GWAT | gwat653 | Journal Name | Manuscript No. | B | Dispatch: November 12, 2009 | Journals: GWAT | CE: Subadra | Author Received: | No. of pages: 4 | TS: Lakshmi

ground water

Technical Commentary/

Methods to Derive the Differential Equation of the Free Surface Boundary

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Introduction

The free surface in an unconfined aquifer is defined as a surface on which the pressure is atmospheric (Bear 1972). The differential equation on the free surface boundary is one of the basic equations in textbooks of hydrogeology and groundwater hydrology. Using a substantial derivative method, or differentiation following the motion of the particle as stated in his original paper, Boulton (1954, p. 568) first derived this equation in radial flow and then simplified it as the boundary condition at the free surface. The derivation of this equation, however, was incorrect, as will be explained later.

Using the same method, Bear derived the wrong equation for three-dimensional flow in his classic book (Bear 1972, p. 258) and then repeated it in his other books (Bear 1979, p. 99; Bear and Verruijt 1987, p. 74; Bear and Verruijt 1994 p. 74). Apart from Bear's books, the authors collected 13 other books with the differential equation in the library of the University of Hong Kong and found that 10 of them included the wrong equation (Polubarinova-Kochina 1962, p. 553; Lohman 1972, p. 34; Hálek and Švec 1979, p. 46; Kovacs 1981, p. 517; Mariño and Luthin 1982, p. 153; de Marsily 1986, p. 141; Dagan 1989, p. 151; Batu 1998, p. 107; Bruggeman 1999, p. 623; Delleur 2007, p. 4–15). Among them, Lohman (1972, p. 34) simply cited Boulton's equation and de Marsily (1986, p. 141) simply cited Bear's equation. Others ended up with the same equation or its variant although they derived it using approaches different from Bear (1972). De Wiest (1965, p. 331); Remson et al. (1971, p. 51) and Pinder and Celia (2006 p. 180) derived the equation correctly. The book by Chen and Lin (1999, p. 33), in Chinese, also presented the equation correctly, but this book is not well known by international readers.

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Because the wrong equation is widely repeated in books, including a very recent one (Delleur 2007), p. 4–15, the authors feel that it is necessary to elaborate how the mistake is made and then present methods to derive the equation correctly in the hope that the mistake will not be repeated in the literature in the future.

Substantial Derivative Method

The substantial derivative method is also called the material derivative method, hydrodynamic derivative method, and total derivative method (Bear 1972). In the following sections, Bear's procedures (1979, p. 98–99) which led to the wrong differential equation, will be quoted first, albeit with some rewording and different symbols to fit the style of this commentary. Then the correct procedures and equation will be presented.

Substantial Derivative Method by Bear

The hydraulic head can be expressed as:

$$h(x, y, z, t) = z + p(x, y, z, t)/\gamma \qquad (1)$$

where h is hydraulic head, x, y, and z are Cartesian coordinates, t is time and γ is specific weight of water. Since the pressure at all points of the free surface, S, is taken as $p = 0$, the above equation becomes:

$$h(x, y, z, t) = z \text{ on } S \qquad (2)$$

S is thus a boundary of prescribed potential. Equation 2 gives at any time t a relationship between the coordinates

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Received April 2009, accepted October 2009.

doi: 10.1111/j.1745-6584.2009.00653.x

of points of the free surface. It may, therefore, be considered the equivalent to $F(x,y,z,t)=0$, describing the geometry of this surface

$$F(x,y,z,t) \equiv h(x,y,z,t) - z = 0 \text{ on } S \tag{3}$$

The unsteady free surface with accretion is a surface on which a certain property is maintained constant, here $F = \text{const.} = 0$. For such a surface, the following relationship can be obtained (Bear 1972, p. 72):

$$\frac{DF}{Dt} \equiv \frac{\partial F}{\partial t} + V \cdot \nabla F = 0 \tag{4}$$

where $D()/Dt$, the substantial derivative, is made equal to zero because no change in F takes place as particles carrying the property F move at a velocity V, which is the velocity of propagation of the free surface.

Continuity requires that at the moving free surface

$$(q - N) \cdot \boldsymbol{n} = n_e V \cdot \boldsymbol{n} \tag{5}$$

where q is specific discharge, N is the rate of accretion (positive downward; $N = -Nk$), $\boldsymbol{n}$ is a unit vector normal to the free surface (outer normal; $n = -\nabla F/|\nabla F|$), and n_e is effective porosity. Equation 5 states that the velocity of the surface depends on the velocities of the water on both sides of the surface; the effective porosity n_e is employed here because as the surface moves, only part of the water is removed from the void space, while the remaining part is retained. When the pores are sufficiently large n_e is close to the porosity n.

Combining Equation 4 with Equation 5 leads to

$$\frac{\partial F}{\partial t} + \frac{1}{n_e}(q - N) \cdot \nabla F = 0 \tag{6}$$

From Equation 3,

$$\nabla F = \frac{\partial h}{\partial x} i + \frac{\partial h}{\partial y} j + \left(\frac{\partial h}{\partial z} - 1\right) k \tag{7}$$

According to Darcy's law, then

$$q - N = -K_x \frac{\partial h}{\partial x} i - K_y \frac{\partial h}{\partial y} j - \left(K_z \frac{\partial h}{\partial z} - N\right) k \tag{8}$$

where K_x, K_y, and K_z are hydraulic conductivities in the directions of x, y, and z coordinates, respectively. Substituting Equations 7 and 8 into Equation 6 leads to:

$$\frac{\partial h}{\partial t} + \frac{1}{n_e}\left[-K_x \frac{\partial h}{\partial x} i - K_y \frac{\partial h}{\partial y} j - \left(K_z \frac{\partial h}{\partial z} - N\right) k\right] \times \left[\frac{\partial h}{\partial x} i + \frac{\partial h}{\partial y} j + \left(\frac{\partial h}{\partial z} - 1\right) k\right] = 0$$

Then the equation for an anisotropic medium is obtained:

$$\frac{\partial h}{\partial t} - \frac{1}{n_e}\left[K_x \left(\frac{\partial h}{\partial x}\right)^2 + K_y \left(\frac{\partial h}{\partial y}\right)^2 + K_z \left(\frac{\partial h}{\partial z}\right)^2 - \frac{\partial h}{\partial z}(K_z + N) + N\right] = 0 \tag{9}$$

Rearranging Equation 9 leads to:

$$K_x \left(\frac{\partial h}{\partial x}\right)^2 + K_y \left(\frac{\partial h}{\partial y}\right)^2 + K_z \left(\frac{\partial h}{\partial z}\right)^2 - \frac{\partial h}{\partial z}(K_z + N) + N = n_e \frac{\partial h}{\partial t} \tag{10}$$

This is the boundary condition to be satisfied on an unsteady free surface with accretion. And this is the differential equation that has been cited in many textbooks. However, it is incorrect. The main mistake lies in the terms related to z (marked in red).

Correction of Bear's Substantial Derivative Method

Equation 10 has two extra terms $K_z(\partial h/\partial z)^2$ and $N\partial h/\partial z$. The mistake stems from taking the derivative of hydraulic head h on the free surface with respect to the independent variable z. As a result, one extra term $\partial h/\partial z$ was added to Equation 7. That is why extra terms in the final differential equation are created. On the free surface, the derivative of h with respect to z is zero because Equation 3 is limited to the free surface only. In order to make Bear's derivation correct, the term $\partial h/\partial z$ in Equation 7 should be deleted. Then the correct differential equation is:

$$K_x \left(\frac{\partial h}{\partial x}\right)^2 + K_y \left(\frac{\partial h}{\partial y}\right)^2 - K_z \frac{\partial h}{\partial z} + N = n_e \frac{\partial h}{\partial t} \tag{11}$$

Equation 11 can also be derived by using the height of the free surface (Remson et al. 1971; Pinder and Celia 2006).

Boulton (1954, p. 568) first derived an equation very similar to Equation 10 in radial flow and then simplified it as the boundary condition at the free surface. Because he did not consider recharge, only one extra term was presented in his equation. This term was then ignored because Boulton assumed that the gradient was very small. So, fortunately, the mistake has no impact on his classical analytical solution (Boulton 1954) on the drawdown of the water-table under nonsteady conditions near a pumped well in an unconfined formation.

Mass Conservation Method

Chen and Lin (1999) first presented this method in their textbook (in Chinese). Consider a control volume of dimensions Δx, Δy, and Δz inside the flow domain in an unconfined aquifer, with the upper surface being the free surface (Figure 1). The aquifer is assumed to be anisotropic with principal directions of anisotropy parallel to the directions x, y, and z.

Applying the mass conservation principle leads to:

$$\begin{aligned}&\left[q_x \Delta y \Delta z|_{(x,y,z,t)} - q_x \Delta y \Delta z|_{(x+\Delta x,y,z,t)}\right]\Delta t \\ &+ \left[q_y \Delta x \Delta z|_{(x,y,z,t)} - q_y \Delta x \Delta z|_{(x,y+\Delta y,z,t)}\right]\Delta t \\ &+ (q_z + N)\Delta x \Delta y \Delta t = n_e(h|_{(x,y,z,t+\Delta t)} \\ &- h|_{(x,y,z,t)})\Delta x \Delta y \quad (z + \Delta z = z_{wt})\end{aligned} \tag{12}$$

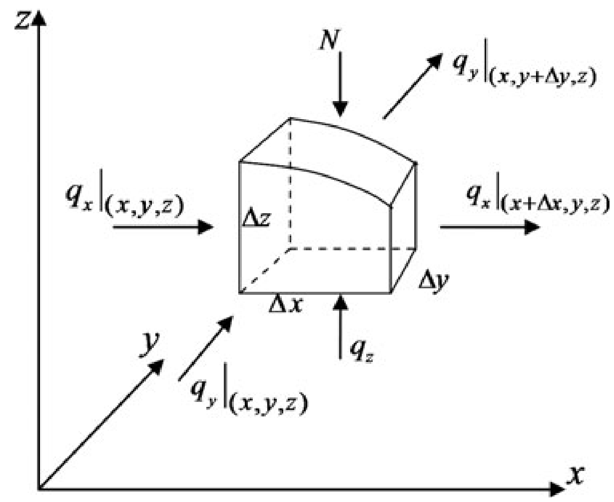

Figure 1. Mass conservation for a control volume.

where q_x, q_y, and q_z are specific discharge in the x, y, and z directions, respectively, z_{wt} is the vertical coordinate of the free surface. Dividing both sides of Equation 12 by $\Delta x \Delta y \Delta t$ leads to:

$$\begin{aligned}&\frac{q_x \Delta y \Delta z|_{(x,y,z,t)} - q_x \Delta y \Delta z|_{(x+\Delta x,y,z,t)}}{\Delta x \Delta y} \\ &\quad + \frac{q_y \Delta x \Delta z|_{(x,y,z,t)} - q_y \Delta x \Delta z|_{(x,y+\Delta y,z,t)}}{\Delta x \Delta y} \\ &\quad + q_z + N \\ &\quad = n_e \frac{h|_{(x,y,z,t+\Delta t)} - h|_{(x,y,z,t)}}{\Delta t}\end{aligned} \tag{13}$$

Let $\Delta x \to 0$, $\Delta y \to 0$, $\Delta t \to 0$, then

$$-\frac{1}{\Delta y}\frac{\partial(q_x \Delta y \Delta z)}{\partial x} - \frac{1}{\Delta x}\frac{\partial(q_y \Delta x \Delta z)}{\partial y} + q_z + N = n_e \frac{\partial h}{\partial t} \tag{14}$$

According to the chain rule of partial differentiation:

$$\frac{\partial(q_x \Delta y \Delta z)}{\partial x} = \frac{\partial q_x}{\partial x}\Delta y \Delta z + q_x \Delta y \frac{\partial(\Delta z)}{\partial x} \tag{15a}$$

$$\frac{\partial(q_y \Delta x \Delta z)}{\partial y} = \frac{\partial q_y}{\partial y}\Delta x \Delta z + q_y \Delta x \frac{\partial(\Delta z)}{\partial y} \tag{15b}$$

Because of $\Delta y \Delta z \to 0$, $\Delta x \Delta z \to 0$, the first term of the right-hand side of Equations 15a and 15b can be neglected, then substituting the second term of the right-hand side of Equations 15a and 15b into Equation 14 leads to:

$$-q_x \frac{\partial(\Delta z)}{\partial x} - q_y \frac{\partial(\Delta z)}{\partial y} + q_z + N = n_e \frac{\partial h}{\partial t} \tag{16}$$

On the free surface, pressure is equal to zero, then

$$\frac{\partial(\Delta z)}{\partial x} = \frac{\partial z|_{p=0}}{\partial x} = \frac{\partial h}{\partial x} \tag{17a}$$

$$\frac{\partial(\Delta z)}{\partial y} = \frac{\partial z|_{p=0}}{\partial y} = \frac{\partial h}{\partial y} \tag{17b}$$

Then Equation 16 can be written as:

$$-q_x \frac{\partial h}{\partial x} - q_y \frac{\partial h}{\partial y} + q_z + N = n_e \frac{\partial h}{\partial t} (z = z_{wt}) \tag{18}$$

Substituting the Darcy equation into Equation 18, again Equation 11 can be obtained. Compared to the substantial derivative method, the advantage of this method is its clear physical meaning because it is directly based on the principle of mass conservation and Darcy's law.

Hypothetical Experiment

A hypothetical experiment is used to test the correctness of Equations 10 and 11. The experiment consists of a vertical column of homogeneous sand and a moveable reservoir at the bottom (Figure 2). The column is initially saturated from below to height L. It is then allowed to drain under the influence of gravity. At the same time, recharge with a rate of N is added to the top. In this case, the difference in hydraulic head $h_1 - h_2$ is equal to the flow length L, so the hydraulic gradient in the column is equal to 1, that is, $\partial h / \partial z = 1$.

Using Equation 10 derived by Bear for this vertical one-dimensional flow leads to:

$$K_z \left(\frac{\partial h}{\partial z}\right)^2 - \frac{\partial h}{\partial z}(K_z + N) + N = n_e \frac{\partial h}{\partial t} \tag{19}$$

Because the hydraulic gradient is equal to 1 in the column, Equation 19 can be written as:

$$K_z - K_z - N + N = n_e \frac{\partial h}{\partial t} \tag{20}$$

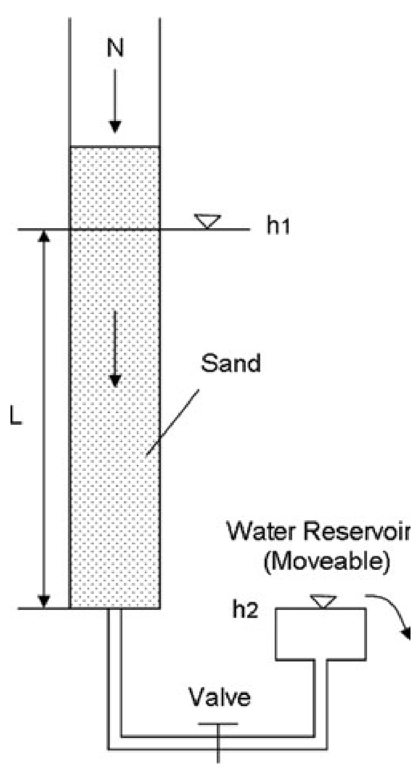

Figure 2. Schematic of the vertical one-dimensional flow.

Equation 20 can be further simplified to $\partial h/\partial t = 0$. This means that steady-state flow can always be maintained no matter what the recharge rate (including $N = 0$). This is obviously contradictory to the physical process of flow in the sand column. This simple experiment demonstrates that Equation 10 is incorrect.

Using the correct Equation 11 for this one-dimensional flow leads to:

$$-K_z \frac{\partial h}{\partial z} + N = n_e \frac{\partial h}{\partial t} \qquad (21)$$

This equation always satisfies the principle of mass conservation. When the system becomes steady, $\partial h/\partial t = 0$, the following equation is obtained:

$$N = K_z \partial h/\partial z \qquad (22)$$

In this experimental setting, because of the unit hydraulic gradient, the flow can be steady only when $N = K_z$, which is physically correct.

Summary

This commentary explained the mistake in the derivation of the differential equation for a free surface boundary presented in the classic paper by Boulton (1954) and several books including Bear (1972). This incorrect differential equation originated from taking the derivative of hydraulic head h on the free surface with respect to the independent variable z. As a result, additional terms were created in the differential equation. When it is recognized that on the free surface z is no longer independent, and this derivative is removed, the substantial derivative method by Bear and others leads to the correct differential equation, which can also be obtained by the mass conservation method, a very different approach based on the principle of mass conservation and Darcy's law. Hopefully the widely used wrong equation will not be included in literature any more.

Acknowledgments

We would like to thank Mary Anderson and other four anonymous reviewers for their insightful comments. The study was partially supported by the Research Grants Council of the Hong Kong Special Administrative Region, China (HKU 701908P).

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