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Numerical evaluation of Theis and Hantush-Jacob well functions

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Abstract

This paper presents a new approach where a numerical quadrature scheme is applied to compute special functions described by integrals, appearing in many groundwater hydrology and pollution problems. The basic idea is to apply a smoothing procedure to the singular integrand and a non-linear coordinate transformation in the quadrature domain. Techniques for lowering the degree of singularity of integrand functions have been successfully applied in physics and computational mechanics, and the self-adaptive co-ordinate transformation used in this work is a well-established procedure in general boundary element integrals quadrature. The main advantage of this joint technique is that it can be directly used to other related functions without further approximations and the user can choose freely the degree of accuracy. Tables included in this paper show the improvement of several orders of magnitude when both techniques are applied simultaneously.

Keywords: Ground water; Leaky aquifers; Theis well function; Hantush-Jacob well function; Numerical Integration; Gauss quadrature

1. Introduction

During the last decades a great number of approximate solutions for evaluation of special functions appearing in well hydraulics and pollutant transport on surface and groundwater problems have been developed, as for instance the M and S Hantush functions, Trefry (1998); Barry et al. (1999). These kind of solutions, which can be applied to steady and unsteady flows, are generally limited to somewhat simple initial and boundary conditions. Due to the large variability of flow patterns, of the porous media properties, and of the need of applying initial and boundary conditions, the utility of semi-analytical solutions is often limited and the use of numerical methods can be helpful. However, analytical solutions are still useful for numerical results validation, for giving initial estimates for pollutant and piezometric head scenarios, in the sensitivity analysis for investigating the effects of several transport parameters and with purpose of extrapolating for large time and distance from the source, where the numerical methods do not apply.

2. Definitions

Being u positive, the Theis (1935) well function, $W(u)$, or well function for confined aquifers or more generically the exponential integral of first order,

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$E_1(u)$, is defined by (Gautschi and Cahill, 1964):

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

The Hantush-Jacob well function (also called well function for leaky aquifers) is defined by (Hantush and Jacob, 1955; Hantush, 1956)

$$W(u, r/B) = \int_u^\infty \frac{1}{y}\exp\left(-y - \frac{r^2}{4B^2 y}\right)\mathrm{d}y \tag{2}$$

More details concerning the variables that appear in expressions (1) and (2) are given in Sections 3.1 and 3.2 of this paper. The Hantush-Jacob well function W (:) presents the following limits:

$$\begin{aligned} &W(0, r/B) = 2K_0(r/B) \quad \text{(modified Bessel function of the second kind of zero order)} \\ &W(u, 0) = E_1(u) \\ &W(\infty, r/B) = 0 \end{aligned} \tag{3}$$

One common aspect to the Theis' function and of the Hantush's leaky aquifer function is that they are singular; the former tend to infinity when $u \to 0$, and the latter tend to infinity when u and r tend to zero simultaneously.

In addition to hydraulics the exponential integral function appears in several fields of mathematics and physics. In reactors physics it occurs in the computation of first flight collision probability in cylindrical and plane geometry (Prabha and Yadav, 1996) or in the evaluation of the electronic energies and properties of molecules when Slater-type orbital are used as a wave function basis. In boundary element method it appears in the fundamental solution (Green's function) for advection-diffusion type equations.

3. Existing approximate solutions

3.1. Theis well function

The first mathematical analysis of transient drawdown effects in a confined aquifer was obtained by Theis (1935). Theis made the following assumptions: (a) The aquifer is top and bottom confined; (b) There is no source of recharge to aquifer; (c) The aquifer is compressible and water is released instantaneously from the aquifer as the head is lowered; (d) The well is pumped at a constant rate, Fetter (1994). The solution of unsteady distribution of drawdown is expressed by:

$$s = \left(\frac{Q}{4\pi T}\right)\int_u^\infty \frac{\mathrm{e}^{-y}}{y}\mathrm{d}y \tag{4}$$

where s, drawdown (L); Q, is the constant pumping rate (L^3/T); $u = r^2S/(4Tt)$; T, aquifer transmissivity (L^2/T); S, aquifer storativity (dimensionless); t, time since pumping began (T); r, radial distance from the pumping well (L).

The Theis well function can not be evaluated analytically in terms of elementary functions. The literature on the subject presents different methods, which are adequate to approximate the W function for different ranges of the argument u and which also vary according to the required degree of accuracy. Tseng and Lee (1998) presented a wide revision of the existing approximations for the evaluation of the function $W(u)$ and they have classified the methodologies more frequently encountered into six classes: series expansions, asymptotic expansions, rational and Chebyshev polynomials, recurrence relations and numerical quadrature.

As stated by Tseng and Lee (1998, pp.39) and quoted in Barry et al. (2000) 'it will always be beneficial to have a simple and handy algorithm for occasional use. An algorithm which is simple and efficient yet satisfies the required accuracy is still highly desirable'. Searching for a unique approximation for $E_1(u)$, Prabha and Yadav (1996) developed a polynomial expression, while Barry et al. (2000) constructed an algorithm based on interpolation between asymptotic expressions to the exponential integral and both obtained a 3S (significant figures) precision. However, under the strict mathematical viewpoint, the construction of such expressions is only suitable to that particular function and thus cannot be generalized to other cases. It is important to observe that Barry et al. (2000) approximation to Theis well function is suitable to hand calculations; in Barry et al. (1999) one can find a simple approximation to Hantush's function which is