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Analytical solution and numerical evaluation of the radial symmetric convection–diffusion equation with arbitrary initial and boundary data

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Abstract The analytical solution to the convection–diffusion equation in a radial velocity field with arbitrary initial data $F(r)$ and an inhomogeneous mixed boundary condition $G(t)$ at the well radius, is presented. These formulas are helpful in the interpretation of tracer injection experiments. To prevent numerical problems during the evaluation of the analytical solution, due to the oscillating character of the integrands, a more appropriate numerical inversion procedure is suggested. This new procedure circumvents oscillating integrands by deforming the Bromwich inversion integral contour through the complex plane using the steepest descent path. Along this path the integrands behave like exponentially decreasing positive functions which makes the integration easier.

Key words Airy function; convection–diffusion; Laplace transform; numerical inversion; radial flow field; steepest descent

INTRODUCTION

Various authors have addressed the convection–diffusion equation in a radial flow field. A purely analytical approach was given by Ogata (1958), Bear (1972, p. 635–637), Tang & Babu (1979), Moench & Ogata (1981), Hsieh (1986), Chen (1987), Chen & Woodside (1988), and Bruggeman (1999). Leijnse *et al.* (1987) published somewhat restricted results as presented below. Their work was based on mathematical results by M. Kopáčková published in an internal report (Beneš *et al.*, 1985).

In this paper we present the analytical solution for the convection–diffusion equation in a radial flow field with full generality with respect to the initial condition and an inhomogeneous mixed boundary condition at the well radius.

STATEMENT OF THE RESULT

In this paper we treat the following problem:

$$\begin{aligned}
&\frac{\partial c}{\partial t} = a|v_r|\frac{\partial^2 c}{\partial r^2} - v_r\frac{\partial c}{\partial r}, && r > r_0, \quad t > 0,\\
&\left(\gamma' c + \delta'\frac{\partial c}{\partial r}\right)\bigg|_{(r_0,t)} = G(t), && t > 0, \\
&c\big|_{(r,0)} = F(r), && r \ge r_0
\end{aligned} \tag{1}$$

with c [ML^{-3}] the resident concentration, t [T] the time, r [L] the radial distance to the well, a [L] the dispersivity, v_r [LT^{-1}] radial velocity, γ' [–], and δ' [L] coefficients for the inhomogeneous mixed boundary condition. Furthermore:

$$v_r = A/r, \qquad A = Q/(2\pi D n_e) \quad [\mathrm{L^2T^{-1}}] \tag{2}$$

with Q [L^{3}T^{-1}] the recharge, D [L] the thickness of the aquifer, and n_e [–] the porosity. So, for an injection ($Q > 0$) we have $v_r > 0$, and the opposite for an extraction. A commonly used boundary condition is a requirement on the so-called flux concentration (see Kreft & Zuber (1978)) $c_F = c - D_r/v_r\ \partial c/\partial r$, with $D_r = a|v_r|$ [L^{2}T^{-1}] the diffusion coefficient. So $c_F = c - a|v_r|/v_r\ \partial c/\partial r = c - a\ \mathrm{sign}(Q)\ \partial c/\partial r$, which means for an injection: $\gamma' = 1$, $\delta' = -a$, and for an extraction: $\gamma' = 1$, $\delta' = a$.

The following cases of equation (1) have been treated in the literature:

- $\gamma' = 1$, $\delta' = 0$, $G(t) = c_0$, $F(r) = 0$: Dirichlet condition: Ogata (1958), Bear (1972, p. 635–637), Tang & Babu (1979), Moench & Ogata (1981), Hsieh (1986), Beneš *et al.* (1985), Leijnse *et al.* (1987), Bruggeman (1999, 820.01),
- $\gamma' = 1$, $\delta' = -a$, $G(t) = c_0$, $F(r) = 0$: mixed boundary condition corresponding to an injection (flux concentration): Chen (1987, with just the Laplace transform $\bar{c}$ and not c),
- $\gamma' = 1$, $\delta' = -a$, $G(t) = \delta(t)$, $F(r) = 0$, $r_0 = 0$: mixed boundary condition corresponding to an injection (flux concentration): Bruggeman (1999, 820.02),
- $\gamma' = 0$, $\delta' = a$, $G(t) = 0$, $F(r) \neq 0$: Neumann condition, extraction: Beneš *et al.* (1985), Leijnse *et al.* (1987), Chen & Woodside (1988).

For the general solution without any restrictions we apply the following transformations:

$$\tau = \left(|A|/a^2\right)t, \qquad \rho = r/a, \qquad \rho_0 = r_0/a \tag{3}$$

$$\begin{aligned}
&\frac{\partial C}{\partial \tau} = \frac{1}{\rho}\left(\frac{\partial^2 C}{\partial \rho^2} \pm \frac{\partial C}{\partial \rho}\right), && \rho > \rho_0, \quad \tau > 0,\\
&\left.(\gamma C + \delta \frac{\partial C}{\partial \rho})\right|_{(\rho_0,\tau)} = g(\tau), && \tau > 0,\\
&C\big|_{(\rho,0)} = f(\rho), && \rho \geq \rho_0
\end{aligned} \tag{4}$$

with $C = c/G_0$, $\gamma = \gamma'$, $\delta = \delta'/a$, $g(\tau) = G(t)/G_0$, $f(\rho) = F(r)/G_0$, and G_0 [ML^{-3}] a normalization constant. Equation (4) is now dimensionless. The upper (plus) sign in the right-hand side of the differential equation in (4) represents an extraction ($Q < 0$), the lower (minus) sign an injection ($Q > 0$). The analytical solution of equation (4) reads:

$$\begin{aligned}
C(\rho,\tau) &= \mathrm{e}^{\mp\rho/2}\int_0^\infty \mathrm{d}s\ s^{-1/3}\,\frac{Ai(z)B_0(z_0) - Bi(z)A_0(z_0)}{A_0^{\,2}(z_0) + B_0^{\,2}(z_0)}\,\mathrm{e}^{-s\tau}\\
&\quad\times\left\{\int_{\rho_0}^\infty \mathrm{d}\rho'\ \rho'\mathrm{e}^{\pm\rho'/2} f(\rho')\left\{Ai(z')B_0(z_0) - Bi(z')A_0(z_0)\right\}\right\}\\
&\quad+ \mathrm{e}^{\mp(\rho-\rho_0)/2}\int_0^\infty \mathrm{d}s\,\frac{Ai(z)B_0(z_0) - Bi(z)A_0(z_0)}{\pi(A_0^{\,2}(z_0) + B_0^{\,2}(z_0))}\int_0^\tau \mathrm{d}\tau'\ g(\tau-\tau')\mathrm{e}^{-s\tau'}
\end{aligned} \tag{5}$$

$$z' = \frac{1-4s\rho'}{4s^{2/3}}, \qquad z_0 = \frac{1-4s\rho_0}{4s^{2/3}}, \qquad z = \frac{1-4s\rho}{4s^{2/3}},$$
$$A_0(z_0) = (\gamma \mp \delta/2)Ai(z_0) - \delta s^{1/3} Ai'(z_0), \quad \alpha = \gamma \mp \delta/2, \tag{6}$$
$$B_0(z_0) = (\gamma \mp \delta/2)Bi(z_0) - \delta s^{1/3} Bi'(z_0) \quad \beta = \delta$$

For the Airy functions, $Ai(z)$, $Bi(z)$ see Abramowitz & Stegun (1964). In particular, for Dirichlet boundary data we have:

$$\gamma' = 1, \quad \delta' = 0, \quad \text{so } A_0(z_0) = Ai(z_0), \quad B_0(z_0) = Bi(z_0)$$

for Neumann boundary data, see also Chen & Woodside (1988):

$$\gamma' = 0, \delta' = \pm a, \quad \text{so } A_0(z_0) = -\frac{1}{2}Ai(z_0) \mp s^{1/3}Ai'(z_0), B_0(z_0) = -\frac{1}{2}Bi(z_0) \mp s^{1/3}Bi'(z_0)$$

and for mixed boundary data, see also Chen (1987):

$$\gamma' = 1, \delta' = \pm a, \quad \text{so } A_0(z_0) = \frac{1}{2}Ai(z_0) \mp s^{1/3}Ai'(z_0), B_0(z_0) = \frac{1}{2}Bi(z_0) \mp s^{1/3}Bi'(z_0)$$

At first sight the result, equation (5), deviates from Chen & Woodside (1988, formula (36)), under the restrictions used by those authors. However, by applying some elementary algebra their solution can be put into the more concise form, i.e. equation (5).

INDICATION OF THE PROOF

The convection term can be removed from the partial differential equation by the substitution $C(\rho,\tau) = D(\rho,\tau)\,e^{\mp\rho/2}$. From the theory given in Naimark (1968, §21.3, 21.4, 21.5) it can be derived that the following transform (for z, z_0, A_0, B_0 see equation (6)):

$$\varphi(s) = T[f] \equiv \int_{\rho_0}^{\infty} \rho f(\rho)\left\{(-\pi s^{-1/3})(Ai(z)B_0(z_0) - Bi(z)A_0(z_0))\right\}\mathrm{d}\rho \tag{7}$$

has the inverse:

$$f(\rho) = T^{-1}[\varphi] = \int_0^{\infty} \varphi(s)\frac{-Ai(z)B_0(z_0) + Bi(z)A_0(z_0)}{\pi(A_0^{\,2}(z_0) + B_0^{\,2}(z_0))}\,\mathrm{d}s \tag{8}$$

with the property:

$$T\left[\frac{1}{\rho}\left(\frac{\partial^2 f}{\partial\rho^2} - \frac{1}{4}f\right)\right] = -sT[f], \quad \text{if } f \text{ satisfies} \left(\alpha f + \beta\frac{\partial f}{\partial\rho}\right)\Bigg|_{(\rho=\rho_0)} = 0 \tag{9}$$

By means of this generalized Hankel transform result equation (5) can be derived. Details will be published elsewhere. Also the traditional Laplace transform technique can deal with this problem, although for initial value problems it is quite involved ($G = 0, F \neq 0$). For $F = 0$, $G \neq 0$, both methods are equally applicable.

NUMERICAL CONSIDERATIONS

Although the analytical solution, equation (5), gives a closed form with all dependencies of the parameters in the problem, in practice, numerical evaluation is difficult due to the oscillating behaviour of the integrand. Therefore, quite often in such cases one just determines the Laplace transform and applies a numerical inversion technique. Nowadays, most authors use the method of de Hoog *et al.* (1982) in this field of convection–diffusion problems. Here, we present another technique which originates from a derivation of asymptotic expressions. We deform the contour in the Bromwich inversion formula for the Laplace transform to the steepest descent path through the complex plane starting from a saddle point on the real axis. This path will be constructed numerically. In the literature on Laplace inversion, this path does not seem to have been considered earlier, although some other methods perform an integration through the complex domain. Therefore, one needs complex versions of the standard mathematical functions. Nowadays, these are easily available, and for the Bessel-type functions one can exploit the library of Amos (1979, 1990, 1995). The starting point is the well-known Bromwich integral for the inversion of the Laplace transform $\overline{f}(s)$, Re $s > p_0$:

$$f(t) = \frac{1}{2\pi \mathrm{i}} \int_L \mathrm{e}^{st} \overline{f}(s) \, \mathrm{d}s, \qquad s \in \mathbf{C} \tag{10}$$

where the contour L is defined by $L = \{s = (p_1, \mathrm{i}q), \quad p_1 > p_0 \text{ fixed}, -\infty < q < \infty\}$. The contour L will be deformed to the steepest descent path L' going through a saddle point s_0 on the real axis. This saddle point will be found by solving $\frac{\mathrm{d}}{\mathrm{d}s}\left(\mathrm{e}^{st}\overline{f}(s)\right) = 0$. This means that the method requires the existence of such a saddle point. One of the two important properties of the steepest descent path L' is that along this contour the Phase$\left(\mathrm{e}^{st}\overline{f}(s)\right)$ is constant. This means that the integrand $\mathrm{e}^{st}\overline{f}(s)$ along L' stays real and of the same sign as $\mathrm{e}^{s_0 t}\overline{f}(s_0)$, which is an important numerical advantage. The other property of the steepest descent path is that along L' Re$\left(\mathrm{e}^{st}\overline{f}(s)\right)$ = $\mathrm{e}^{st}\overline{f}(s)$ decreases as an exponential. This ensures the fastest convergence of the integral. The steepest descent path will be found by successively determining points s_i in the complex plane such that the Phase$\left(\mathrm{e}^{s_i t}\overline{f}(s_i)\right)$ = 0. More details will be published elsewhere.

For the case of Dirichlet boundary data (α = 1, β = 0) with $f(\rho) = 0, g(\tau) = 1$, ρ = 10.1, ρ_0 = 10, τ = 0.01, we show the steepest descent path (Fig. 1(a)) and the integrand along that path (Fig. 1(b)). We compare this numerical Laplace inversion with the numerical evaluation of the second term in the right-hand side of equation (5) (Fig. 2). As can be seen in Fig. 1(b), the integrand function through the complex plane is a nice exponentially decreasing function, while the integrand in the second term of the analytical expression in equation (5) is a slowly decreasing oscillating function (Fig. 2). Both methods give to high precision, the same result:

$C(10.1, 0.01) = 2.619\,477\,443 \times 10^{-2}$.

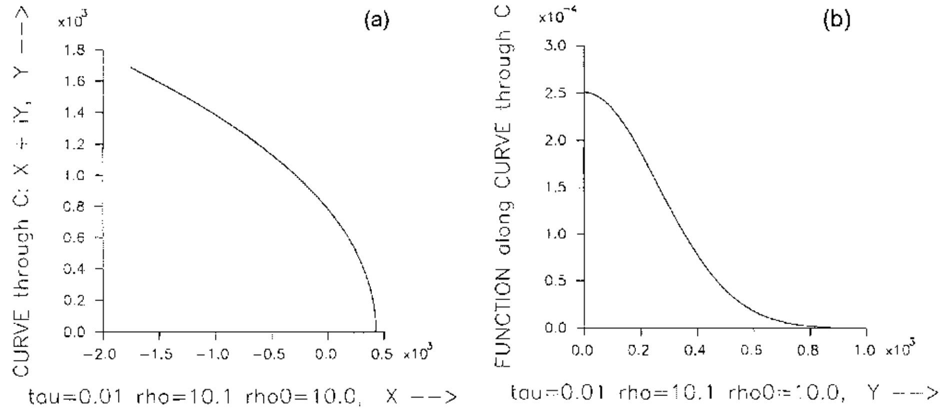

Fig. 1 (a) Path through the complex plane as found by the Steepest Descent Method for the case $f(\rho) = 0$, $g(\tau) = 1$, $\alpha = 1$, $\beta = 0$, $\rho = 10.1$, $\rho_0 = 10$, $\tau = 0.01$. (b) Function (with abscissa the distance to the real axis) along the path through the complex plane as found by the Steepest Descent Method for the case in (a).

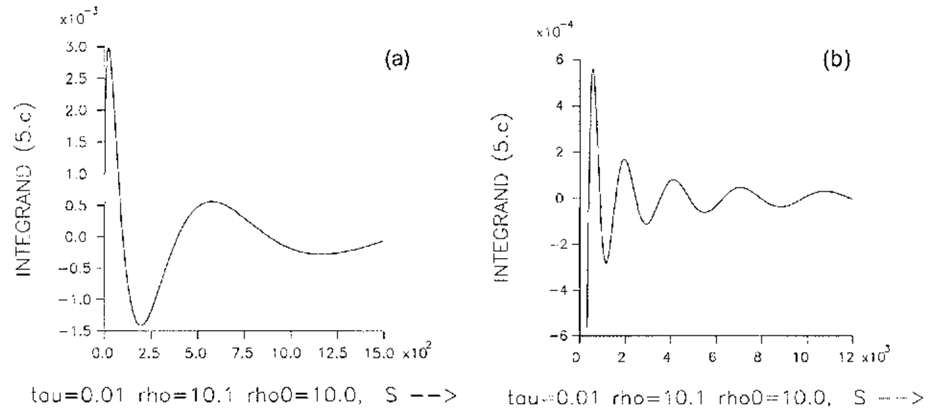

Fig. 2 Integrand function with respect to s for the second term of the analytical expression in equation (5) for the case in Fig. 1(a): (a) $0 \le s \le 1500$; (b) $300 \le s \le 12\,000$.

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