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New Approach for Calculate Exponential Integral Function

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Abstract

This manuscript presents a new approach to accurately calculating exponential integral function that arises in many applications such as contamination, groundwater flow, hydrological problems and mathematical physics. The calculation is obtained with easily computed components without any restrictive assumptions

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A detailed comparison of the execution times is performed. The calculated results by the suggested approach are better and faster accuracy convergence than those calculated by other methods. Error analysis of the calculations is studied using the absolute error and high convergence is achieved. The suggested approach out-performs all previous methods used to calculate this function and this decision is based on the getting results.

Keywords: Theis well function, Exponential integral, Chebyshev approximation, Rational approximation, Exponential integral.

اسلوب جديد لحساب تكامل دالة أسية

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الخلاصة

يتضمن البحث اسلوب جديد لحساب تكامل دالة اسية بدقة و التي تظهر في تطبيقات عديدة مثل التلوث, جريان المياه الجوفية, مشاكل الموارد المائية و الرياضيات الفيزيائية. الحسابات حصلت بحساب المركبات بسهولة دون قيود فرضيات للمعالجة. تم عمل مقارنة تفصيلية للزمن المستغرق في الحساب. النتائج المحسوبة بالأسلوب المقترح احسن دقة و اسرع تقارب مقارنة بتلك المحسوبة بطرق اخرى . تحليل الخطأ للحسابات درس باستخدام الخطأ المطلق و حصلنا على تقارب عالي. الاسلوب المقترح يختلف عن اداء جميع الطرق السابقة التي استخدمت لحساب هذه الدالة و هذا القرار مستند على النتائج التي تم الحصول عليها

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1. Introduction

The exponential integral is an important integral because it is used in many physical problems such as groundwater flow models, reactor physics and others [1]. In addition, many integrals and complex functions can be represented by exponential integrals. The important point is how to estimate this function which denoted (well function), W(u) = - E_i(-u). Theis [2] was the beginning of the appearance of exponential integration in groundwater models. Properly calculating the well function is very important in the calculations of the pumping tests which is used to determine the coefficients of confined or leakage aquifers. Formerly, the well function are based on the approximate values in the form of tables for small values or used numerical integrations. Recently, approximations of the well function are valid for the entire range of arguments that have been proposed for both confined and leaky aquifers by Swamee and Ojha see [3-5]. Finding an analytical solution for exponential integration is not possible, so numerical methods must be used. Our purpose in this paper is to find a reliable and easy implementation approximate for $E_1(u)$. This approximate is appropriate for the aquifer systems, such approximate will be involved only common mathematical functions and be less computationally intensive to evaluate as well as simple and quick to program, it will also involve errors that are less than would occur in hydrological data sets such that using the formula does not consist any additional errors.

The importance of the calculated exponential integral function is appeared in solving Theis equation which studied the groundwater flow model in confined aquifers in the unsteady state case and it is defined as follows [6-8]:

$$s_r = \frac{Q}{4\pi T_r}\int_u^\infty \frac{e^{-\tau}}{\tau}d\tau = \frac{Q}{4\pi T_r} W(u)$$

where Q is discharge or volume flow rate, T_r is the transmissivities in the r direction.

This article has been arranged as follows: In section 2, we present the exponential integral function. In section 3, we briefly review the most approximate methods. A suggested approach with implementation and discussions for the results will be given in section 4. Finally, the conclusion is given in section 5.

2. Exponential Integral Function

The exponential integral function is also called Theis function or First order $E_1(u)$ which is applying to confined aquifers, it is denoted by W(u) and defined as follows [9-11]:

$$W(u) = E_1(u) = -E_i(-u) = \int_u^\infty \frac{e^{-y}}{y}dy, \quad u > 0 \tag{1}$$

Where u is a dimensionless variable and y is a dummy variable. The integral in eq. (1) is a function of the lower integration limit u. This function tends to be infinity, thus it fails to be defined when u approaches zero. The integral in eq. (1) can be expanded in a convergent series that is given in most groundwater textbooks.

Lebedev (1965) see [12] and Van der Laan and Temme (1984) see [13] discussed this integral in complex domain, for $u = \frac{r^2\delta}{4T\tau}$, where T: transmissivity, δ : storativity, r : radial distance, and τ : the time.

As we mentioned earlier, the well function cannot be analytically solved. Therefore, different methods and techniques have been used to approximate this function which varies according to the required of accuracy. For u < 1, we can use the Maclaurin series to the exponential function in equation (1) and then integrate this series term by term to get:

$$E_1(u) = -\gamma - \ln(u) + \sum_{n=1}^{\infty} \frac{(-1)^{n+1} u^n}{n.n!} \qquad (2)$$

where γ = 0.5772156649015328606 is the Euler constant. There are some efficient approaches that have been successfully used to calculate Euler constant such as those was suggested by Lebedev (1965) see [14-16] and Andrews (1985) see [17-19]. But the accurate value of this constant is up to 50 decimal places proposed by Murnaghan and Wrench (1963) see [20-23].

Here by using MATLAB code, the authors calculate the value of well function for any number of the series terms in equation (2). In the interval (0, 1], it is found that the values of the function are matching with 50 decimal places when calculated for 20 or more terms of the series in equation (2). Table 1 illustrates the matching of the values when calculating the function with 20-terms and 200-terms for different values within the interval (0, 1]. Therefore, we will approximate the following function instead of approximate equation (2)

$$E_1(u) = -\gamma - \ln(u) + \sum_{n=1}^{20} \frac{(-1)^{n+1} u^n}{n.n!} \;, u \in (0,1] \qquad (3)$$

Table 1: The values of exponential integral function with n= 20 and n= 200

u	n= 20	n= 200
0.00001	10.93571980004369414984921604627743363380432128906 25	10.93571980004369414984921604627743363380432128906 25
0.00006	9.144010329940652326285999151878058910369873046875	9.144010329940652326285999151878058910369873046875
0.0001	8.633224704574702812465147871989756822586059570312 5	8.633224704574702812465147871989756822586059570312 5
0.0006	6.841965147858592999341453833039849996566772460937 5	6.841965147858592999341453833039849996566772460937 5
0.001	6.331539364136149039552492467919364571571350097656 25	6.331539364136149039552492467919364571571350097656 25
0.006	4.544771156839062520305105863371863961219787597656 25	4.544771156839062520305105863371863961219787597656 25
0.01	4.037929576538114240236154728336259722709655761718 75	4.037929576538114240236154728336259722709655761718 75
0.06	2.295306918143782848318323885905556380748748779296 875	2.295306918143782848318323885905556380748748779296 875
0.1	1.822923958419390366714196716202422976493835449218 75	1.822923958419390366714196716202422976493835449218 75
0.2	1.222650544183892629135357310588005930185317993164 0625	1.222650544183892629135357310588005930185317993164 0625
0.3	0.905676651675846433597882878530072048306465148925 78125	0.905676651675846433597882878530072048306465148925 78125
0.4	0.702380118865662428362384162028320133686065673828 125	0.702380118865662428362384162028320133686065673828 125
0.5	0.559773594776160732244818518665852025151252746582 03125	0.559773594776160732244818518665852025151252746582 03125
0.6	0.454379503189402178531253184701199643313884735107 421875	0.454379503189402178531253184701199643313884735107 421875
0.7	0.373768843233509229229127868165960535407066345214 84375	0.373768843233509229229127868165960535407066345214 84375
0.8	0.310596578545542900684495180030353367328643798828 125	0.310596578545542900684495180030353367328643798828 125
0.9	0.260183939325999646907661144723533652722835540771 484375	0.260183939325999646907661144723533652722835540771 484375
1.0	0.219383934395520285853820041666040197014808654785 15625	0.219383934395520285853820041666040197014808654785 15625

3. Approximate Methods

There is various approximation methods have been used and developed to approximate the exponential integral because their nonanalytic nature, each one of them is suitable in some range for the values of u. It will be beneficial to have a simple and handy algorithm for occasional use Barry et al., 2000, see [24]. In the following, most of these methods are reviewed briefly.

3.1. Series expansion

The power series in equation (2) is converging with any $u < 1$, that is

$$\begin{cases} E_1(u) = -\gamma - \ln(u) + \sum_{n=1}^{\infty} \frac{(-1)^{n+1} u^n}{n.n!} < \infty & if\ u < 1 \\ E_1(u) = -\gamma - \ln(u) + \sum_{n=1}^{\infty} \frac{(-1)^{n+1} u^n}{n.n!}\ diverge & otherwise \end{cases}$$

But for large values of u, the rate of convergence becomes slow. For example, in 1942, Coulson and Duncanson see [25-26] showed to compute up to 75 terms to get accuracy with two significant figures, we need to take u = 20. Therefore, Harris in 1957, see [27] showed that equation (2) is valid if "u < 4", or preferably if "u < 1" (Cody and Thacher, 1968; Stegun and Zucker, 1974, see [28, 29]). But, if "u < 0.01" Cooper and Jacob, in 1946, see [30] used the approximation $w(u) \cong -\gamma - \ln(u)$ for the practical pump-test problems.

3.2. Rational Chebyshev approximation

This method is suggested by Cody and Thacher in 1968, see [31] and the idea of the method is based on Chebyshev approximation polynomial to find a new formula for evaluation $E_1(u)$as follows:

$$E_1(u) \cong -\ln(u) + \frac{\sum_{s=0}^{n} p_s\, u^s}{\sum_{s=0}^{n} q_s\, u^s}\ , u \in (0,1] \qquad (4)$$

and the suitable result when n = 6 is got in [32].

3.3. Asymptotic expansion

Integration by parts can be used to equation (1) to get the following asymptotic expansion of the exponential integral (1):

$$E_1(u) \cong \frac{e^{-u}}{u} \sum_{n=0}^{\infty} \frac{(-1)^n\, n!}{u^n} \qquad (5)$$

Coulson and Duncanson in 1942 [33] used equation (5) to approximate $E_1(u)$ when u >15 , while Harris in 1957, see [34] used equation (5) when u >50. Bleistein and Handelsman in 1975 see [35] got the best approximation of equation (5) if n (greatest integer) $\leq u$.

3.4. Continued Fraction

Gautschi and Cahill in 1964 see [36] suggest another useful representation of E_1(u) which was the continued fraction as:

$$E_1(u) = e^{-u}\left(\frac{1}{u+}\frac{1}{1+}\frac{1}{u+}\frac{2}{1+}\frac{2}{u+}\cdots\right) \qquad (6)$$

Van der Laan and Temme in 1984 see [37] discussed the properties of this representation in detail. The generalized of $E_n(u)$ when u > 1 has been approximated as the even form of the continued fraction by Stegun and Zucker in 1974. Stegun and Zucker in 1974 see [38] showed that the continued fraction converges more rapidly than the asymptotic expansion for large u.

3.5. Polynomial, Rational and Chebyshev polynomial approximations

Polynomials are one of the most common methods of approximating functions in a given interval. Nevertheless, the optimal rational function, which is the ratio of two polynomials, is able to achieve higher accuracy than the optimal polynomial with the same number of coefficients. The best rational approximation is difficult to be obtained using easy methods; therefore, many techniques have been proposed based on minimizing some measure of errors (Hamming, 1973, see [39]). The widely used rational approximation of functions is the so-called minimax or Chebyshev approximation, which minimizes the maximum error. Many authors used this technique to approximate the exponential integral; Gautschi and Cahill in 1964 see [40] approximated $E_1(u)$ for u∈[0, 1] by a polynomial of degree five. Rational functions with the same degree in numerator and denominator have been developed to approximate the expression "$ue^u E_l(u)$" in the Chebyshev sense by Hastings in 1955, see [41]. Cody and Thacher in 1968 see [42] introduced rational Chebyshev approximations in three intervals, later in 1969 see [43]; they used the method to approximate the exponential integral in four intervals.

3.6. Other Approximate Methods

There are some other methods used to approximate the exponential integral such stehfest algorithm of the inverse Laplace transform, finite difference and numerical quadrature formulas such as trapezoidal, Simpson, and Gauss-Laguerre. Moreover, Prodanoff et al., in 2006 see [44] and Nadarajah in 2007 see [21] used smoothing techniques to approximate the well function which is employed whenever the integrand gradient is high around a point, or even when it is singular. Some approximations of Theis' solution are reviewed and compared with the numerical evaluation of the exponential integral by means of a short FORTRAN code suggested by Giao, in 2003, see [45]. While Swamee with Ojha, in 1990, see [41] and Vatankhah in 2014 see [24] proposed full-range approximations valid for all values but got the result with less accuracy.

The results obtained by previous methods were even less accurate than required, so we suggest the following approach.

4. Suggested Approach

Here, we suggest the following algorithm to approximate equation (3) based on optimal rational Chebyshev approximation and to compute the best approximation.

4.1. Suggested Algorithms

Let g(u) be a continuous function in $[a, b]$ which is defined as follows:

$$g(u) = \frac{p_0 + p_1 u + \cdots + p_n u^n}{1 + q_1 u + \cdots + q_m u^m} \tag{7}$$

Now, we have to find p_0 , p_1, … , p_n ; q_1, … , q_m ; by using Chebyshev polynomial to minimize:

$$\max_{[a,b]} |E_1(u) - g(u)| \tag{8}$$

That is: minimize $\max_{[a,b]} |E_1(u) - g(u)|$ (9)

Attained N+2 times, N = n + m, so that the suggested algorithm is stated as follows:

i. Choose an initial set of N + 2 ordered points $\left\{u_i^{(1)}\right\}$, i =1, …, N + 2 in [a, b] so that

$$a \leq u_1^{(1)} < u_2^{(1)} < \cdots < u_{N+2}^{(1)} \leq b.$$

ii. We get the system of N+2 equations and N+1 unknown coefficients as:

$$E_1\left(u_i^{(1)}\right) - g\left(u_i^{(1)}\right) = -1^i r \qquad (10)$$

This can be solved for a function $g^{(1)}(u)$ and $r = \max_{[a,b]}|E_1(u) - g(u)|$ is constant.

iii. Each of the points $u_i^{(1)}$, i = 1, …, N + 2 is replaced by a nearby point at which $\left|E_1(u) - g^{(1)}(u)\right|$ has an extremum.

iv. Repeat steps (ii) and (iii) at the k^{th} time using the set of points $\left\{u_i^{(1)}\right\}$.

4.2. The Implementation and Results

To solve equation (3) by using the suggested algorithm, we use the following expression:

$$C(u) = \frac{p_0 + p_1 u + \cdots + p_5 u^5}{1 + q_1 u + \cdots + q_5 u^5} \qquad (11)$$

That is N = 10, [a, b] = [0, 1], and the coefficients p_i, q_i are constructed using Chebyshev polynomial with satisfies equation (9), and the results are given in Table 2.

Table 2: The coefficients of suggested solution

i	p_i	q_i
0	-0.577215664901532754527124779997 39	1
1	0.7534273070245228742791709919 4019	0.4271760244371237691396459013049
2	0.1305984613689932238855817558 9424	0.0806935187322509184237873114 3981
3	0.0245261388193113889777396963 15439	0.0085391469049514896749730752 389951
4	0.0013834734635821579855352592 14771	0.0005156278099577269206574281 4904183
5	0.0000723098331210997113211932 92956622	0.0000145889001020922358929123 03052427

4.3. Discussion

From the previous studies, we note that the results obtained by using rational Chebyshev approximation which is suggested by Cody and Thacher, is the best compared with those obtained by using other methods which are studied in section three. However, the results of our proposed method are more accurate and have fewer calculations than others as illustrated in Figure 1 and Table 3.

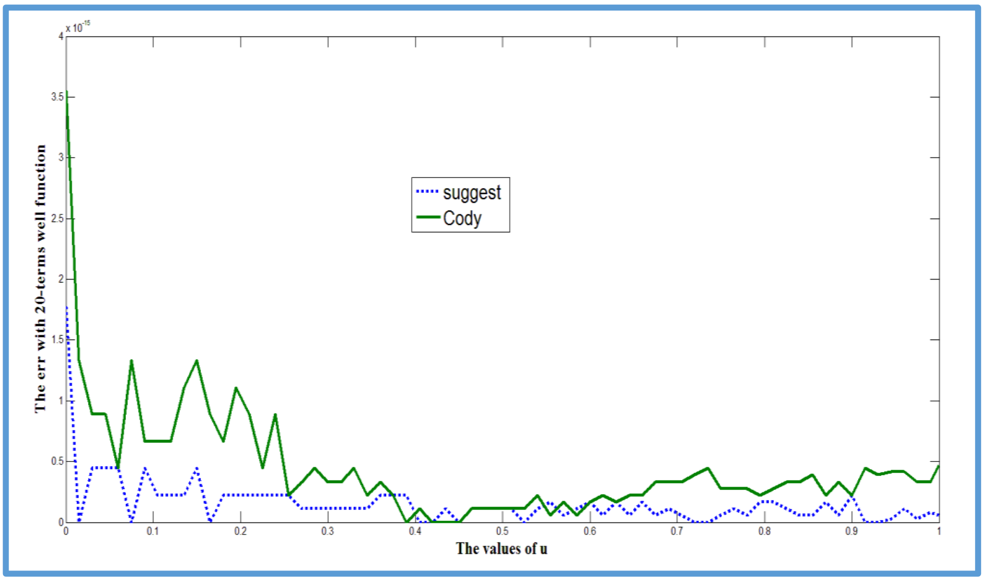

Figure 1: Accuracy of our solution and Cody solution

Table 3: The error $\left|E_1(u) - g^{(1)}(u)\right|$ in suggested solution and Cody solution

u	Suggest solution	Cody solution
0.000000	1.77636E-15	3.55271E-15
0.000003	1.77636E-15	3.55271E-15
0.000005	0	1.77636E-15
0.000007	0	1.77636E-15
0.000009	1.77636E-15	1.77636E-15
0.00001	1.77636E-15	3.55271E-15
0.00003	0	1.77636E-15
0.00005	1.77636E-15	1.77636E-15
0.00007	1.77636E-15	3.55271E-15
0.00009	1.77636E-15	1.77636E-15
0.0001	1.77636E-15	3.55271E-15
0.0003	8.88178E-16	8.88178E-16
0.0005	0	1.77636E-15
0.0007	0	1.77636E-15
0.0009	0	1.77636E-15
0.001	0	1.77636E-15
0.003	0	8.88178E-16
0.005	0	1.77636E-15
0.007	0	1.77636E-15
0.009	0	8.88178E-16
0.01	8.88178E-16	8.88178E-16
0.03	0	1.33227E-15
0.05	0	1.33227E-15
0.07	4.44089E-16	8.88178E-16
0.09	8.88178E-16	4.44089E-16
0.1	0	1.33227E-15
0.3	2.22045E-16	6.66134E-16
0.5	1.11022E-16	0
0.7	0	3.33067E-16
0.9	5.55112E-17	3.88578E-16
1	2.77556E-17	3.88578E-16

5. Conclusion

In this article, we present a comprehensive review and study of the numerical calculations for exponential integral function (also called the Theis well function) that is frequently appearing in well-hydraulic literature. We suggest an efficient approach to calculate this function. We see that all previous studies until now do not give the best approximations to exponential integral that are valid for the full range of u. The suggested method in this work achieves this aim. For small u, the series representation is still the most widely used technique among all these methods which is used to calculate E1(u). For large u, an effort and special techniques are required. The practical results show the suggested approach can be easily evaluated this value in software algorithms with acceptable accuracy.

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