The Application of Numerical Laplace Inversion Methods to Groundwater Flow and Solute Transport Problems

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ABSTRACT

In the past decades, numerous analytical or semianalytical solutions for groundwater problems have been obtained with the Laplace transform technique. As the physical understanding of realistic groundwater problems evolves, the corresponding mathematical models become more complicated, to which analytical solutions are no longer easily obtainable. Therefore, a great deal of interest has been focused on finding semianalytical solutions for groundwater problems. The semianalytical solutions are the result of numerical inversion of the Laplace domain solutions. Many different Laplace numerical inversion methods have been employed to determine the semianalytical solutions. Here, eight different Laplace numerical inversion methods are examined; they are the Stehfest [Stehfest, 1970], Schapery [Schapery, 1962], Widder [Widder, 1934], Dubner and Abate [Dubner and Abate, 1968], Koizumi [see Squire, 1984], Crump [Crump, 1975], Weeks [Weeks, 1966] and Talbot [Talbot, 1979] methods. These eight methods are tested for their accuracy and computational efficiency on groundwater problems. It is found that the Crump method is suggested for use in groundwater problems because it can successfully invert functions which are oscillatory, smooth, or of discontinuities in the first derivative. In addition to this suggestion, we noted that for oscillatory functions, the Talbot method may be used instead of the Crump method for less CPU times are needed by the Talbot method. For smooth functions, due to its simplicity in application the Stehfest method may be used with care, noting that it yields spurious oscillatory results at large times for transport problems. Other methods such as Schapery's, Widder's, Dubner and Abate's, Koizumi's, and Weeks's methods are not recommended for groundwater problems because they have the limitation in accuracy or computational efficiency.

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Chapter 1.

INTRODUCTION

Mathematical modeling has been an important theoretical approach in studying groundwater problems. Generally, it involves finding the solutions to the mathematical model constructed to investigate the problem of interest. Usually, a mathematical model consists of a set of differential equation(s) (i.e., the governing equation(s)) mathematically describing the physical conditions of the problem and a set of boundary and initial conditions appropriately prescribed. Many analytical/semianalytical solutions for various groundwater mathematical models have been obtained with the aid of the Laplace transform technique in the past decades. The Laplace transform of $f(\underline{x}, t)$ with respect to t is formally defined as

$$F(\underline{x}, s) = \int_0^\infty e^{-st} f(\underline{x}, t) dt \tag{1}$$

where s is the transform parameter being complex, $\underline{x}$ denotes the spatial coordinates, and t represents temporal variable. Applications of the Laplace transform to the mathematical models simplifies the models by reducing the degree of freedom (i.e., the independent variables). By doing so, the solutions for the transformed models in the Laplace domain can be easier obtained. If the Laplace domain solutions are determined, they need to be inverted to the original domain such that the true solutions can be known. The Laplace inversion of $F(\underline{x}, s)$ can be formally defined by the Mellin integral (e.g., Krylov and Skoblya [1977], Lepage [1961]) as

$$f(\underline{x}, t) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} F(\underline{x}, s) e^{st} ds \tag{2}$$

where γ is a positive real number so chosen that all the singularities of the integrand lie left of the vertical line defined by $\gamma - i\infty$ to $\gamma + i\infty$ in the complex plane, and i represents the complex number defined to be $\sqrt{-1}$.

Calculation of (2) can be carried out by making use of the Cauchy integral theorem to find the sum of residues of the integrand at each of its singularities within the region bounded by the contour in the complex plane. A number of analytical solutions based on this analytical inversion method have been determined. Chen and Woodside [1988] obtained the analytical solution for a mathematical model investigating aquifer decontamination by a single withdrawl well. This analytical solution studied concentration variation inside the aquifer during the withdrawal process. Chen [1987] determined the analytical solutions for four different radial dispersion problems from an injection well; namely, resident and flux concentration distributions dealing with a continuous or a pulse injection, respectively. The well bore was simulated as a Cauchy boundary condition. To the similar problems studied by Chen [1987] yet subject to a Dirichlet boundary condition at the well bore, Tang and Babu [1979], and Hsieh [1986] gave analytical solutions in terms of Bessel and Airy functions, respectively. Boulton and Streltsova [1977] derived the equation for the drawdown in a fissured water-bearing formation, which was idealized as an aquifer-aqitard combination, assumed an impermeable boundary at the top of the aquitard. Numan and Witherspoon [1969] obtained an analytical solution for the problem of groundwater flowing into a well in an infinite radial system composed of two aquifers that are seperated by an aquitard. Other analytical solutions for groundwater problems can be found in Bear [1972] or Hantush [1964, p.281-432].

In general, the most difficult task in using (2) for analytical solutions is to find the singularities of the integrand involved. If the integrand is complicated and its singularities are difficult to know, sometimes the so-called asymptotic solutions are desired. The asymptotic solutions are the inversion of the simplified Laplace domain solutions evaluated at large or small arguments. Many asymptotic solutions for groundwater problems have been obtained. Chen [1987] gave the short-time asymptotic solutions for resident concentration dealing with a continuous injection from a single well. Chen [1986] obtained the short-time asymptotic solution for radionuclide transport from an injection well into a single fracture by radial advection and longitudinal dispersion. Chen [1985] dealt with comtaminat transport from an injection well into an aquifer with simultaneous diffusion into adjacent aquitards. Voigt and Haefner [1987], and Chen and Reddel [1983] determined the short and long time asymptotic solutions for heat transfer in aquifers with finite thickness caprock during a thermal injection process. Sageev [1986] presented the early and late time asymptotic solutions for head response in an aquifer to a slug test in a fully penetrating well with well bore storage and the skin effect around the active well. Hantush [1960] determined the short and long time drawdown distributions in leaky aquifers.

Since the asymptotic solutions are only valid for short or long time periods of the problems, they do not provide information for the intermidiate time periods. Therefore, hydrologists have been interested in finding semianalytical solutions that are useful for any time periods. These semianalytical solutions were obtained by numerically inverting the Laplace domain solutions; they are called semianalytical solutions because usually the Laplace domain solutions are in terms of analytical functions yet their inversions are calculated by numerical methods instead of analytical or asymptotic techniques. The Stehfest method [Stehfest, 1970] has been widely applied to invert the transformed solutions in Laplace domain for various groundwater problems. The following works used the Stehfest method to obtain the semianalytical solutions. Karasaki et al. [1988] gave the semianalytical solutions for various models of slug tests. Hemker and Maas [1987] applied the Stehfest method to obtain a semianalytical solution for the drawdowns in leaky and confined multi-aquifer systems, results were compared with a analytical solutions developed by Maas [1987] and excellent agreement was noted. Sageev [1986] generated the intermediate time type curves of slug test by the Stehfest method. Moench [1985] used this method to find the semianalytical solutions for the groundwater flow toward a large-diameter well in a leaky aquifer. Barker [1985] evaluated the generalized well function for homogeneous and fissured aquifer. Moench [1984] provided double-porosity models for a fissured groundwater reservoir with fracture skin. Moench and Ogata [1984] noted that the Stehfest method gave good results for various groundwater flow problems. Moench and Ogata [1981], and Chen [1985, 1986] applied this method to determine semianalytical solutions for radial dispersion from an injection well into a granular or fracture aquifers.

Chen [1989] obtained semianalytical solutions for solute transport in a leaky aquifer receiving wastewater injection by making use of three different numerical inversion methods; namely, Stehfest [1970], Dubner and Abate [1968], and Crump [1976]. He noted that both Dubner and Abate's and Crump's method gave essentially the same results, yet the Stehfest method showed oscillatory results at small dimensionless time periods. Kipp [1985] used the Crump method to analyze the response of a well to a slug test. He found that the Stehfest method could not accurately invert a decaying sinusoid analytical function. Barker [1982] presented graphs for solute migration in fissured aquifer by using the Crump [1976] and Durbin [1974] methods. Valocchi [1985] used Durbin's and Stehfest's method to enhance the reliability of the calculated results for the validity of the local equilibrium assumption for modeling sorbing solute transport through homogeneous soils. He found that results by these two methods generally agreed to within a few percent. Durbin's method is based on Fouier cosine and sine series, an approach used in Crump's method. However, Davies and Martine [1979] noted that Crump's method is computaionally more efficient.

Barker and Black [1983] applied the Talbot method [Talbot, 1979] to determine the head solutions of slug tests in fissured aquifers. Sposito et al. [1986] used the same method to obtain semianalytical solutions for a transfer function of solute transport through soil.

Chen [1980] used the Schapery method [Schapery, 1962] to acquire steady state semianalytical solutions for an aquifer thermal injection problem; satisfactory results were noted. Clegg [1967] used this method for some simple problems in plane radial flow;

accurate results were obtained. He noted that the Schapery method was satisfactory provided that the function $s \bullet F(s)$ satisfies the condition that it was approximately a linear function of $ln(s)$.

Another useful numerical Laplace inversion method has been proposed by Weeks [1966]. Wada [1981] used the Weeks method to obtain accurate results in mechanical engineering problem for the transient torsional vibrations of a rigid mass connected to an elastic half-space by an elastic circular rod. Although the Weeks method has not been used in the area of groundwater, we feel that it may be an effective technique in dealing with groundwater problems. In addition to the Weeks method, the Koizumi method (see Squire [1984]) may be a successful method for numerically inverting the Laplace domain solutions of groundwater problems, because it is based on the Fourier series, an approach used in Crump's, and Dubner and Abate' methods. Widder [1934] gave a numerical Laplace inversion formula which is employed in this study due to the simple structure. Piessens [1975], and Piessens and Dang [1976] provided detailed bibliography for Laplace numerical inversion methods. Davies and Martine [1979] gave a suvey and comparison of methods for numerical inversion of Laplace transform.

As discussed earlier, the semianalytical solutions can usually be obtained with appropriate numerical inversion methods. However, their accuracy depends on the chosen methods. Therefore, the objective of this study is to evaluate the applicability of eight different numerical Laplace inversion methods that have been used in dealing with groundwater or other practical problems. Specifically, these eight methods are Stehfest, Schapery, Widder, Dubner and Abate, Koizumi, Crump, Weeks, and Talbot.

Chapter 2.

NUMERICAL LAPLACE INVERSION METHODS

This section discusses the eight numerical inversion methods mentioned earlier. They are the Stehfest, Schapery, Widder, Dubner and Abate, Koizumi, Crump, Weeks, and Talbot methods.

§2.1 The Stehfest Method:

Stehfest [1970] gave the following formula to numerically invert F(s) as

$$f(t) \simeq \left[s \bullet \sum_{n=1}^{N} K_n \bullet F(ns)\right]_{s=ln(2/t)} \tag{3}$$

where the transform parameter s is defined in calculations to be $ln(2/t)$. The weighting coefficients K_n are given by

$$K_n = (-1)^{n+N/2} \bullet \sum_{k=(n+1)/2}^{min(n,N/2)} \frac{k^{N/2}(2k)!}{(N/2-k)!k!(k-1)!(n-k)!(2k-n)!} \tag{4}$$

In (4) N must be even. According to Stehfest, the accuracy can be improved by increasing N. However, roundoff error limits the value of N. Moench and Ogata [1981] obtained accurate results by using $N = 18$ for duouble precision. They noted that the limiting factor in the accuracy of the results is the number of significant figures that the computer is capable of holding.

§2.2 The Schapery Method:

Schapery [1962] proposed a numerical inversion formula for F(s) as

$$f(t) \simeq [s \bullet F(s)]_{s=1/2t} \tag{5}$$

where the transform parameter s is defined to be $1/2t$. The formula of (5) is simple in structure and no weighting coefficients need to be calculated.

§2.3 The Widder Method:

Widder [1934] obtained a formula to numerically invert F(s) as

$$f(t) \simeq [(-1)^n (n!)^{-1} s^{(n+1)} F^{(n)}(s)]_{s=n/t} \tag{6}$$

where the transform parameter s is defined to be n/t. $F^{(n)}(s)$ is the n-th derivative of F(s) with respect to s. In general using higher derivatives (i.e., large value of n) gives higher accuracy, but tests by Davies and Martine [1979] indicated that convergence was slow.

§2.4 Methods approximate the Laplace inversion by expressing the transformed function in a Fourier series:

In (1), s is a complex variable which can be expressed as $s = a + i\omega$, where a is an arbitrary real number and ω will be defined later. Substituting the s into (1) and by the identity $e^{i\omega} = cos(\omega t) + isin(\omega t)$ for the exponential term of (1), the integral can be replaced by

$$F(s) = \int_0^\infty e^{-at} f(t) cos(\omega t) dt - i \int_0^\infty e^{-at} f(t) sin(\omega t) dt \tag{7}$$

or

$$F(s) = Re[F(a + i\omega)] + iIm[F(a + i\omega)] \tag{8}$$

where

$$Re[F(a + i\omega)] = \int_0^\infty e^{-at} f(t) cos(\omega t) dt \tag{9}$$

$$Im[F(a + i\omega)] = -\int_0^\infty e^{-at} f(t) sin(\omega t) dt \tag{10}$$

Introducing (8) with $s = a + i\omega$ and $ds = id\omega$ into (2) and rearraging the integral of (2) gives

$$f(t) = \frac{e^{at}}{2\pi} \{ \int_{-\infty}^{+\infty} [Re[F(s)] cos\omega t - Im[F(s)] sin\omega t] \, d\omega$$

$$+i\int_{-\infty}^{+\infty}\left[Im[F(s)]cos\omega t+Re[F(s)]sin\omega t\right]d\omega\} \quad (11)$$

By substituting (9) and (10) into (11), the imaginary part can be expressed as

$$\int_{-\infty}^{+\infty}\left[Im[F(s)]cos\omega t+Re[F(s)]sin\omega t\right]d\omega\} =$$

$$-\int_{-\infty}^{+\infty}[\int_{0}^{\infty}e^{-at}f(t)sin(\omega t)dt]\bullet cos(\omega t)d\omega$$

$$+\int_{-\infty}^{+\infty}[\int_{0}^{\infty}e^{-at}f(t)cos(\omega t)dt]\bullet sin(\omega t)d\omega=0 \quad (12)$$

According to (12), (11) reduces to

$$f(t)=\frac{e^{at}}{2\pi}\int_{-\infty}^{+\infty}\left[Re[F(s)]cos\omega t-Im[F(s)]sin\omega t\right]d\omega$$

which can be simplified to the following equation by noting that the integrand is an even function

$$f(t)=\frac{e^{at}}{\pi}\int_{0}^{\infty}\Big(Re[F(s)]cos(\omega t)-Im[F(s)]sin(\omega t)\Big)d\omega \quad (13)$$

§2.4.1 The Crump Method:

Crump [1975] approximated the Lapalce inversion by writting (13) as an infinite series which was constructed to be an infinite set of even periodic functions $g_n(t)$ and odd periodic functions $K_n(t)$, each with period 2T. For n=0,1,2,3,.. $g_n(t)$ and $K_n(t)$ are given by

$$g_n(t)=\begin{cases} h(t) & nT\le t\le(n+1)T; \\ h(2nT-t) & (n-1)T\le t\le nT. \end{cases} \quad (14)$$

$$K_n(t)=\begin{cases} h(t), & nT\le t\le(n+1)T; \\ -h(2nT-t), & (n-1)T\le t\le nT. \end{cases} \quad (15)$$

where h(t) is a real function and $h(t)=0$ for $t<0$. Therefore, the Fourier cosine representation of each $g_n(t)$ is

$$g_n(t)=\frac{a_{n,0}}{2}+\sum_{m=1}^{\infty}a_{n,m}cos(\frac{m\pi t}{T}) \quad (16)$$

where

$$a_{n,m} = \frac{2}{T}\int_{nT}^{(n+1)T} h(t)cos(\frac{m\pi t}{T}) \quad n = 0, 1, 2, 3, ... \tag{17}$$

The Fourier sine representation of each $K_n(t)$ is

$$K_n(t) = \sum_{m=0}^{\infty} b_{n,m} sin(\frac{m\pi t}{T}) \tag{18}$$

where

$$b_{n,m} = \frac{2}{T}\int_{nT}^{(n+1)T} h(t)sin(\frac{m\pi t}{T})dt \quad n = 0, 1, 2, 3, ... \tag{19}$$

It is seen from (17) and (19) that convert the finite Fourier cosine transform to a true integral transform is to sum over n so that the upper limit becomes infinite. Summing (16) over n and replacing $h(t) = e^{-at}f(t)$ gives

$$\sum_{n=0}^{\infty} g_n(t)e^{at} = \frac{2e^{at}}{T}[\frac{A_{m=0}}{2} + \sum_{m=1}^{\infty} A_m cos(\frac{m\pi t}{T})] \tag{20}$$

where

$$A_{m=0} = \int_0^{\infty} e^{-at}f(t)dt = Re[F(a)] \tag{21a}$$

$$A_m = \int_0^{\infty} e^{-at}f(t)cos(\frac{m\pi t}{T})dt = Re[F(a+i\omega)]_{\omega=m\pi/T} \tag{21b}$$

Summing (18) over n and replacing $h(t) = e^{-at}f(t)$ yields

$$\sum_{n=0}^{\infty} e^{at}K_n(t) = \frac{2e^{at}}{T}[\sum_{m=0}^{\infty} B_m sin(\frac{m\pi t}{T})] \tag{22}$$

where

$$B_m = \int_0^{\infty} e^{-at}f(t)sin(\frac{m\pi t}{T})dt = -Im[F(a+i\omega)]_{\omega=m\pi/T} \tag{23}$$

Dividing (20) and (22) by two and adding together obtains

$$\frac{1}{2}\sum_{n=0}^{\infty} e^{at} g_n(t) + \frac{1}{2}\sum_{n=0}^{\infty} e^{at} K_n(t) =$$

$$\frac{2e^{at}}{T}[\frac{A_{m=0}}{2} + \sum_{m=1}^{\infty} A_m cos(\frac{m\pi t}{T}) + \sum_{m=0}^{\infty} B_m sin(\frac{m\pi t}{T})] \tag{24}$$

Equation (24) contained an error term which can be carried out by summing (14) over n and multiplying e^{at} to both sides, then

$$\sum_{n=0}^{\infty} e^{at} g_n(t) = \sum_{n=0}^{\infty} e^{at} h(2nT+t) + \sum_{n=1}^{\infty} e^{at} h(2nT-t) \tag{25}$$

Furthermore, making the substitution $h(t) = e^{-at} f(t)$ into (25) becomes

$$\sum_{n=0}^{\infty} e^{at} g_n(t) = \sum_{n=0}^{\infty} e^{-2nTa} f(2nT+t) + \sum_{n=1}^{\infty} e^{2at} e^{-2nTa} f(2nT-t) \tag{26}$$

Seperating the $n = 0$ term out of the summation in (26) gives

$$\sum_{n=0}^{\infty} e^{at} g_n(t) = f(t)_{(n=0)} + \sum_{n=1}^{\infty} e^{-2nTa}[f(2nT+t) + e^{2at} f(2nT-t)] \tag{27}$$

with $\sum_{n=1}^{\infty} e^{-2nTa}[f(2nT+t) + e^{2at} f(2nT-t)]$ being one part of error term. (27) can be rewritten as

$$\sum_{n=0}^{\infty} e^{at} g_n(t) = f(t) + ERROR1 \tag{28}$$

By using the same procedures of (25)-(28), (15) with the other part of error term can be expressed as

$$\sum_{n=0}^{\infty} e^{at} K_n(t) = f(t) + ERROR2 \tag{29}$$

where ERROR2= $\sum_{n=1}^{\infty} e^{-2nTa}[f(2nT+t) - e^{2at}f(2nT-t)]$. Again dividing (28) and (29) by two and adding generates

$$\frac{1}{2}\sum_{n=0}^{\infty} e^{at}g_n(t) + \frac{1}{2}\sum_{n=0}^{\infty} e^{at}K_n(t) = f(t) + \frac{1}{2}ERROR1 + \frac{1}{2}ERROR2 \qquad (30)$$

By noting (24), (30) can be rewritten as

$$\frac{2e^{at}}{T}[\frac{A_{m=0}}{2} + \sum_{m=1}^{\infty} A_m cos(\frac{m\pi t}{T}) + \sum_{m=0}^{\infty} B_m sin(\frac{m\pi t}{T})] = f(t) + ERROR3 \qquad (31)$$

where the truncation error ERROR3 is equal to $(1/2)ERROR1 + (1/2)ERROR2$. It is clear that (31) combines the Fourier cosine and sine series to be the approximate formula for the Laplace inversion of (13). In essence, (31) given by Crump is calculated with the aid of epsilon algorithm (e.g., MacDonald [1964]).

§2.4.2 The Dubner and Abate Method:

Dubner and Abate [1968] approximated (13) by expressing the transformed function in Fourier cosine series, neglecting the term involving $sin(\omega t)$ in (13). By noting (20), (28) can be rewritten as

$$\frac{2e^{at}}{T}[\frac{A_{m=0}}{2} + \sum_{m=1}^{\infty} A_m cos(\frac{m\pi t}{T})] = f(t) + ERROR1 \qquad (32)$$

Clearly, (32) is an approximate formula for the Laplace inversion with an error term named ERROR1. In (32) the Fourier cosine series is computed with the fast Fourier transform (FFT) method (see, for example, Cooley and Tukey [1965]).

§2.4.3 The Koizumi Method:

The development of the Koizumi method (see Squire [1984]) is very similar to that of Dubner and Abate. Koizumi, however, approximated (13) by writting the transformed function in Fourier sine series, neglecting the term involving $cos(\omega t)$ in (13). By noting (22), (29) can be rewritten as

$$\frac{2e^{at}}{T}[\sum_{m=0}^{\infty} B_m sin(\frac{m\pi t}{T})] = f(t) + ERROR2 \tag{33}$$

Obviously, (33) is an approximate formula given by Koizumi for the Lapalce inversion with an error term called ERROR2. The Fourier sine series is evaluated by a modification of Clenshaw's recursive procedures (e.g., Mattheman [1963]). In the next section more details about those errors will be discussed.

§2.4.4 Error Analysis:

Some conclusions regarding the best method can be draw by analyzing the errors associated with thses three methods. If $f(t) \leq c$ for all t and c is a constant, then ERROR1 in (32) can be written as

$$\begin{aligned} ERROR1 &\leq \sum_{n=1}^{\infty} e^{-2anT}\left[c + ce^{2at}\right] \\ &\leq c \bullet \sum_{n=1}^{\infty} e^{-2anT}\left[1 + e^{2at}\right] \\ &\leq c \bullet [1 + e^{2at}] \bullet \frac{e^{-2aT}}{1 - e^{-2aT}} \\ &\leq c \bullet e^{(-aT+at)} \frac{cosh(at)}{sinh(aT)} \end{aligned} \tag{34}$$

In (34) ERROR1 is bounded as $0 \leq t \leq T$. When $t \rightarrow T$, ERROR1 approches to coth(aT) which becomes prohibitively large when aT is less than 1.2 (Abramowitz and Stegun [1970, p.83]). Therefore, the representation is restricted to the interval $0 \leq t \leq T/2$ (i.e., $T \geq 2t_{max}$) with an error of the order $c \bullet e^{-aT}$. For example , suppose after determing T($\geq 2t_{max}$), a value is chosen such that aT=10, then for the case under consideration, our approximation of f(t) on the interval(0,T/2) is good to within an error of the order $c \bullet 10^{-5}$. Similarly the error term of (33) can be shown by

$$ERROR2 \leq c \bullet e^{(-aT+at)} \frac{sinh(-at)}{sinh(aT)} \tag{35}$$

ERROR2 is also bounded as $0 \leq t \leq T$. When $t \to T$, ERROR2 approches to a constant c which may be large. Moreover, the representation is also restricted to the interval $0 \leq t \leq T/2$. It is clear that neither of these formulas (34) and (35) shows any specific advantage because both error terms contain a factor which is expoentially increasing with t

If f(t) is again bounded by a constant c for all t, then in (31) the error term gives

$$\begin{aligned} ERROR3 &\leq c \bullet \sum_{n=1}^{\infty} e^{-2nTa} \\ &\leq c \bullet \frac{e^{-2aT}}{1 - e^{-2aT}} \\ &\leq c \bullet \frac{1}{e^{2aT} - 1} \end{aligned} \tag{36}$$

The interest of (36) is twofold by Durbin [1974]: First of all, ERROR3 is now bounded by a fixed quantity; allowing us to use reprsentation of f(t) on the interval (0,2T) instead of (0,T/2). Secondly, This fixed bound depends only on the product aT. For example, when aT=10 the $ERROR3 \leq c \bullet 10^{-9}$, whereas the Dubner and Abate, and Koizumi methods give only $c \bullet 10^{-5}$ and $0 \leq t \leq T/2$. This implies that the Crump method is capable of obtaining more accurate results.

§2.5 The Weeks Method:

Weeks [1966] developed a method for the numerical inversion of Laplace transform, in which the Laplace inversion was obtained as an expansion in terms of orthonormal Laguerre functions.

If the function f(t) satisfies the conditions

$$\int_0^{\infty} e^{-ct} |f(t)| dt < \infty \tag{37a}$$

and

$$\int_0^{\infty} e^{-ct} |f(t)|^2 dt < \infty \tag{37b}$$

, then from Schohat [1940] and Widder [1935], (2) can be approximated by a function $f_N(t)$ as

$$f_N(t) = e^{ct} \sum_{n=0}^{N} a_n \phi(\frac{t}{T}) \tag{38}$$

In (38), the function of $\phi(t/T)$ is defined by

$$\phi(\frac{t}{T}) = e^{-\frac{t}{2T}} L_n(\frac{t}{T}) \tag{39}$$

where $L_n(t/T)$ is the Laguerre polynomial of degree n. These polynomials are determined by the orthogonality condition as

$$\int_0^\infty e^{-x} L_n(x) L_m(x) = \begin{cases} 0, & n \neq m; \\ 1, & n = m\ . \end{cases} \tag{40}$$

In essence, (36) indicates that the Laguerre polynomials $L_n(x)$ are orthogonal on $(0,\infty)$ with respect to the weight function e^{-x}.

In (38), T must be greater than zero. Weeks [1966, p.424] empirically found that a satisfactory choice was

$$T = \frac{t_{max}}{N} \tag{41}$$

A satisfactory choice of c given by Weeks [1966, p424] was

$$c = (c_0 + \frac{1}{t_{max}}) \bullet u(c_0 + \frac{1}{t_{max}}) \tag{42}$$

where c_0 is the abscissa of convergence of the Laplace integral and u(x) is the Unit step function described as

$$u(x) = \begin{cases} 0, & \text{if } x < 0; \\ 1, & \text{if } x \geq 0. \end{cases} \tag{43}$$

The coefficients a_n in (38) are determined by the following procedures. Let $F_N(s)$ be the Laplace transform of $f_N(t)$, that is

$$F_N(s) = \int_0^\infty f_N(t) e^{-st} dt \tag{44}$$

Introducing (38) to (44) gives

$$F_N(s) = \int_0^\infty e^{(c-s)t} \sum_{n=0}^{N} a_n \phi(\frac{t}{T}) dt \tag{45}$$

Calculating the Laplace transform of $e^{ct}\phi(\frac{t}{T})$ with the inversion formula tabulated by Magnus and Oberhettinger [1954, p.129] yields

$$F_N(s) = \sum_{n=0}^{N} a_n \bullet \frac{(s-c-1/2T)^n}{(s-c+1/2T)^{n+1}} \tag{46}$$

The function $f_N(t)$ approximates f(t) in the sense that for any $\epsilon > 0$, there exists an integer N, such that

$$\int_0^\infty e^{-2ct} |f(t) - f_N(t)|^2 dt < \epsilon \tag{47}$$

If f(t) is absolutely integrable, and bounded, then f(t) and F(s) can be related by the formula of Parseval theorem as

$$\int_0^\infty |f(t)|^2 dt = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} |F(s)|^2 ds \tag{48}$$

Therefore, it follows that the function $f(t) - f_N(t)$ can be related to its Laplace transform $F(s) - F_N(s)$ by Parseval theorem.

$$\int_0^\infty e^{-2ct} |\ f(t) - f_N(t)\ |^2 dt = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} |\ F(s) - F_N(s)\ |^2 ds \tag{49}$$

By noting (47), (49) can be rewritten as

$$\frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} |F(s) - F_N(s)|^2 ds < \epsilon \tag{50}$$

Introducing (46) with $s = c + i\omega$ and $ds = id\omega$ into (50) yields

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} \left|\ F(c + i\omega) - \sum_{n=0}^{N} a_n \bullet \frac{(i\omega - \frac{1}{2T})^n}{(i\omega + \frac{1}{2T})^{n+1}}\ \right|^2 d\omega < \epsilon \tag{51}$$

By making change of the variable $\omega = [(1/2T)cot(\theta/2]$, (51) can be rearranged as

$$\frac{T}{2\pi}\int_{-\pi}^{+\pi} \mid (\frac{1}{2T} + \frac{i}{2T}cot\frac{\theta}{2})F(c + i\frac{cot\frac{\theta}{2}}{2T}) - \sum_{n=0}^{N} a_n \bullet e^{in\theta} \mid^2 d\theta < \epsilon \qquad (52)$$

It is seen from (52) that

$$(\frac{1}{2T} + i\frac{cot\frac{\theta}{2}}{2T})F(c + i\frac{cot\frac{\theta}{2}}{2T}) \simeq \sum_{n=0}^{N} a_n \bullet e^{in\theta} \qquad (53)$$

, indicating that the right hand side of (53) converges in the mean to the left hand side with increasing N.

$F_1(c,\omega)$ and $F_2(c,\omega)$ represent the real and imaginary parts, respectively, of $F(c + i\omega)$, then

$$F(c + i\omega) = F_1(c,\omega) + iF_2(c,\omega) \qquad (54)$$

By making use of the identity $e^{in\theta} = cos(n\theta) + isin(n\theta)$ for the exponential term of the right hand side of (53), it can be rewritten as

$$(\frac{1}{2T} + i\frac{1}{2T}cot\frac{\theta}{2})[F_1(c,\omega + iF_2(c,\omega)] \simeq \sum_{n=0}^{N} a_n \bullet [cos(n\theta) + isin(n\theta)] \qquad (55)$$

By separating both sides of (55) into real and imaginary part, the real part is taken as

$$\frac{1}{2T}F_1(c, \frac{1}{2T}cot\frac{\theta}{2}) - \frac{1}{2T}F_2(c, \frac{1}{2T}cot\frac{\theta}{2})cot\frac{\theta}{2} \simeq \sum_{n=0}^{N} a_n \bullet cos(n\theta) \qquad (56)$$

and the imaginary part is taken as

$$\frac{1}{2T}F_2(c, \frac{1}{2T}cot\frac{\theta}{2}) + \frac{1}{2T}F_1(c, \frac{1}{2T}cot\frac{\theta}{2})cot\frac{\theta}{2} \simeq \sum_{n=0}^{N} a_n \bullet sin(n\theta) \qquad (57)$$

By applying the trigonometric interpolation formula (e.g., Hildebrand [1956]) to $cos(n\theta)$ in (56), coefficients a_n when n=0 can be determined as

$$a_0 = \frac{1}{N+1}\sum_{j=0}^{N}[\frac{1}{2T}F_1(c, \frac{1}{2T}cot\frac{\theta}{2}) - \frac{1}{2T}F_2(c, \frac{1}{2T}cot\frac{\theta}{2})cot\frac{\theta}{2}]_{\theta=\theta_j} \qquad (58a)$$

For $n = 1, 2, 3...$ the coefficients a_n are written as

$$a_n = \frac{2}{N+1}\sum_{j=0}^{N}[\frac{1}{2T}F_1(c, \frac{1}{2T}cot\frac{\theta}{2}) - \frac{1}{2T}F_2(c, \frac{1}{2T}cot\frac{\theta}{2})cot\frac{\theta}{2}]_{\theta=\theta_j} cos(n\theta_j) \qquad (58b)$$

By applying the trigonometric interpolation formula to $sin(n\theta)$ in (57), coefficients a_n when n=0 can be given as

$$a_0 = 0 \qquad (59a)$$

For $n = 1, 2, 3...$ the coefficients a_n are generated as

$$a_n = \frac{2}{N+1}\sum_{j=0}^{N}[\frac{1}{2T}F_1(c, \frac{1}{2T}cot\frac{\theta}{2}) - \frac{1}{2T}F_2(c, \frac{1}{2T}cot\frac{\theta}{2})cot\frac{\theta}{2}]_{\theta=\theta_j} sin(n\theta_j) \qquad (59b)$$

Finally, Weeks [1966] applied the coefficients of (58) to (38) and by making use of the recurrence relations for Laguerre polynomial given as

$$L_0(\frac{t}{T}) = 1$$

$$L_1(\frac{t}{T}) = 1 - \frac{t}{T}$$

$$nL_n(\frac{t}{T}) = (2n - 1 - \frac{t}{T})L_{n-1}(\frac{t}{T}) - (n-1)L_{n-2}(\frac{t}{T}) \qquad (60)$$

, so that the approximate function $f_N(t)$ given in (38) to numerically invert F(s) is readily obtained.

§2.6 The Talbot Method:

Talbot [1979] provided a method for the numerical inversion of Laplace transform, in which the Laplace inversion is approximated by trapezoidal integration along a special contour.

(2) can be rewritten as

$$f(t) = \frac{1}{2\pi i}\int_B e^{st}F(s)ds \qquad (61)$$

where B is the Bromwich contour from $r - i\infty$ to $r + i\infty$ and $t > 0$, so that B is to the right of all singularities of F(s). However, in the fromal definition of Lapalce inversion as shown in (61) t can be any real number (e.g., Lepage [1961, p.324]). Therefore, the condition of $t > 0$ in the Talbot method indicates a restriction of its usage. For example, if F(s) has the function of $e^{(t-k)s}$, then the Talbot method gives accurate results as $t > k$, k is any positive real number. Direct numerical integration along B may be difficult for some problems, Talbot overcome the difficulty by replacing B with the aid of an equivalent contour L, such that

(a) L includes all singularities of F(s)

(b) F(s) uniformly converge as $|s| \to \infty$

Condition (a) may well not be satisfied with this particular L by a given F(s). However, this condition can be made to hold in general for the modified function $F(\lambda s + \sigma)$ by a suitable choice of the scaling parameter λ defined later and shift parameter σ which is zero for most functions of F(s). For example, if F(s) has a singularity s_0, then $F(\lambda s + \sigma)$ has the corresponding singularity

$$s_0^* = \frac{s_0 - \sigma}{\lambda} \tag{62}$$

and (61) can be replaced by

$$f(t) = \frac{\lambda e^{\sigma t}}{2\pi i} \int_L e^{\lambda st} F(\lambda s + \sigma) ds \tag{63}$$

Let z be a complex variable, M the imaginary interval from $z = -2\pi i$ to $+2\pi i$ and s=S(z) a real uniform analytical function of z which (i) has singularities at $\pm 2\pi i$, and residues there with imaginary part positive and negative, respectively. (ii) has no singularities in the interval from $z = -2\pi i$ to $+2\pi i$ (i.e., $|y| < 2\pi$) (iii) maps M onto a contour L in the s-plane, which encloses all singularities of $F(\lambda s + \sigma)$ for some λ and σ. (iv) maps the half strip H: $x > 0, |y| < 2\pi$ into the exterior of L.

Introducing (i), (ii), (iii), and (iv) into (63) and rewritting terms yields

$$f(t) = \frac{1}{2\pi i}\int_M Q(z)dz = \frac{1}{2\pi}\int_{-2\pi}^{+2\pi} Q(iy)dy \tag{64}$$

where $Q(z) = \lambda e^{[\lambda S(z)+\sigma]t} \bullet F(\lambda S(z)+\sigma)S'(z)$. A trapezoidal approximation to f(t) in the real integral (64) is

$$f(t) \simeq \overline{f(t)} = \frac{2}{N}\sum_{k=0}^{N-1} Re[Q(z_k)] \tag{65}$$

where $z_k = \frac{2k\pi i}{N}$. Therefore, (65) is the general inversion formula considered in Talbot's method. Theoretically, the accuracy in (65) can be improved by increasing the value of N.

Talbot [1979] selected a mapping function for S(z) given by

$$S(z) = \frac{z}{1-e^{-z}} + az = \frac{z}{2}(coth\frac{z}{2} + \nu) \tag{66}$$

where $a = \frac{(\nu-1)}{2}$; ν generally can be set to 1 (i.e., $a = 0$). Substituting $z = 2\theta i$ into (66) and rearranging terms yields

$$S(\theta) = \theta cot\theta + i\nu\theta \tag{67}$$

In (65), $S'(z) = dS/dz = (dS/d\theta) \bullet (d\theta/dz)$; $dz/d\theta = 2i$ and $dS/d\theta = S'(\theta)$. Thus

$$S'(z) = \frac{S'(\theta)}{2i} = \frac{(\nu + i\beta)}{2} \tag{68}$$

where $\beta = \theta + \frac{\theta cot\theta \bullet (\theta cot\theta - 1)}{\theta}$

Introducing (67) and (68) into (65), the approximate function of f(t) becomes

$$f(t) \simeq \overline{f(t)} = \frac{\lambda e^{\sigma t}}{N}\sum_{k=0}^{N-1} Re\left[(\nu + \beta i)e^{S(\theta)\tau}F[\lambda S(\theta) + \sigma]\right]_{\theta=\theta_k} \tag{69}$$

where $\theta_k = \frac{k\pi}{N}$, k=0,1,2....N-1 and $\tau = \lambda t$.

or

$$\overline{f(t)} = \frac{\lambda e^{\sigma t}}{N} \bullet Re\left[\sum_{k=0}^{N-1} a_k \bullet e^{ki\varphi}\right] \tag{70}$$

where $\alpha = \theta cot\theta$

$$a_k = e^{\alpha\tau}(\nu + i\beta)F[\lambda S(\theta) + \sigma]$$

$$\varphi = \frac{\tau\nu\pi}{N}$$

Therefore, (70) is a workable form applied by Talbot for (65) and the sum $\sum$ in (70) can be evaluated by an algorithm almost identical to Clenshaw's recursive procedure for Chebyshev sums.

Chapter 3.

RESULTS AND DISCUSSIONS

To evaluate the applicability of eight different numerical Laplace inversion methods described previously, two numerical examples are tested with those methods. The applicability is concerned with the accuracy of the results obtained by those methods. If they can provide accurate results, then the computational efficience (i.e., CPU time) will be considered.

§3.1 The Unit Step Function Tests:

The first example is the Laplace transform of the following function

$$F(s) = \frac{1}{s} \bullet e^{-ks} \tag{71a}$$

The Laplace inversion of (71a) is

$$f(t) = u(t-k) = \begin{cases} 0, & \text{if } t < k; \\ 1, & \text{if } t > k. \end{cases} \tag{71b}$$

where u(t-k) is the Unit step function, k is an arbitrary real number. The Unit step function has a sharp front (i.e., a first derivative discontinuity) at $t = k$. This function is involved in solutions for advection dominant solute transport problems. The Unit step function is chosen to test the applicability of eight Laplace numerical inversion methods because the sharp front condition is difficult to handle numerically.

The calculated results by those eight different methods for (71a) when k is ten are tabulated in Table 1-6. All the calculations were carried out on Micro Vax II at New Mexico Institute of Mining and Technology. In those tables, CPU times are given in the bottom row. The first column gives values of independent variable t and the second column lists the exact values of f(t) (i.e., u(t-k)). The rest column(s) give(s) the approximate values of f(t) (i.e., semianalytical solutions numerically inverted by those eight methods).

In Table 1, the results inverted by Stehfest's method are presented. Three different numbers of weighting points (i.e., N=16, 18 and 24) were used. The weighting number of 24 gives the maximum allowable length for the decimal figures of double precision in Micro Vax II. It is seen from Table 1 that accuracy of numerical results are not significantly improved by using more weighting points. The Stehfest method fails to give accurate results for the sharp front functions.

In Table 2, the results inverted by Schapery's method are presented. Although Schapery's method is simple in structure and no weighting coefficients are needed, it dose not give accurate results for the sharp front functions.

In Table 3, the results inverted by Widder's method are presented. Three different derivatives (i.e., N=1, 4, and 10) were used. Although accuracy of numerical inversion is improved by using higher derivatives, yet when N is equal to ten the calculated results do not converge to the true solutions. In general, for groundwater problems the Laplace domain solutions may be complicated so that their higher derivatives are difficult to obtain. Therefore, Widder's method is not suggested to use.

In Table 4, the results inverted by Crump's, Dubner and Abate's, and Koizumi's methods are presented. For these calculations, a fixed value of aT was selected. Subject to this consistent aT, the truncation error (see (34) and (35)) for Dubner and Abate's, and Koizumi's methods is about 10^{-2}, and 10^{-4} for Crump's method (see (36)). Theoretically, Crump's method is capable of obtaining most accurate results due to the small truncation error. To further evaluate accuracy of the three methods, we define the percentage error as

$$\text{percentage error} = \frac{|\text{calculated results-exact solutions}|}{\text{exact solutions}} \% \qquad (72)$$

The maximum percentage error of calculated results for Crump's method is about 0.8% at t=11 that is less than 1 % at t=20 given by Dubner and Abate's, and 3 % at t=9.95

given by Koizumi's methods. This indicates that Crump's method indeed gives most accurate results as aT is fixed. Regarding computaional efficiency, the Crump method used the least CPU time (i.e., 58.5 seconds for Crump's method that is less than Dubner and Abate's 4 minutes and Koizumi's 1 minute). Therefore, we suggest that among the three methods based on Fourier series expansion, the Crump method be used for sharp front functions.

In Table 5, the results inverted by Weeks's method are presented. Because Weeks's method is written in an infinite series form, we choose four different numbers of terms (i.e., N=50, 70, 100, and 150) to test its applicability. Although the accuracy of numerical inversion is improved by increasing the number of terms, the maximum percentage error is about 45.8 % at t=10.01 when N is equal to 150. It is clear that the Weeks method dose not give accurate results for the sharp front functions.

In Table 6, the results inverted by Talbot's method are presented. As Talbot's method is expressed in an infinite series form, four different numbers of terms (i.e., N=5, 15, 30, 45) were selected to test its applicability. In general, accuracy of numerical inversion is improved by increasing the number of terms; when N is equal to 45 accurate results (i.e., the maximum percentage error occuring at t=10.01 is about 1.1 %) are observed as the values of t are greater than 10(=k). However, inaccurate results exist for t being less than 10. This indicates that the Talbot method is only appropriate for the range of $t > k$ as discussed earlier. To further quantitatively examine this limitation, we chose another two problems. The first one is

$$F(s) = \frac{1}{s^2} e^{-ks} \qquad (73a)$$

where k is 5. The Laplace inversion of (73a) is given by

$$f(t) = (t - k) u(t - k) \qquad (73b)$$

Results of numerically inverting (73a) by Talbot's method are plotted in Figure 1a. Very good agreement between the exact solutions and the calculated results is observed when t is greater than 5; poor agreement exists for t less than 5. The second test function is

$$F(s) = \frac{1 - e^{-ks}}{s} \tag{74a}$$

where k has the same value of 5 as used in (73a). The Laplace inversion of (74a) is

$$f(t) = u(t) - u(t-k) \tag{74b}$$

The inversion results of (74a) by Talbot's method are ploted against the exact solution of (74b). Again it is noted that Talbot's method fails to yield accurate results for $t < k$.

§3.2 Oscillatory function Tests:

The second example is the Laplace transform of a sinusoid function described by

$$F(s) = \frac{s}{(s^2+1)^2} \tag{75a}$$

The Laplace inversion of (74a) is

$$f(t) = \frac{t \bullet sin(t)}{2} \tag{75b}$$

Equation (75a) is selected because this kind oscillatory behavior is related to groundwater problems associated with the decaying sinusoidal displacement of the well water level (e.g., Kipp [1988]; van der Kamp [1976]). The calculated results for (75a) by those eight methods are tabulated in Table 7-12, which have the similar format as used in Table 1-6.

In Table 7, the results inverted by Stehfest's method are presented. Three different numbers of weghting points (i.e., N=16, 18, and 24) were used. It is noted that for all of N, Stehfest's method dose not give accurate results for oscillatory functions.

In Table 8, the results inverted by Schapery's method are presented. It is also noted that the Schapery method dose not give accurate results for oscillatory functions.

In Table 9, the results inverted by Widder's method are presented. Four different numbers of derivatives (i.e., N=1, 2, 3, and 4) were used. The accuracy of numerical inversion dose not improved by using higher derivatives for the oscillatory function. For all of N, the Widder method dose not give accurate results.

In Table 10, the results inverted by Crump's, Dubner and Abate's, and Koizumi's methods are presented. A fiexed value of 15 for aT was chosen for these calculations. The truncation error (see (34) and (35)) for Dubner and Abate's, and Koizumi's methods is about 10^{-7} , and 10^{-14} for Crump's method (see (36)). Accurate results are obtained by all of three methods (i.e., the maximum percentage error occuring at t=20 is less than 10^{-3} % for all the three methods). However, the Crump method is most computationally efficient (i.e., 7.2 seconds CPU time for Crump's method that is less than Dubner and Abate's 26.4 seconds, and Koizumi's 9.5 seconds).

In Table 11, the results inverted by the Talbot method are presented. The number of N has the same definition as used in Table 6. Three different numbers (i.e., N=10, 15 and 64) were used. Accuracy of numerical inversion can be improved by increasing the number of terms. When N is equal to 64, accurate results (i.e., the percentage error is less than 10^{-5} % for all values of t) are obseved. Although the Talbot and Crump methods give the same level of accuracy for the oscillatory function tested, the Talbot method is suggested to use because less CPU times are needed by Talbot's method (i.e., for Talbot's method CPU time is 1.2 seconds while 7.2 seconds by Crump's method).

In Table 12, the results inverted by Weeks's method are presented. The number of N has the same definition as used in Table 5. Four different numbers (i.e., N=30, 40, 53 and 70) were used. In principle, the accuracy of numerical inversion can be improved by increasing the number of terms. However, roundoff error limits the value of N so that the accurate results (i.e., the maximun percentage error occuring at t=10 is about 2.4 %) are obtained when N is 53 instead of 70. The Weeks method utilizes about 1 minute CPU time which is much longer than 1.2 seconds by Talbot's method or 7.2 seconds by Crump's method. The Weeks method dose not appear to be a computationally efficient technique, supporting the conclusion noted by Lyness and Giunta [1986]. However, they described a modification for Weeks's method which could improve the computational efficiency of Weeks's method. We did not use this improved scheme because Talbot's method has been noted to be appropriate method for oscillatory functions in this study.

Comparisons between (75b) and results numerically inverted by those eight methods for (75a) are also shown in the Figure 2. Good agreement provided by the Crump, Dubner and Abate, Koizumi, Weeks, and Talbot methods can be noted in Figure 2a; poor agreement by the Stehfest, Schapery, and Widder methods is shown in Figure 2b.

According to the earlier discussions, the four methods of Schapery, Widder, Dubner and Abate, and Koizumi will not be used for further tests because they have limitation in accuracy or compuational efficiency. The other four methods of Stehfest, Crump, Weeks, and Talbot will be used for testing groundwater problems which do not possess sharp front, or oscillatory functions.

§3.3 Radial Dispersion Tests:

In this section, the four Laplace inversion methods of Stehfest, Crump, Weeks, and Talbot are tested against various analytical radial dispersion solutions given by Chen [1987]. In Figure 3, results of the resident concentration distributions for continuous injection from a single well [Chen, equation 21] are compared with appropriate semianalytical solutions for equation (12) of Chen [1987]. In Figure 4, results of the flux concetration distributions for continuous injection from a single well [Chen, equation 30] are compared with appropriate semianalytical solutions for the concentration transformation of equation (12) described in Chen [1987]. In Figure 5, results of the resident concentration distributions dealing with pulse injection from a single well [Chen, equation 28] are compared with the appropriate semianalytical solutions for equation (12) without (1/p) term of Chen [1987]. In Figure 6, results of the flux concentration for pulse injection from a single well [Chen, equation 32] are compared with the appropriate semianalytical solutions for the concentration transformation of equation (12) and without (1/p) term in Chen [1987].

In preparation of these four figures, the semianalytical solutions were determined by all the four numerical methods. Evaluation of these analytical solutions become uneasy as the dimensionless time is large. This is due to the difficulty involved in the necessary numerical integrations of pertinent functions. Therefore, the numerical inversion methods offer an alternative to obtain the desired solutions at large times. The semianalytical solutions at dimensionless time of 5000 are given in Figure 3 and 4 for demenstration purposes. It is seen from these four figures that the Crump, Weeks, and Talbot methods give accurate results for all dimensionless times. The Stehfest method yields accurate results for small dimensionless times and gives spurious oscillatory results for large dimensionless time.

To the similar problem studied by Chen [1987] yet subject to a Dirichlet boundary condition at the well bore, Moench and Ogata [1981] also noted that for large dimensionless times, the accuracy of the Stehfest method was limited by the number of significant digits that the computer could hold.

§3.4 Radial Flow Tests:

Karasaki et al. [1988] provided a linear radial flow model which was a composite system with two concentric regions. The flow was assumed to be linear in the inner region and radial in the outer region. The inner region was composed of a finite number of fractures whose flow characteristics and properties were different from the average values for the entire system. In the outer region the flow took place in a sufficient number of fractures so that the flow was radial. Analytical solutions were not given in his paper, but semianlytical solutions by Stehfest method were given. Here we use the four numerical methods to find the semianalytical solutions of the problem given by Karasaki [1988]. Results of dimensionless pressure heads at well bore for different dimensionless diffusivity α_c and dimensionless transmissivity β are shown in Figure 7 and 8. Very good agreement for these four methods is observed. As opposed to the test results discussed in section 3.3, the Stehfest method dose not yield oscillatory results at large times. Since the Stehfest method is the easiest one to use, it appears to be the best method for this particular test.

t	EXACT f(t)	APPROXIMATE f(t)		
		N=16	N=18	N=24
1.00	0.00000	0.00000	0.00000	0.00000
2.00	0.00000	-0.00014	-0.00013	-0.00002
3.00	0.00000	-0.00099	0.00261	-0.00072
4.00	0.00000	-0.00247	-0.01163	0.00495
5.00	0.00000	0.03469	0.02894	-0.01510
6.00	0.00000	-0.03419	0.00035	0.03708
7.00	0.00000	-0.09548	-0.09113	-0.02807
8.00	0.00000	0.00975	-0.02631	-0.08671
9.00	0.00000	0.25372	0.22094	0.13293
9.95	0.00000	0.51522	0.51049	0.49948
10.00	0.50000	0.52824	0.52508	0.51879
10.01	1.00000	0.53083	0.52798	0.52263
11.00	1.00000	0.75562	0.77774	0.84277
12.00	1.00000	0.91002	0.94058	1.01354
13.00	1.00000	0.99817	1.02311	1.06072
14.00	1.00000	1.03857	1.05141	1.04665
15.00	1.00000	1.04959	1.05014	1.01752
16.00	1.00000	1.04517	1.03656	0.99500
17.00	1.00000	1.03433	1.02063	0.98419
18.00	1.00000	1.02225	1.00702	0.98270
19.00	1.00000	1.01149	0.99730	0.98639
20.00	1.00000	1.00305	0.99140	0.99186
CPU TIME		00:00.00.130	00:00.00.130	00:00.00.150

Table 1. Using the Stehfest method [Stehfest, 1970] to numerically invert (71a) at three different numbers of weighting points.

t	EXACT $f(t)$	APPROXIMATE $f(t)$
1.00	0.000	0.00674
2.00	0.000	0.08209
3.00	0.000	0.18888
4.00	0.000	0.28650
5.00	0.000	0.36788
6.00	0.000	0.43460
7.00	0.000	0.48954
8.00	0.000	0.53526
9.00	0.000	0.57375
9.95	0.000	0.60501
10.00	0.500	0.60653
10.01	1.000	0.60683
11.00	1.000	0.63474
12.00	1.000	0.65924
13.00	1.000	0.68071
14.00	1.000	0.69967
15.00	1.000	0.71653
16.00	1.000	0.73162
17.00	1.000	0.74519
18.00	1.000	0.75747
19.00	1.000	0.76862
20.00	1.000	0.77880
CPU TIME		00:00.00.16

Table 2. Using the Schapery method [Schapery, 1962] to numerically invert (71a).

t	EXACT $f(t)$	APPROXIMATE $f(t)$		
		$N=1$	$N=4$	$N=10$
1.00	0.00000	0.00050	0.00000	0.00000
2.00	0.00000	0.04043	0.00002	0.00000
3.00	0.00000	0.15459	0.00294	0.00000
4.00	0.00000	0.28730	0.02925	0.00059
5.00	0.00000	0.40601	0.09963	0.01081
6.00	0.00000	0.50367	0.20563	0.05733
7.00	0.00000	0.58201	0.32512	0.15745
8.00	0.00000	0.64464	0.44049	0.29681
9.00	0.00000	0.69496	0.54268	0.44586
9.95	0.00000	0.73391	0.62491	0.57479
10.00	0.50000	0.73576	0.62884	0.58100
10.01	1.00000	0.73613	0.62962	0.58223
11.00	1.00000	0.76915	0.69947	0.69096
12.00	1.00000	0.79676	0.75649	0.77397
13.00	1.00000	0.81981	0.80218	0.83306
14.00	1.00000	0.83921	0.83867	0.87288
15.00	1.00000	0.85570	0.86783	0.89799
16.00	1.00000	0.86980	0.89118	0.91224
17.00	1.00000	0.88196	0.90994	0.91863
18.00	1.00000	0.89251	0.92508	0.91943
19.00	1.00000	0.90171	0.93735	0.91632
20.00	1.00000	0.90980	0.94735	0.91050
CPU TIME		00:00.00.070	00:00.00.060	00:00.00.080

Table 3. Using the Widder method [Widder, 1934] to numerically invert (71a), N is the n-th derivative.

t	EXACT f(t)	APPROXIMATE f(t)		
		DUBNER &ABATE aT=4.5	KOIZUMI aT=4.5	CRUMP aT=4.5
1.00	0.00000	0.0002803	0.0000313	0.0000000
2.00	0.00000	0.0003197	0.0000969	0.0000006
3.00	0.00000	0.0003691	0.0001188	0.0000202
4.00	0.00000	0.0004309	0.0001033	0.0000063
5.00	0.00000	0.0005085	0.0002570	0.0000084
6.00	0.00000	0.0006060	0.0005430	-0.0000043
7.00	0.00000	0.0007289	0.0004718	-0.0000345
8.00	0.00000	0.0008848	0.0000535	0.0004516
9.00	0.00000	0.0010899	0.0008197	-0.0003940
9.95	0.00000	0.0043174	-0.0293063	0.0010010
10.00	0.50000	0.5012920	0.5007749	0.4947337
10.01	1.00000	0.9990843	1.0067979	0.9994454
11.00	1.00000	1.0015535	1.0013345	1.0083534
12.00	1.00000	1.0019403	1.0028337	1.0013146
13.00	1.00000	1.0024091	1.0021769	1.0015003
14.00	1.00000	1.0029921	1.0019945	0.9993314
15.00	1.00000	1.0037203	1.0034824	1.0009883
16.00	1.00000	1.0046313	1.0050749	0.9992479
17.00	1.00000	1.0057716	1.0055323	1.0010493
18.00	1.00000	1.0071993	1.0062767	1.0006855
19.00	1.00000	1.0089870	1.0087461	1.0002603
20.00	1.00000	1.0112256	1.0117089	1.0000605
CPU TIME		00:04.15.180	00:01.04.050	00:00.58.490

Table 4. Using the Dubner and Abate [1968], Koizumi [see Squire, 1984] and Crump [1975] method to numerically invert (71a) with $aT = 4.5$ chosen for an error of order in (34), (35) and (36).

t	EXACT f(t)	APPROXIMATE f(t)			
		N=50	N=70	N=100	N=150
1.00	0.00000	0.03982	0.06250	0.07588	0.02499
2.00	0.00000	0.09084	-0.05568	0.04512	-0.02665
3.00	0.00000	-0.02774	-0.01306	-0.05664	-0.05116
4.00	0.00000	0.01287	-0.04089	0.01586	-0.00628
5.00	0.00000	0.03637	-0.06927	0.04207	-0.00540
6.00	0.00000	-0.07690	-0.06362	-0.00198	0.04146
7.00	0.00000	0.04613	-0.02420	-0.06641	0.02742
8.00	0.00000	0.00594	0.01092	-0.02438	-0.04283
9.00	0.00000	-0.07470	0.01321	0.03948	-0.02395
9.95	0.00000	0.43481	0.39423	0.39253	0.34284
10.00	0.50000	0.49421	0.47096	0.50585	0.50887
10.01	1.00000	0.50609	0.48650	0.52852	0.54219
11.00	1.00000	1.09245	1.01918	0.95663	1.02263
12.00	1.00000	0.94169	1.04700	0.97383	0.98407
13.00	1.00000	1.04632	0.95842	0.97632	1.01253
14.00	1.00000	0.95559	1.01257	0.98158	0.99221
15.00	1.00000	1.03406	1.00486	0.99544	0.99104
16.00	1.00000	0.97754	0.98121	1.01026	1.00278
17.00	1.00000	0.99806	1.01915	1.00798	1.00560
18.00	1.00000	1.01874	0.97649	0.99020	1.00182
19.00	1.00000	0.96913	1.01853	0.98969	0.99773
20.00	1.00000	1.01497	0.97818	1.00692	0.99537
CPU TIME		00:01.51.390	00:03.41.300	00:07.35.860	00:17.08.830

Table 5. Using the Weeks method [Weeks, 1966] to numerically invert (71a) with four different numbers of term in series of (38).

t	EXACT f(t)	APPROXIMATE f(t)			
		N= 5	N=15	N=30	N=45
1.00	0.00000	0.76030	0.56063	-1.03809	-9.40436
2.00	0.00000	0.84924	0.88349	0.81893	0.65816
3.00	0.00000	0.87232	0.92881	0.92740	0.90604
4.00	0.00000	0.88279	0.94512	0.95562	0.95342
5.00	0.00000	0.88876	0.95330	0.96747	0.97023
6.00	0.00000	0.89260	0.95817	0.97377	0.97823
7.00	0.00000	0.89529	0.96139	0.97760	0.98274
8.00	0.00000	0.89727	0.96366	0.98016	0.98558
9.00	0.00000	0.89879	0.96536	0.98198	0.98750
9.95	0.00000	0.89995	0.96661	0.98327	0.98883
10.00	0.50000	0.90000	0.96667	0.98333	0.98889
10.01	1.00000	0.90001	0.96668	0.98335	0.98890
11.00	1.00000	0.90098	0.96771	0.98438	0.98993
12.00	1.00000	0.90179	0.96856	0.98521	0.99073
13.00	1.00000	0.90247	0.96926	0.98588	0.99137
14.00	1.00000	0.90305	0.96985	0.98644	0.99189
15.00	1.00000	0.90355	0.97036	0.98691	0.99232
16.00	1.00000	0.90399	0.97079	0.98731	0.99268
17.00	1.00000	0.90437	0.97118	0.98765	0.99298
18.00	1.00000	0.90471	0.97151	0.98795	0.99325
19.00	1.00000	0.90502	0.97181	0.98822	0.99348
20.00	1.00000	0.90529	0.97208	0.98845	0.99368
CPU TIME		00:00.00.170	00:00.00.430	00:00.00.800	00:00.01.190

Table 6. Using the Talbot method [Talbot, 1979] to numerically invert (71a) with four different numbers of term in series of (70).

t	EXACT f(t)	APPROXIMATE f(t)		
		N=16	N=18	N=24
0.10	0.00499	0.00499	0.00499	0.00499
0.50	0.11986	0.11985	0.11986	0.11986
0.80	0.28694	0.28691	0.28693	0.28697
1.00	0.42074	0.42088	0.42070	0.42074
2.00	0.90930	0.89325	0.90649	0.90929
3.00	0.21168	0.33501	0.25352	0.21047
4.00	-1.51360	-1.89921	-1.59339	-1.49978
5.00	-2.39731	-2.35135	-2.73089	-2.40929
6.00	-0.83825	0.56260	0.17794	-1.04662
7.00	2.29945	2.16533	2.78985	2.91773
8.00	3.95743	1.33167	1.90496	4.08613
9.00	1.85453	-0.00410	-0.18198	0.16514
10.00	-2.72011	-0.66477	-1.21222	-3.29330
15.00	4.87716	0.09808	0.28655	0.84362
20.00	9.12945	0.03281	-0.01266	-0.21756
30.00	-14.82047	-0.00586	-0.00308	0.00183
CPU TIME		00:00.00.030	00:00.00.040	00:00.00.040

Table 7. Using the Stehfest method [Stehfest, 1970] to numerically invert (75a) at three different numbers of weighting points.

t	EXACT $f(t)$	APPROXIMATE $f(t)$
1.00	0.42074	0.16000
2.00	0.90930	0.05536
3.00	0.21168	0.02630
4.00	-1.51360	0.01515
5.00	-2.39731	0.00980
6.00	-0.83825	0.00685
7.00	2.29945	0.00505
8.00	3.95743	0.00388
9.00	1.85453	0.00307
10.00	-2.72011	0.00249
CPU TIME		00:00.00.11

Table 8. Using the Schapery method [Schapery, 1962] to numerically invert (75a).

t	EXACT f(t)	APPROXIMATE f(t)			
		N=1	N=2	N=3	N=4
1.00	0.42074	0.25000	0.46080	0.51192	0.51842
2.00	0.90930	-0.03200	0.00000	0.10646	0.22528
3.00	0.21168	-0.05400	-0.15126	-0.25000	-0.32388
4.00	-1.51360	-0.04234	-0.11520	-0.20676	-0.31250
5.00	-2.39731	-0.03129	-0.07126	-0.10875	-0.14627
6.00	-0.83825	-0.02345	-0.04320	-0.04864	-0.04117
7.00	2.29945	-0.01803	-0.02683	-0.01940	0.00174
8.00	3.95743	-0.01422	-0.01724	-0.00630	0.01408
9.00	1.85453	-0.01146	-0.01147	-0.00072	0.01492
10.00	-2.72011	-0.00941	-0.00788	0.00148	0.01241
CPU TIME		00:00.00.030	00:00.00.030	00:00.00.030	00:00.00.030

Table 9. Using the Widder method [Widder, 1934] to numerically invert (75a), N is the n-th derivative.

t	EXACT f(t)	APPROXIMATE f(t)		
		DUBNER &ABATE aT=15	KOIZUMI aT=15	CRUMP aT=15
1.00	0.4207355	0.4207355	0.4207358	0.4207355
2.00	0.9092974	0.9092974	0.9092978	0.9092974
3.00	0.2116800	0.2116800	0.2116805	0.2116800
4.00	-1.5136050	-1.5136050	-1.5136042	-1.5136050
5.00	-2.3973107	-2.3973107	-2.3973093	-2.3973107
6.00	-0.8382465	-0.8382465	-0.8382439	-0.8382465
7.00	2.2994531	2.2994532	2.2994579	2.2994531
8.00	3.9574330	3.9574331	3.9574420	3.9574330
9.00	1.8545332	1.8545328	1.8545497	1.8545332
10.00	-2.7201056	-2.7201101	-2.7200771	-2.7201056
CPU TIME		00:00.26.370	00:00.09.490	00:00.07.170

Table 10. Using the Dubner and Abate [1968], Koizumui [see Squire, 1984] and Crump [1975] methods to numerically invert (75a) with $aT = 15$ chosen for an error of order in (34), (35) and (36)

t	EXACT $f(t)$	APPROXIMATE $f(t)$		
		N=10	N=15	N=64
1.00	0.42074	0.50574	0.42075	0.42074
2.00	0.90930	1.24187	0.90924	0.90930
3.00	0.21168	0.95902	0.21180	0.21168
4.00	-1.51360	-0.20037	-1.51381	-1.51360
5.00	-2.39731	-0.38939	-2.39702	-2.39731
6.00	-0.83825	2.01086	-0.83859	-0.83825
7.00	2.29945	6.08566	2.29980	2.29945
8.00	3.95743	8.75194	3.95720	3.95743
9.00	1.85453	7.77161	1.85446	1.85453
10.00	-2.72011	4.32564	-2.71946	-2.72011
CPU TIME		00:00.00.220	00:00.00.310	00:00.01.200

Table 11. Using the Talbot [1979] method to numerically invert (75a) with three different numbers of term in series of (70).

t	EXACT $f(t)$	APPROXIMATE $f(t)$			
		N=30	N=40	N=53	N=70
1.00	0.42074	0.41355	0.29263	0.41150	0.46126
2.00	0.90930	0.89735	0.95500	0.90796	0.91040
3.00	0.21168	-0.05569	0.26329	0.20978	0.18795
4.00	-1.51360	-1.94160	-1.46274	-1.47956	-1.53035
5.00	-2.39731	-2.36232	-2.43940	-2.35763	-2.39853
6.00	-0.83825	-0.55415	-0.94550	-0.82686	-0.75585
7.00	2.29945	2.58485	2.19855	2.25357	2.36127
8.00	3.95743	4.25247	3.85280	3.87481	3.90863
9.00	1.85453	1.37869	2.08978	1.81374	1.71744
10.00	-2.72011	-3.32702	-2.38632	-2.65465	-2.83802
CPU TIME		00:00.20.290	00:00.35.900	00:01.03.160	00:01.50.540

Table 12. Using the Weeks [1966] method to numerically invert (75a) at four different numbers of term in series of (38).

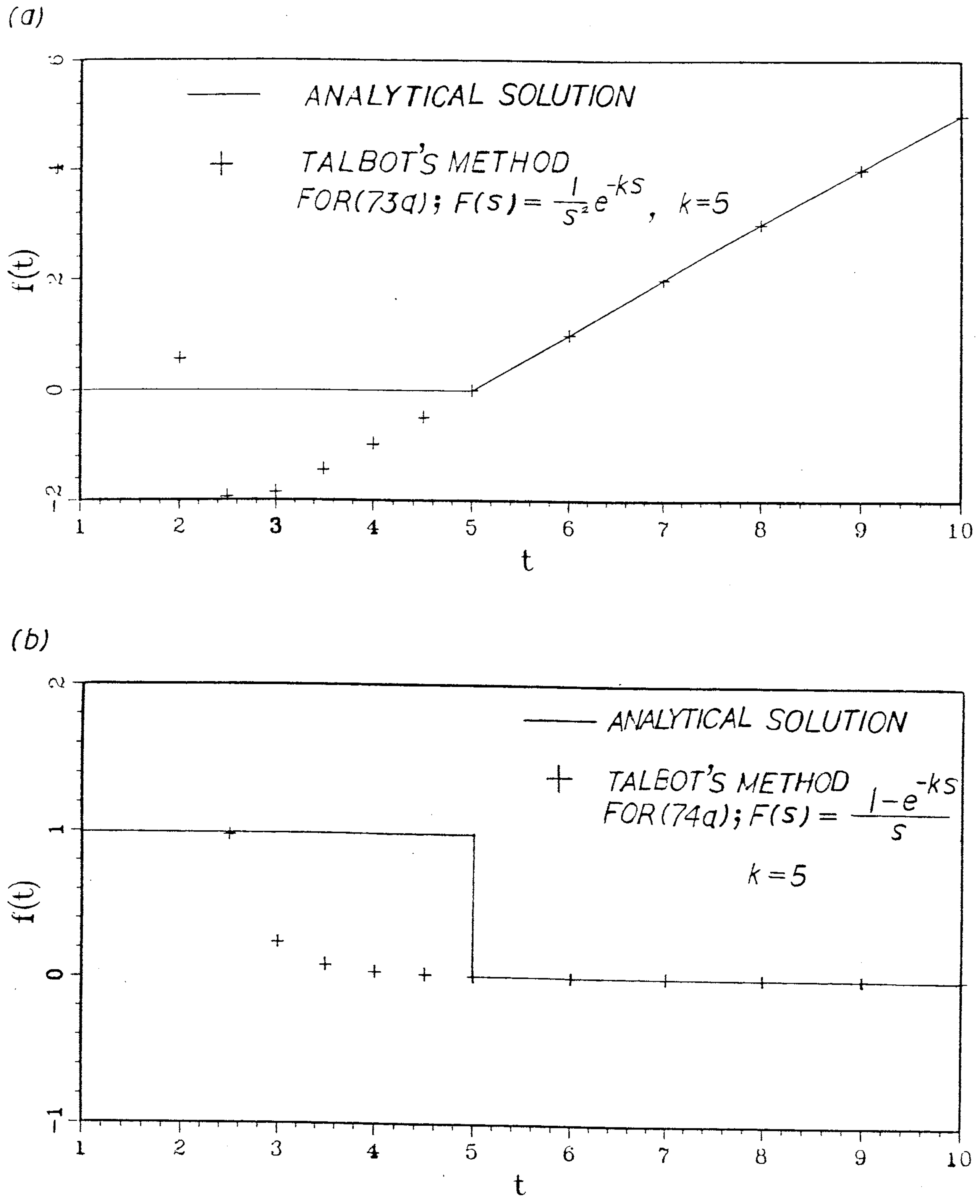

Fig. 1 Comparisons showing Talbot's method is not appropriate for inverting functions of $e^{(t-k)}$ as $t < k$. (a) Results inverted by Tablot's method for (73a); (b) Results inverted by Talbot' method for (74a)

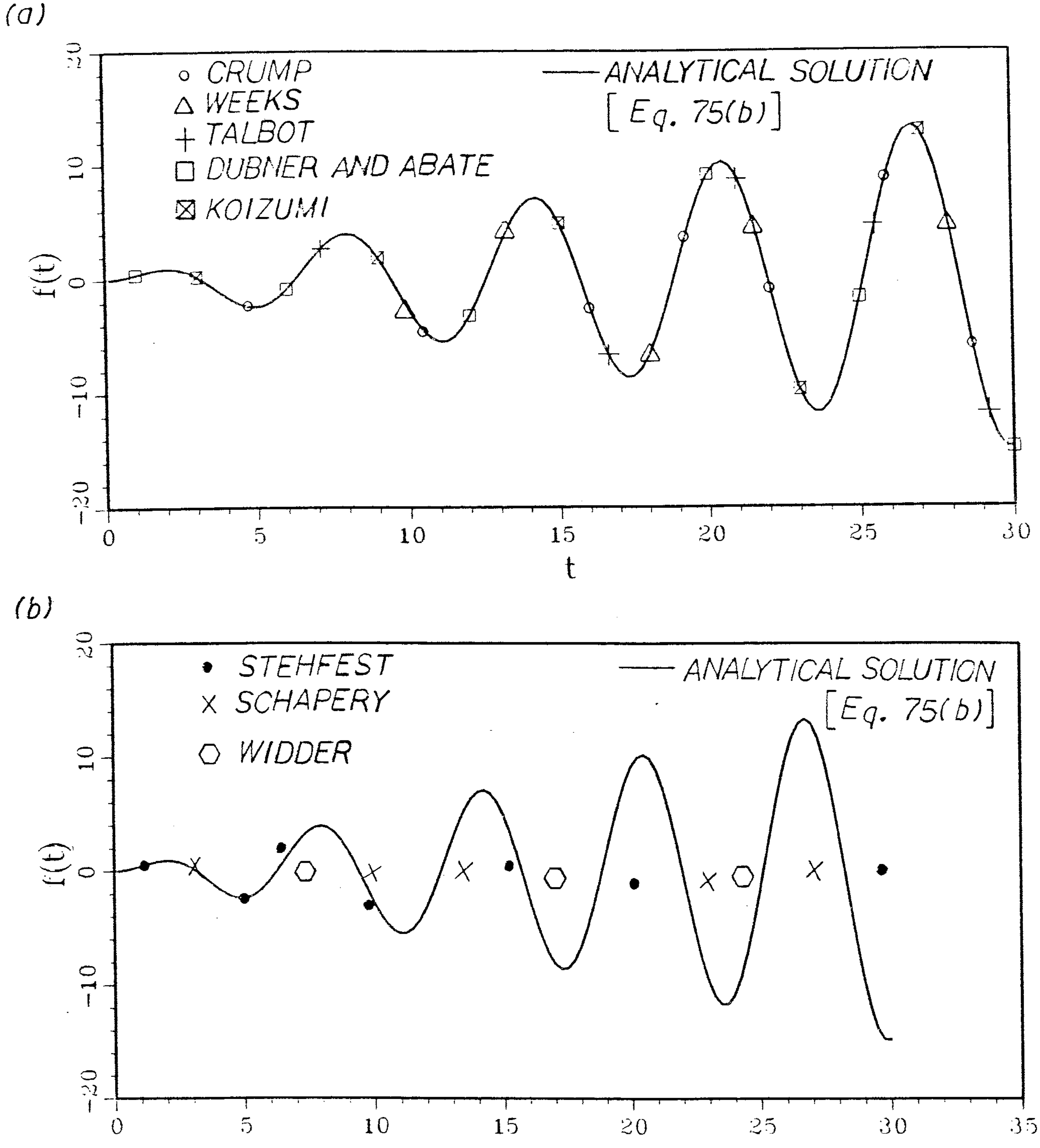

Fig. 2 Comparisons between the analytical solution of (75b) and semianalytical solutions for (75a) by eight different numerical inversion methods. (a) Good agreement by Crump, Dubner and Abate, Koizumi, Weeks and Talbot methos; (b) Poor agreement by Stehfest, Schapery and Widder nethods

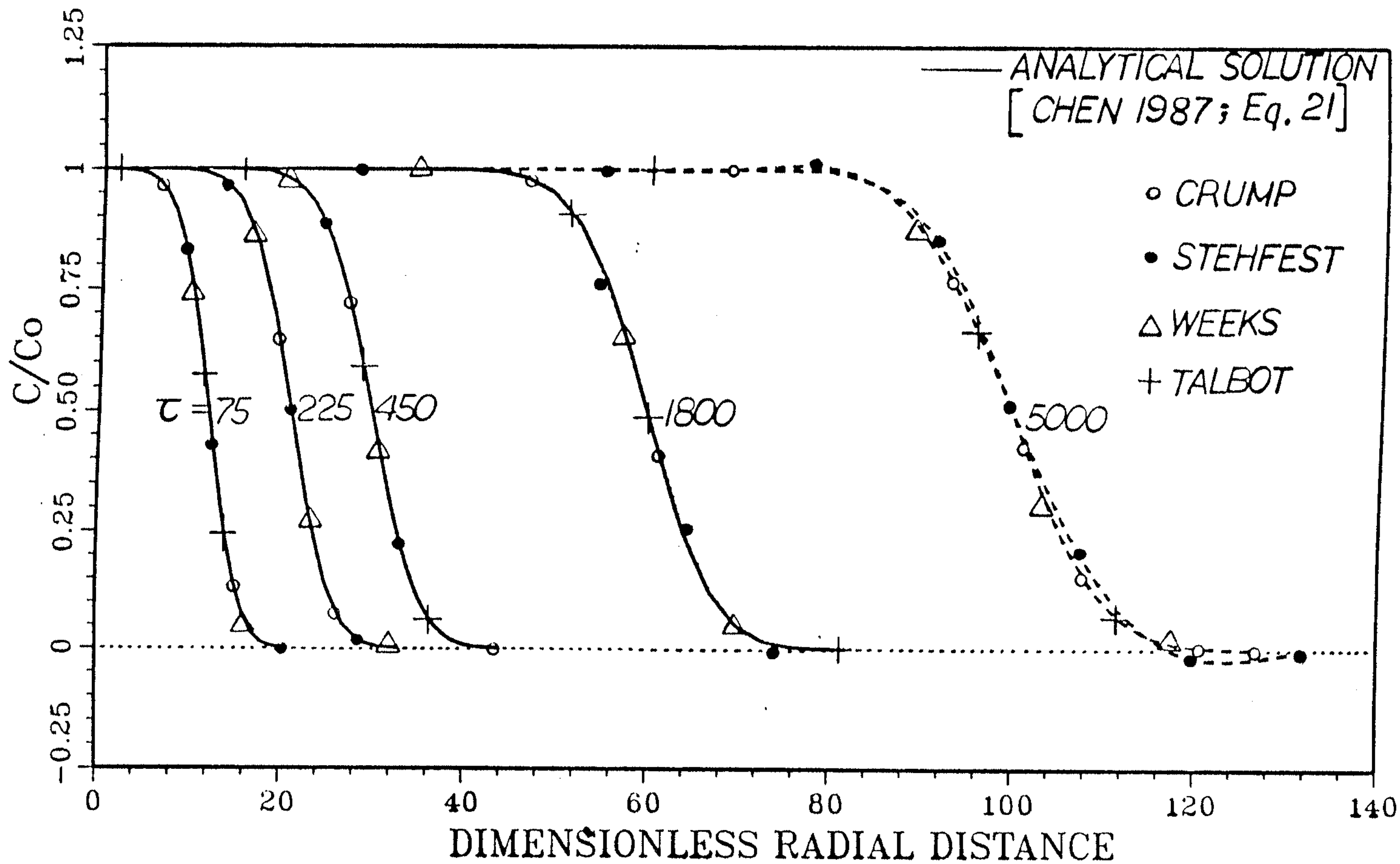

Fig. 3 Comparisons of different numerical inversion methods with analytical solutions for resident concentration dealing with a continuous injection from a single well at various dimensionless time

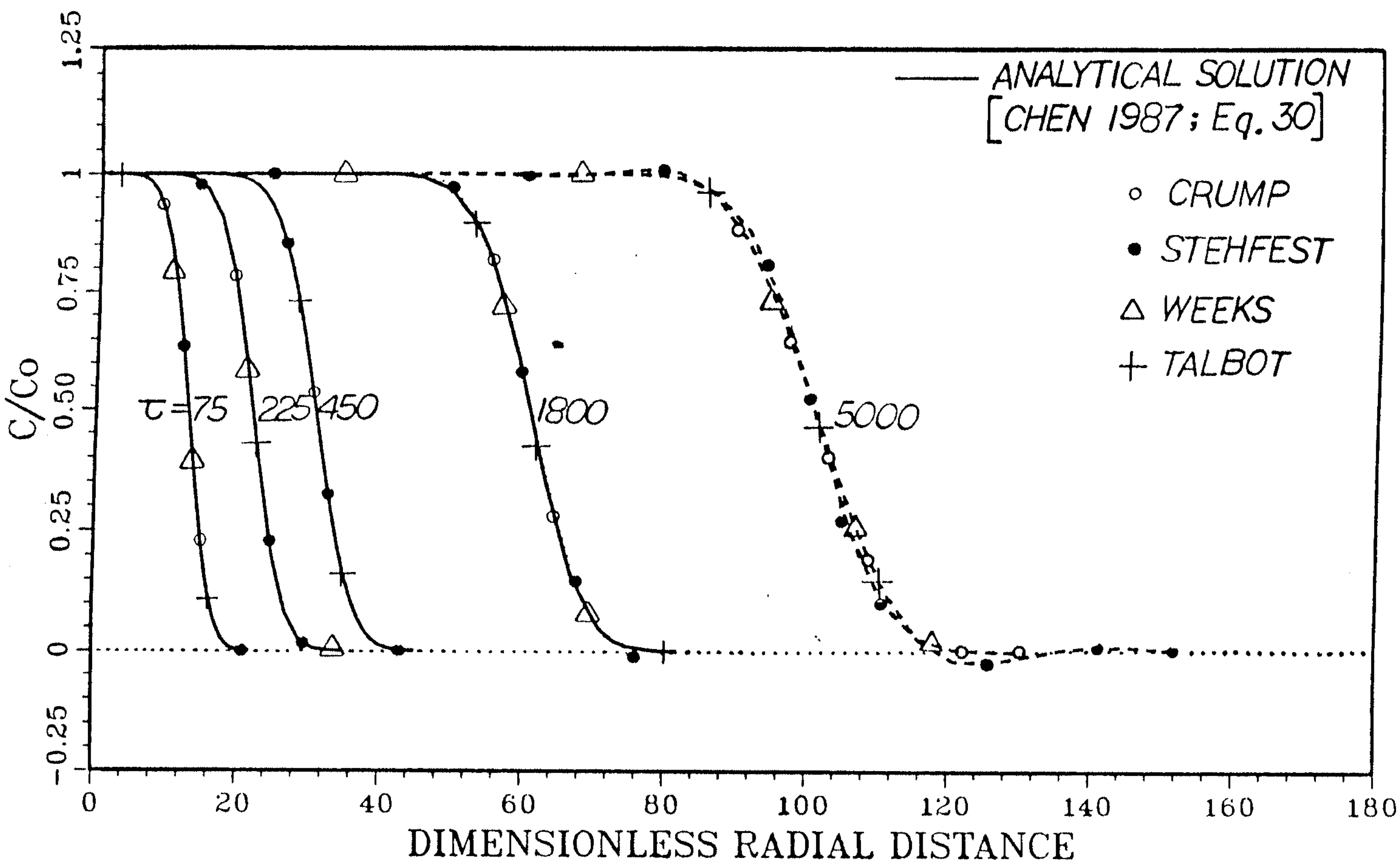

Fig. 4 Comparisons of different numerical inversion methods with analytical solutions for flux cincentration dealing with a continuous injection from a single well at various dimensionless time

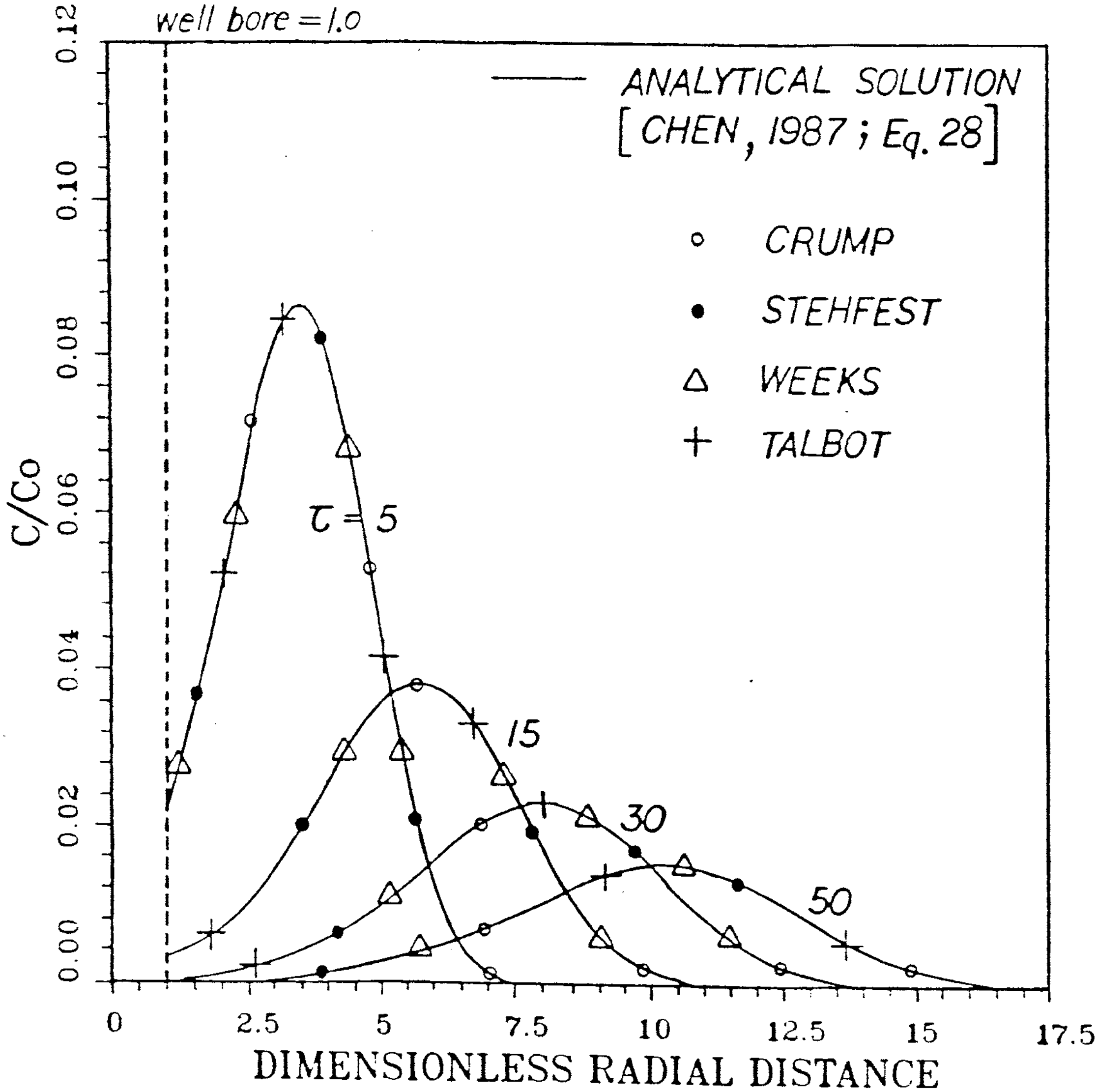

Fig. 5 Comparisons of different numerical inversion methods with analytical solutions for resident concentration dealing with a pluse injection from a single well at various dimensionless time

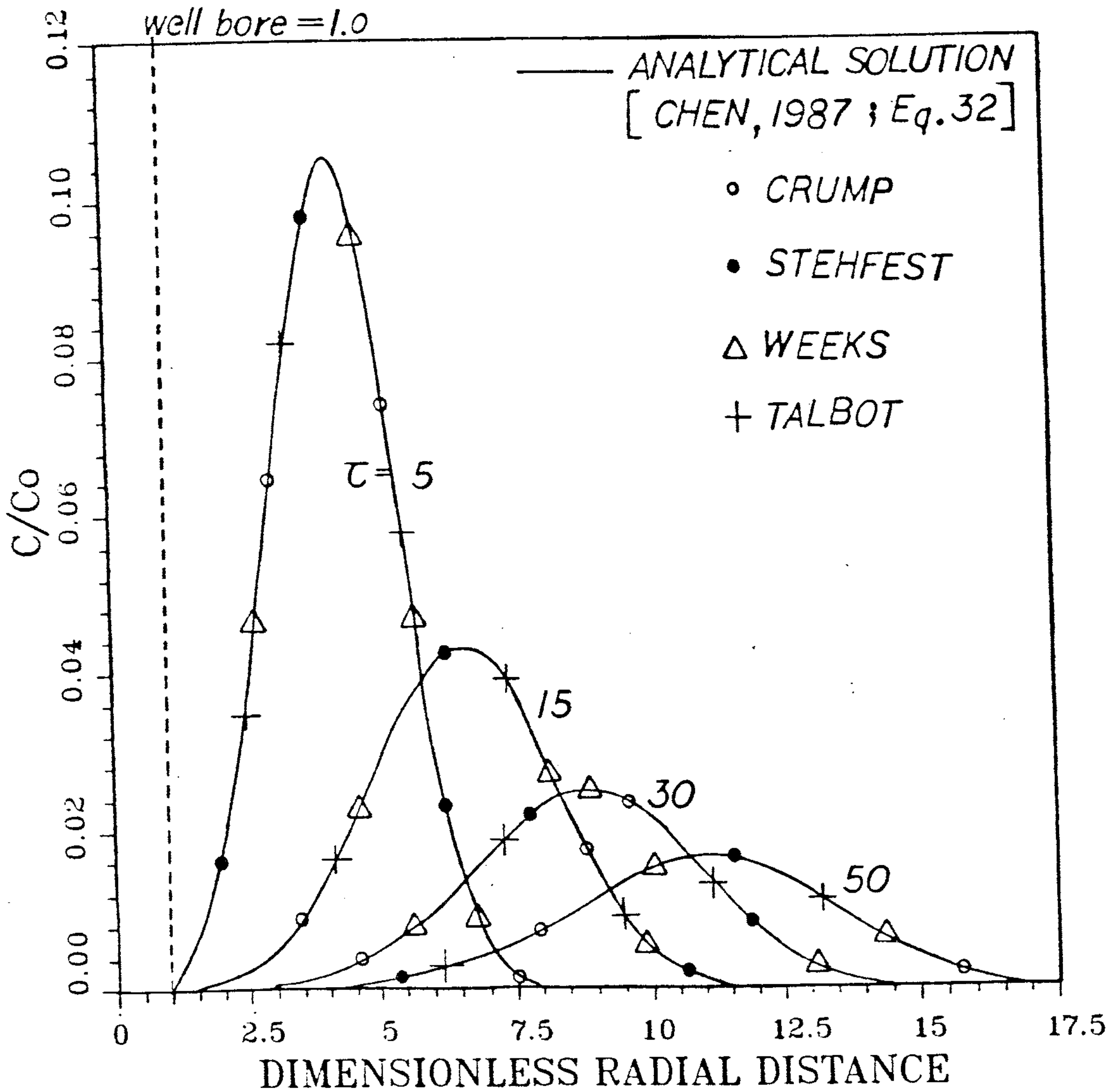

Fig. 6 Comparisons of different numerical inversion methods with analytical solutions for flux concentration dealing with a pulse injection from a single well at various dimensionless time

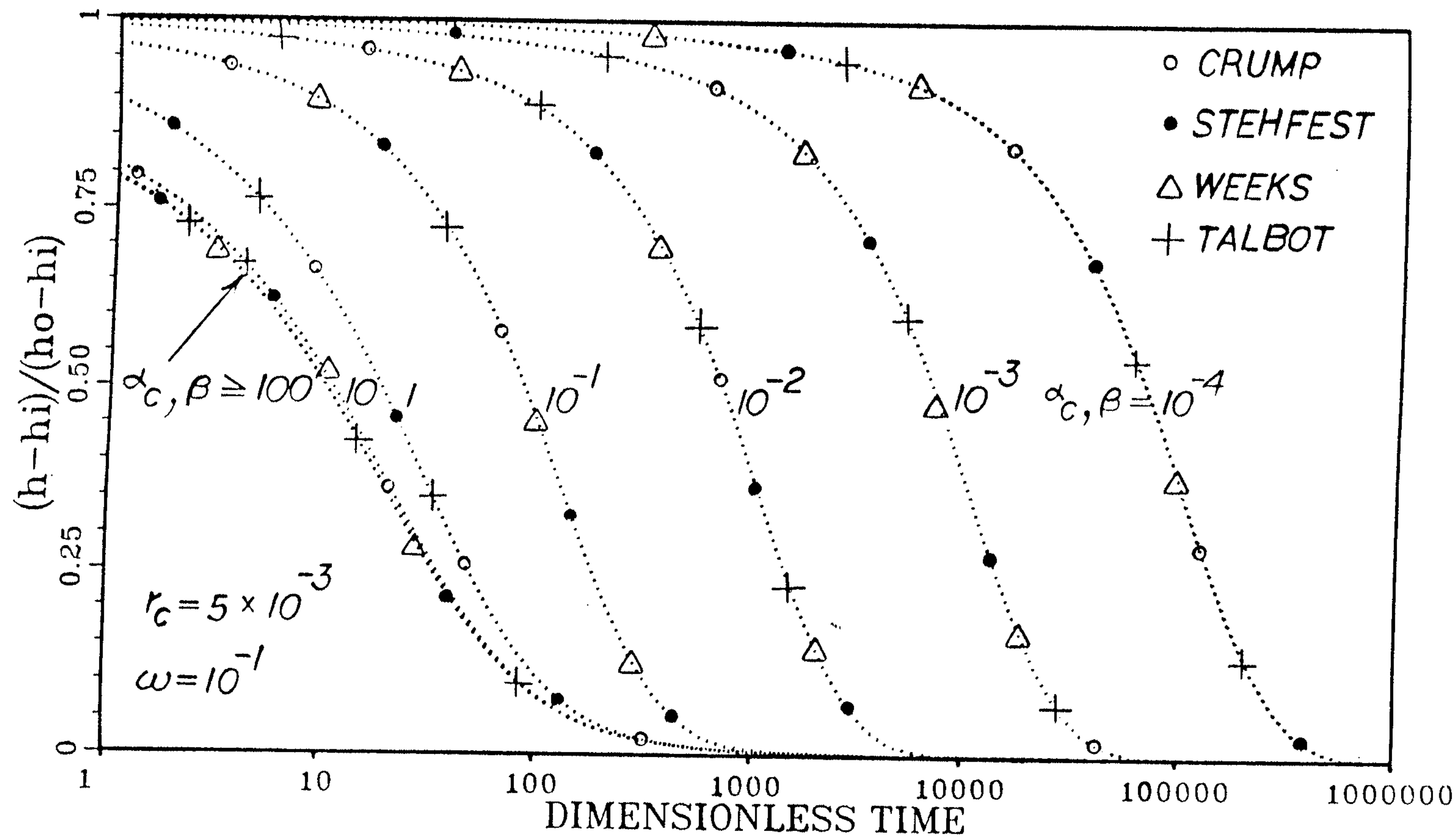

Fig. 7 Comparisons of semianalytical solutions inverted by four different numerical inversion methods for linear radial flow model of the slug test present by Karasaki et al. [1988] at $r_c = 5 \bullet 10^{-3}$ and $\omega = 10^{-1}$

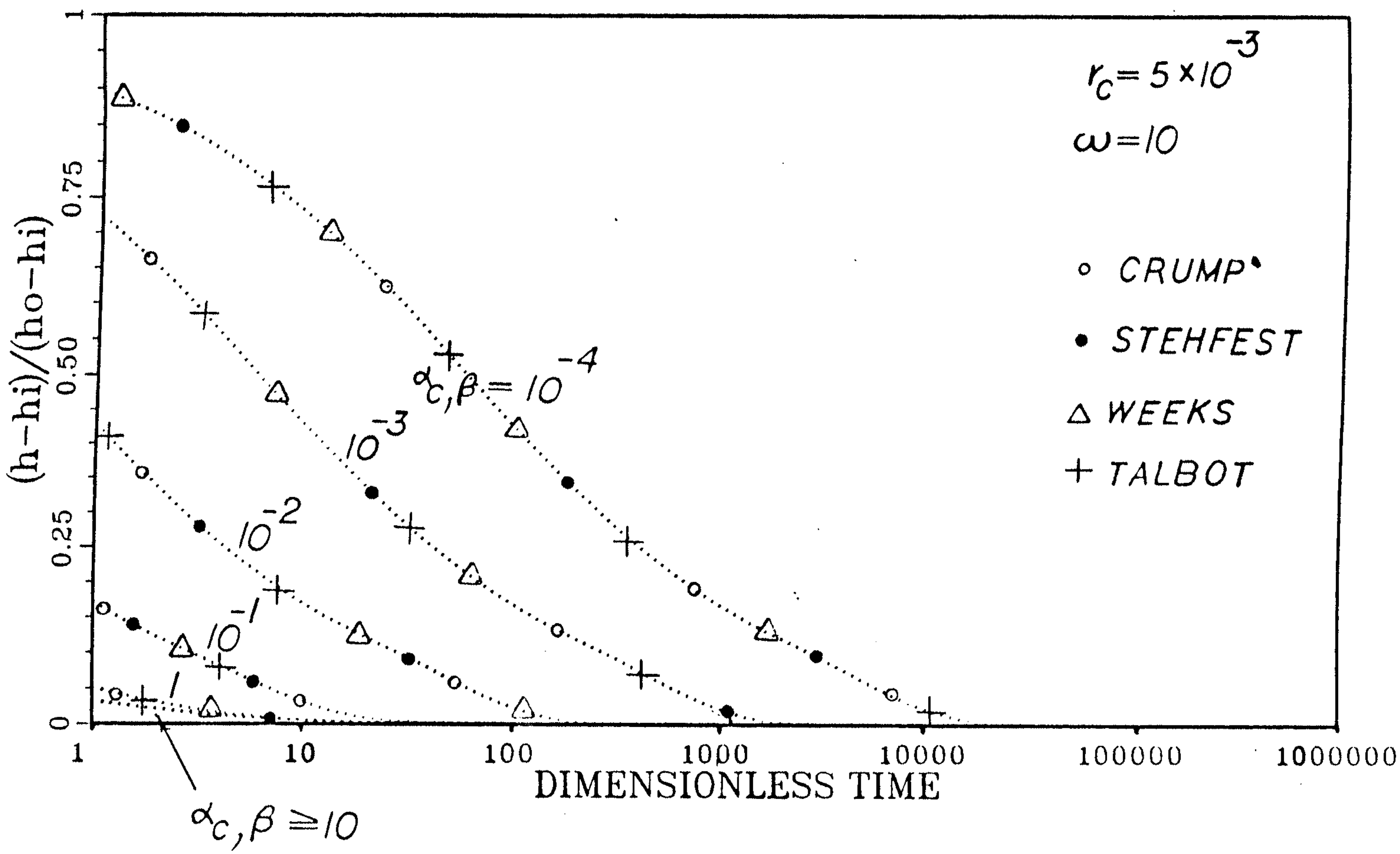

Fig. 8 Comparisons of semianalytical solutions inverted by four different numerical inversion methods for linear radial flow model of the slug test present by Karasaki et al. [1988] at $r_c = 5 \bullet 10^{-3}$ and $\omega = 10$

Chapter 4.

CONCLUSIONS AND SUGGESTIONS

This study permitted the following conclusions to be drawn.

1. For functions with a steep first derivative (e.g., sharp concentration front resulted from advection dominant transport process), the Sthefest, Schapery, Widder, Weeks and Talbot methods do no give accurate results. The accurate results can be obtained by the Crump, Dubner and Abate and Koizumi methods. The Crump method is most computationally efficient (i.e., least CPU time) among these three successful methods.

2. For functions having oscillatory behavior, the Stehfest, Schapery, and Widder methods do not provide accurate results. The Crump, Koizumi, Dubner and Abate, Weeks and Talbot methods generate accurate results. Among these five successful methods, the Talbot method is most efficient (i.e., least CPU time).

3. In dealing with groundwater solute transport and flow problems without sharp front conditions, or rapid oscillations, the Stehfest, Crump, Weeks and Talbot methods give essentially the same results. However, the Stehfest method yields spurious oscillatory results at large dimensionless times for transport problems. Computationally, the Stehfest method is the easiest to use; the Crump, Weeks, and Talbot methods involve complex number calculations for the Laplace transform parameter needs to be declared as complex.

Therefore, among the eight numerical Laplace inversion methods, we suggest that the Crump method be used for groundwater problems because it can successfully invert functions that are oscillatory, smooth, or of discontinuities in the first derivative. In addition to this suggestions, we offer the following comments:

(1) For oscillatory functions, the Talbot method may be used instead of the Crump method for less CPU time are needed by the Talbot method.

(2) For smooth functions, due to its simplicity in application the Stehfest method

may be used with care, noting that it may give spurious oscillatory results at large times for transport problems.

(3) Other methods such as Schapery's, Weeks's, Dubner and Abate's, Koizumi's, and Weeks's methods are not recommended for groundwater problems. However, We noted that Lyness and Giunta [1986] gave a modified Weeks's method that may improve its computational efficiency. This improvement has not been tested here for groundwater problems.

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