper by Tomasko, 1987.

Table 5.1 General summary

CASE	EXAMPLE		Given Aquifer Parameters	Observed Data	MARQUARDT ALGORITHM (PRESENT STUDY)				TYPE CURVE
					Determined Parameter(s)	Number of iterations	E(p) (Residual Squares)	Results	Results
Constant Drawdown	1	Synthetic Data	$T^*=2\times10^{-3}$ m^2/s $S^*=2\times10^{-4}$	s(x,t)	T/S	7	0	$T_{OPT}=2\times10^{-3}$ m^2/s $S_{OPT}=2\times10^{-4}$	$T=2.031\times10^{-3}$ m^2/s $S=2.031\times10^{-4}$
				Q(t)	T.S	1	0		
Constant Discharge	2	Synthetic Data	$T^*=2\times10^{-2}$ m^2/s $S^*=2\times10^{-3}$	s(x,t)	T and S	6	0	$T_{OPT}=2\times10^{-2}$ m^2/s $S_{OPT}=2\times10^{-3}$	$T=2.025\times10^{-2}$ m^2/s $S=2.025\times10^{-3}$
	3	Field Data	$T^*=2.7\times10^{-6}$ m^2/s $S^*=2\times10^{-5}$	s(x,t)	T and S	21	0.23	$T_{OPT}=2.243\times10^{-6}$ m^2/s $S_{OPT}=1.445\times10^{-5}$	$T=2.502\times10^{-6}$ m^2/s $S=1.334\times10^{-5}$

5.2 Conclusions

The following conclusions are drawn from this study:

1. The parameters estimated using the present method are reliable since the sums of residual squares almost vanish after a few iterations.

2. Convergence is reached quickly, and unique estimates of the parameters are obtained for different initial estimates; which means that the method is stable.

3. Although the proposed method is applicable to one-dimensional *confined* flow in a homogeneous isotropic aquifer which is bounded on one side by a stream, it also provides a good approximation for *unconfined* flow if changes in water levels are small in comparison with saturated thickness (Önder, 1994).

4. The method is developed mainly for constant drawdown in the stream or constant discharge due to pumping from the aquifer. Therefore, the method developed in this work is not applicable to the cases where there is an arbitrary variation in the stream stage or in the pumping pattern.

5.3 Future Recommendations

This work can be expanded to the following cases:

1. There may exist cases where the observation is performed at different locations for a specific value of time (unlike the current study; where t

is constant and x is variable). In these cases, observed drawdown values are function of space rather than time in Eqs. (2.10) and (2.29). The Marquardt optimization procedure presented in this study is also applicable for such cases. Since there will be only one observed discharge value, β can be determined in one computation step directly from Eq. (2.20) without iteration.

2. For arbitrary variation of stream stage or pumping rate, the use of convolution integral in discrete form may be considered. Then the present method must be adapted.

3. In the present work, hydraulic parameters of a semi-infinite aquifer are determined. By using appropriate analytical models; other types, such as finite aquifer, may also be considered.

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APPENDIX

ITERATION TABLES

Iteration tables for constant drawdown case, constant discharge case, and the example of Tomasko (1987) for constant discharge case are presented. The first and the last iterations for each example are given.

Table A.1 Iteration table for constant drawdown, k = 1

ITERATION 1 (k = 1)											
	α_{k-1} =	0,1m^2/s		β_{k-1} =	0,001m^2/s		λ_k =	0	A_k for α	A_k for β	
i	t_i [s]	u_i	erfc(u_i)	$s_i^c(\alpha)$ [m]	$s_i^{obs} - s_i^c(\alpha)$	$Q_i^c(\beta)$ [m^2/s]	$\psi_i^c(\beta)=(Q_i^c)^2$	$\psi_i^{obs} - \psi_i^c(\beta)$	$(\partial s/\partial\alpha)_i$	$(\partial\psi/\partial\beta)_i$
1	30	14,434	0	0	0,0989444	0,01563528	0,0002445	-0,0002444	6,5E-89	0,24446
2	60	10,206	0	0	0,3573954	0,01105581	0,0001222	-0,0001222	8E-44	0,12223
3	120	7,2169	0	0	0,7378427	0,00781764	6,112E-05	-6,109E-05	2,3E-21	0,06112
4	300	4,5644	1E-10	2,6E-10	1,244652	0,00494431	2,445E-05	-2,444E-05	5,5E-08	0,02445
5	600	3,2275	5E-06	1,2E-05	1,5553725	0,00349615	1,222E-05	-1,222E-05	0,00131	0,01222
6	900	2,6352	0,0002	0,000465	1,702066	0,0028546	8,149E-06	-8,145E-06	0,0344	0,00815
7	1200	2,2822	0,0012	0,002997	1,7895283	0,00247215	6,112E-06	-6,109E-06	0,16906	0,00611
8	1500	2,0412	0,0039	0,009342	1,8454502	0,00221116	4,889E-06	-4,887E-06	0,42852	0,00489
9	1800	1,8634	0,0084	0,020179	1,8809746	0,00201851	4,074E-06	-4,073E-06	0,78338	0,00407
10	2400	1,6137	0,0225	0,053949	1,9127954	0,00174808	3,056E-06	-3,055E-06	1,6162	0,00306
11	3600	1,3176	0,0624	0,149778	1,8954516	0,0014273	2,037E-06	-2,036E-06	3,1437	0,00204
12	7200	0,9317	0,1876	0,450318	1,6980971	0,00100925	1,019E-06	-1,018E-06	5,29564	0,00102
13	10800	0,7607	0,282	0,67681	1,517574	0,00082405	6,791E-07	-6,788E-07	5,7748	0,00068
14	18000	0,5893	0,4047	0,971176	1,2694314	0,00063831	4,074E-07	-4,073E-07	5,63824	0,00041
15	28800	0,4658	0,51	1,224046	1,0498886	0,00050463	2,546E-07	-2,545E-07	5,07729	0,00025
16	43200	0,3804	0,5906	1,417527	0,8795164	0,00041203	1,698E-07	-1,697E-07	4,45659	0,00017
17	86400	0,269	0,7037	1,688823	0,6383585	0,00029135	8,488E-08	-8,485E-08	3,38769	8,5E-05
18	129600	0,2196	0,7561	1,814715	0,5258235	0,00023788	5,659E-08	-5,657E-08	2,83354	5,7E-05
19	172800	0,1902	0,788	1,89111	0,4573927	0,00020601	4,244E-08	-4,242E-08	2,48368	4,2E-05
20	259200	0,1553	0,8262	1,982834	0,3751176	0,00016821	2,829E-08	-2,828E-08	2,05252	2,8E-05

CALCULATION OF α_k :	
$A_k^T A_k$ =	182,031
$\lambda_k I$ =	0
$A_k^T A_k + \lambda_k I = K_{1x1}$ =	182,031
K^{-1} =	0,00549
$A_k^T[s_i^{obs} - s_i^c(\alpha)]_k = L_{1x1}$ =	51,3999
$\Delta\alpha_k = K^{-1} * L$ =	0,28237
α_k [m^2/s] = $\alpha_{k-1} + \Delta\alpha_k$ =	0,38237
E(α) =	34,6527

CALCULATION OF β_k :	
$A_k^T A_k$ =	0,07934
$\lambda_k I$ =	0
$A_k^T A_k + \lambda_k I = M_{1x1}$ =	0,07934
M^{-1} =	12,6034
$A_k^T[s_i^{obs} - s_i^c(\beta)]_k = N_{1x1}$ =	-7,9E-05
$\Delta\beta_k = M^{-1} * N$ =	-0,001
β_k [m^2/s] = $\beta_{k-1} + \Delta\beta_k$ =	4E-07
E(β) =	7,9E-08

Table A.2 Iteration table for constant drawdown, k = 10

ITERATION 10 (k = 10)

i	t_i [s]	u_i	erfc(u_i)	$s_i^c(\alpha)$ [m]	$s_i^{obs} - s_i^c(\alpha)$	$Q_i^c(\beta)$ [m²/s]	$\psi_i^c(\beta)=(Q_i^c)^2$	$\psi_i^{obs} - \psi_i^c(\beta)$	A_k for α: $(\partial s/\partial\alpha)_i$	A_k for β: $(\partial\psi/\partial\beta)_i$
	α_{k-1} =	10m²/s		β_{k-1} =	0,0000004m²/s		λ_k =	0		
1	30	1,4434	0,0412	0,098944	0	0,00031271	9,778E-08	0	0,02434	0,24446
2	60	1,0206	0,1489	0,357395	0	0,00022112	4,889E-08	0	0,04877	0,12223
3	120	0,7217	0,3074	0,737843	0	0,00015635	2,445E-08	0	0,05805	0,06112
4	300	0,4564	0,5186	1,244652	0	9,8886E-05	9,778E-09	0	0,05018	0,02445
5	600	0,3227	0,6481	1,555384	0	6,9923E-05	4,889E-09	0	0,03938	0,01222
6	900	0,2635	0,7094	1,702531	0	5,7092E-05	3,259E-09	0	0,03329	0,00815
7	1200	0,2282	0,7469	1,792526	0	4,9443E-05	2,445E-09	0	0,02933	0,00611
8	1500	0,2041	0,7728	1,854792	0	4,4223E-05	1,956E-09	0	0,02651	0,00489
9	1800	0,1863	0,7921	1,901154	0	4,037E-05	1,63E-09	0	0,02437	0,00407
10	2400	0,1614	0,8195	1,966745	0	3,4962E-05	1,222E-09	0	0,02129	0,00306
11	3600	0,1318	0,8522	2,045229	0	2,8546E-05	8,149E-10	0	0,01753	0,00204
12	7200	0,0932	0,8952	2,148415	0	2,0185E-05	4,074E-10	0	0,01251	0,00102
13	10800	0,0761	0,9143	2,194384	0	1,6481E-05	2,716E-10	0	0,01024	0,00068
14	18000	0,0589	0,9336	2,240608	0	1,2766E-05	1,63E-10	0	0,00795	0,00041
15	28800	0,0466	0,9475	2,273935	0	1,0093E-05	1,019E-10	0	0,00629	0,00025
16	43200	0,038	0,9571	2,297043	0	8,2405E-06	6,791E-11	0	0,00514	0,00017
17	86400	0,0269	0,9697	2,327181	0	5,8269E-06	3,395E-11	0	0,00364	8,5E-05
18	129600	0,022	0,9752	2,340539	0	4,7577E-06	2,264E-11	0	0,00297	5,7E-05
19	172800	0,019	0,9785	2,348503	0	4,1203E-06	1,698E-11	0	0,00257	4,2E-05
20	259200	0,0155	0,9825	2,357951	0	3,3642E-06	1,132E-11	0	0,0021	2,8E-05

CALCULATION OF α_k :	
$A_k^T A_k$ =	0,01486
$\lambda_k I$ =	0
$A_k^T A_k + \lambda_k I = K_{1x1}$ =	0,01486
K^{-1} =	67,3019
$A_k^T[s_i^{obs} - s_i^c(\alpha)]_k = L_{1x1}$ =	0
$\Delta\alpha_k = K^{-1} * L$ =	0
α_k [m²/s] = $\alpha_{k-1} + \Delta\alpha_k$ =	10
$E(\alpha)$ =	0

CALCULATION OF β_k :	
$A_k^T A_k$ =	0,07934
$\lambda_k I$ =	0
$A_k^T A_k + \lambda_k I = M_{1x1}$ =	0,07934
M^{-1} =	12,6034
$A_k^T[s_i^{obs} - s_i^c(\beta)]_k = N_{1x1}$ =	0
$\Delta\beta_k = M^{-1} * N$ =	0
β_k [m²/s] = $\beta_{k-1} + \Delta\beta_k$ =	4E-07
$E(\beta)$ =	0

Table A.3 Iteration table for constant discharge, k = 1

ITERATION 1 (k = 1)											
T_{k-1} =		0,1m^2/s		S_{k-1} =	0,1	λ_k =	5000000	A_k for p		$A_k^T A_k$	
i	**t_i [s]**	**u_i**	**erfc(u_i)**	**s_i^{obs} [m]**	**$s_i^c(p)$ [m]**	**s_i^{obs} - $s_i^c(p)$**	**exp(-u_i^2)**	**($\partial s/\partial T)_i$**	**($\partial s/\partial S)_i$**	117,5866578	151,055693
1	30	4,56435	1,082E-10	0,0538457	3,596E-13	0,00538457	8,9577E-10	7,65E-11	-8,0096E-11	151,055693	200,2184321
2	60	3,22749	5,01E-06	0,3338131	3,206E-08	0,03338128	2,9929E-05	3,4641E-06	-3,7847E-06		
3	120	2,28218	0,0012488	1,1353673	1,499E-05	0,11352173	0,00547078	0,00082841	-0,00097834	**$A_k^T A_k + \lambda_k I = K_{2x2}$**	
4	300	1,44338	0,0412268	3,5084721	0,0010769	0,3497703	0,12451447	0,02443808	-0,03520722	5000117,587	151,055693
5	600	1,02062	0,1489147	6,7062517	0,0066763	0,66394891	0,35286608	0,07434057	-0,1411032	151,055693	5000200,218
6	900	0,83333	0,238593	9,3166143	0,0143926	0,91726879	0,49935179	0,10063014	-0,24455649		
7	1200	0,72169	0,3074345	11,572677	0,0227073	1,13456031	0,59402532	0,1088551	-0,33592855	**K^{-1}**	
8	1500	0,6455	0,3613104	13,587419	0,0310896	1,32765226	0,65924063	0,10591653	-0,41681268	1,99995E-07	-6,0418E-12
9	1800	0,58926	0,4046568	15,424518	0,039342	1,50310981	0,70664828	0,09601058	-0,48943034	-6,0418E-12	1,99992E-07
10	2400	0,51031	0,4704864	18,712439	0,055211	1,81603287	0,77073038	0,06428513	-0,61639546		
11	3600	0,41667	0,5556898	24,27678	0,0842826	2,34339542	0,84062374	-0,01943808	-0,82338743	**$A_k^T[s_i^{obs} - s_i^c(p)]_k = L_{2x1}$**	
12	7200	0,29463	0,6769222	36,950285	0,1560742	3,53895426	0,91685536	-0,29069942	-1,27004294	-435,1896487	
13	10800	0,24056	0,7337007	46,725569	0,21408	4,45847693	0,94377228	-0,53965582	-1,60114412	-576,422927	
14	18000	0,18634	0,7921474	62,267366	0,3084904	5,91824626	0,96587368	-0,9694285	-2,11547508		
15	28800	0,14731	0,8349687	80,565026	0,4213917	7,63511091	0,97853239	-1,50295924	-2,71095794	**ΔT =**	-8,7032E-05
16	43200	0,12028	0,8649288	100,21979	0,543733	9,47824608	0,98563656	-2,09299308	-3,3443368	**ΔS =**	-0,00011528
17	86400	0,08505	0,9042603	144,6188	0,821964	13,6399156	0,9927923	-3,45569653	-4,76394351		
18	129600	0,06944	0,9217661	178,70208	1,0363829	16,8338255	0,99518908	-4,5151275	-5,84870117	**T [m^2/s] =**	0,099912968
19	172800	0,06014	0,9322203	207,4406	1,2174593	19,5266003	0,99638963	-5,41294723	-6,76164553	**S =**	0,099884723
20	259200	0,0491	0,9446359	255,65588	1,5215901	24,0439979	0,99759164	-6,92462024	-8,29128091	**E(p) =**	1659,904133

Table A.4 Iteration table for constant discharge, k = 9

ITERATION 9 (k = 9)											
	T_{k-1} =	0,02m^2/s		S_{k-1} =	0,002	λ_k =	0	A_k for p		$A_k^T A_k$	
i	**t_i [s]**	**u_i**	**erfc(u_i)**	**s_i^{obs} [m]**	**$s_i^c(p)$ [m]**	**$s_i^{obs} - s_i^c(p)$**	**exp($-u_i^2$)**	**$(\partial s/\partial T)_i$**	**$(\partial s/\partial S)_i$**	1067420,3	11636362,58
1	30	1,44338	0,0412268	0,0538457	0,0053846	2,5153E-17	0,12451447	0,61095212	-8,80180606	11636362,58	127637171,7
2	60	1,02062	0,1489147	0,3338131	0,0333813	1,1796E-16	0,35286608	1,85851435	-35,2758005		
3	120	0,72169	0,3074345	1,1353673	0,1135367	0	0,59402532	2,72137738	-83,9821365	**$A^T A + \lambda I = K_{2x2}$**	
4	300	0,45644	0,518605	3,5084721	0,3508472	0	0,81193635	0,60752728	-181,49888	1067420,3	11636362,58
5	600	0,32275	0,6480769	6,7062517	0,6706252	0	0,90107511	-5,04548921	-284,857695	11636362,58	127637171,7
6	900	0,26352	0,7093881	9,3166143	0,9316614	0	0,93291196	-10,4626129	-361,204585		
7	1200	0,22822	0,7468856	11,572677	1,1572677	0	0,94924976	-15,424645	-424,387377	**K^{-1}**	
8	1500	0,20412	0,77283	13,587419	1,3587419	0	0,95918946	-19,9923101	-479,447838	0,000152389	-1,3893E-05
9	1800	0,18634	0,7921474	15,424518	1,5424518	0	0,96587368	-24,2357125	-528,868769	-1,3893E-05	1,27442E-06
10	2400	0,16137	0,819477	18,712439	1,8712439	0	0,97429449	-31,9612737	-616,009213		
11	3600	0,13176	0,8521789	24,27678	2,427678	0	0,98278872	-45,2807274	-761,031712	**$A_k^T[s_i^{obs} - s_i^c(p)]_k = L_{2x1}$**	
12	7200	0,09317	0,8951729	36,950285	3,6950285	0	0,99135701	-76,1869667	-1085,64458	2,346E-16	
13	10800	0,07607	0,9143266	46,725569	4,6725569	0	0,99422968	-100,278792	-1333,49054	-4,38257E-15	
14	18000	0,05893	0,9335865	62,267366	6,2267366	0	0,9965338	-138,784979	-1725,51852		
15	28800	0,04658	0,9474727	80,565026	8,0565026	0	0,99783221	-184,278004	-2185,47128	**ΔT =**	9,66373E-20
16	43200	0,03804	0,9571013	100,21979	10,021979	0	0,99855429	-233,240786	-2678,58167	**ΔS =**	-8,8445E-21
17	86400	0,0269	0,9696587	144,6188	14,46188	0	0,99927688	-344,011205	-3790,82774		
18	129600	0,02196	0,9752245	178,70208	17,870208	0	0,99951786	-429,118771	-4643,91647	**T [m^2/s] =**	0,02
19	172800	0,01902	0,9785429	207,4406	20,74406	0	0,99963838	-500,905038	-5362,97939	**S =**	0,002
20	259200	0,01553	0,9824797	255,65588	25,565588	0	0,9997589	-621,372056	-6569,07344	**E(p) =**	1,45475E-32

Table A.5 Iteration table for field data of Tomasko, 1987 (constant discharge, k = 1)

ITERATION 1 (k = 1)											
	T_{k-1} =	1E-10m^2/s		S_{k-1} =	1E-10	λ_k =	0	A_k for p		$A_k^T A_k$	
i	**t_i [s]**	**u_i**	**erfc(u_i)**	**s_i^{obs} [m]**	**s_i^c(p) [m]**	**$s_i^{obs} - s_i^c(p)$**	**exp($-u_i^2$)**	**$(\partial s/\partial T)_i$**	**$(\partial s/\partial S)_i$**	1,66047E+32	1,80108E+32
1	108088	0,11406	0,8718502	3,48	264026,78	-264023,298	0,98707401	-1,0331E+15	-1,6071E+15	1,80108E+32	1,95721E+32
2	877943	0,04002	0,9548642	13,44	863706,01	-863692,566	0,99839953	-4,0042E+15	-4,6328E+15		
3	2E+06	0,02401	0,9729093	24	1481813,9	-1481789,86	0,99942353	-7,0888E+15	-7,7293E+15	**$A_k^T A_k + \lambda_k I = K_{2x2}$**	
4	5E+06	0,01755	0,9802011	34,56	2051431	-2051396,46	0,99969211	-9,9345E+15	-1,058E+16	1,66047E+32	1,80108E+32
5										1,80108E+32	1,95721E+32
6											
7										**K^{-1}**	
8										3,26952E-30	-3,0087E-30
9										-3,0087E-30	2,77382E-30
10											
11										**$A_k^T[s_i^{obs} - s_i^c(p)]_k = L_{2x1}$**	
12										3,46149E+22	
13										3,75823E+22	
14											
15										**ΔT =**	9,99959E-11
16										**ΔS =**	1,00001E-10
17											
18										**T [m^2/s] =**	1,99996E-10
19										**S =**	2,00001E-10
20										**E(p) =**	7,2196E+12

Table A.6 Iteration table for field data of Tomasko, 1987 (constant discharge, k = 21)

ITERATION 21 (k = 21)											
	T_{k-1} =	$2{,}2E\text{-}06 m^2/s$		S_{k-1} =	1,445E-05	λ_k =	0	A_k for p		$A_k^T A_k$	
i	**t_i [s]**	**u_i**	**erfc(u_i)**	**s_i^{obs} [m]**	**$s_i^c(p)$ [m]**	**$s_i^{obs} - s_i^c(p)$**	**$\exp(-u_i^2)$**	**$(\partial s/\partial T)_i$**	**$(\partial s/\partial S)_i$**	7,85319E+13	1,49344E+13
1	108088	0,28948	0,682257	3,48	3,2571227	0,22287726	0,91961688	-279732,779	-181955,728	1,49344E+13	2,86884E+12
2	877943	0,10157	0,8857816	13,44	13,531899	-0,0918994	0,98973625	-2436381,17	-558114,276		
3	2E+06	0,06094	0,9313183	24	24,330353	-0,33035301	0,99629284	-4813036,28	-936352,592	**$A_k^T A_k + \lambda_k I = K_{2x2}$**	
4	5E+06	0,04454	0,9497806	34,56	34,310913	0,24908674	0,99801858	-7025127,63	-1283544,05	7,85319E+13	1,49344E+13
5										1,49344E+13	2,86884E+12
6											
7										**K^{-1}**	
8										1,2704E-12	-6,6134E-12
9										-6,6134E-12	3,47762E-11
10											
11										**$A_k^T[s_i^{obs} - s_i^c(p)]_k = L_{2x1}$**	
12										1690,761014	
13										349,6638429	
14											
15										**ΔT =**	-1,6451E-10
16										**ΔS =**	9,78303E-10
17											
18										**T [m^2/s]=**	2,2435E-06
19										**S =**	1,44523E-05
20										**E(p) =**	0,229297094