



Closed-form analytical solutions for steady-state density-dependent flow and transport in a layered vertical soil column

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Abstract

Closed-form analytical solutions are derived for steady-state ground water flow and solute transport phenomena when the ground water density depends on the solute concentration. The flow and transport under consideration are one dimensional vertical as they occur in a vertical soil column. The soil column can be inhomogeneous, consisted of two layers where transport related properties are uniform within each layer, but there can be jump discontinuities across the layer interface. Transport mechanisms considered are advection, molecular diffusion, and velocity-dependent mechanical dispersion. Therefore, all relevant transport mechanisms are accounted for. The closed-form solutions derived herein can be used to assess accuracies of various numerical codes which simulate density-dependent flow and transport.

1 Introduction

Predicting ground water flow and solute transport phenomena when ground water density depends on the solute concentration is a challenging problem. Even a small density difference would cause significant changes in the flow pattern.

Many numerical codes have been developed to simulate the phenomena. Recent developments include Huyakorn and Taylor[1], Intera[2], Kipp[3], Voss and Souza[4], Herbert et al[5], and Oldenburg and Pruess[6]. Since no exact solutions were available, numerical codes were applied to a few reference problems. These problems include the so-called Henry's problem[7], Elder's experiments[8], and the HYDROCOIN problems[9].



The Henry's problem is by far the most popular problem because an approximate solution is available. Numerical codes applied to these problems resulted in solutions differing from other numerical solutions by a varying degree. However, to date it was not possible to determine which code is more accurate because exact solutions were unavailable.

Park[10] has developed exact solutions for the flow and transport phenomena. His solutions are quite simple: steady state in the vertical direction. However, his solutions are general in that all transport mechanisms such as advection, molecular diffusion and velocity-dependent mechanical dispersion are accounted for. In this study his solutions are extended to layered soil columns. For brevity we consider a soil column composed of two layers only. Lengths of layers are L_1^* and L_2^* , respectively. However, the methodology developed herein can be applied to a soil column of any number of layers. Each layer is associated with constant flow and transport related parameters, but there may be jump discontinuities across layer interface.

2 Governing equations

The governing equations for general ground water flow and solute transport are coupled nonlinear partial differential equations. However, for the case considered herein, steady state in one dimension, the governing equations reduce to a set of ordinary differential equations.

The conservation equation for the solute can be written as:

$$\frac{dm_s^*}{dz^*} = 0 \quad (1)$$

where z^* is positive upward. The superscript * indicates that the quantity is dimensional. Equation (1) states that the solute mass flux must be constant throughout the column. The solute mass flux is due to advection and dispersion.

$$m_s^* = \theta \left(v^* c^* - D^* \frac{dc^*}{dz^*} \right) \quad (2)$$

where θ is the effective porosity, v^* is the pore water velocity, and c^* is the solute concentration expressed as mass of solute per volume of solution. The dispersion is controlled by the dispersion coefficient, D^* , consisted of molecular diffusion and mechanical dispersion (Bear[11]):

$$D^* = \alpha^* |v^*| + D_m^* \quad (3)$$

where α^* is the dispersivity and D_m^* is the molecular diffusion coefficient.

The conservation equation for ground water flow is:

$$\frac{dm_f^*}{dz^*} = 0 \quad (4)$$

where the constant ground water mass flux is

$$m_f^* = \theta \rho^* v^* \quad (5)$$

in which ρ^* is the ground water density which depends on the solute concentration. The following linear relationship is assumed between the density and the solute concentration.

$$\rho^* = \rho_f^* + \hat{a}c^* \quad (6)$$

where ρ_f^* is the density of freshwater and \hat{a} is the dimensionless constant of proportionality.

The pore water velocity is related to the pressure via the modified Darcy's law:

$$v^* = -\frac{k^*}{\mu^* \theta} \left(\frac{dp^*}{dz^*} + \rho^* g^* \right) \quad (7)$$

where μ^* is the coefficient of viscosity, k^* is the intrinsic permeability, p^* is the ground water pressure, and g^* is the gravitational acceleration.

Above dimensional equations are nondimensionalized using the following set of normalization variables:

$$\begin{aligned} z^* &= L^* z \\ v^* &= V^* v \\ c^* &= c_s^* c \\ \rho^* &= \rho_f^* \rho \\ p^* &= \rho_f^* g^* L^* p \\ k^* &= k_r^* k \end{aligned} \quad (8)$$

where $L^*(= L_1^* + L_2^*)$ is the total length of the column, V^* is the reference velocity, c_s^* is the maximum solute concentration, and k_r^* is the reference intrinsic permeability.

With these normalization variables the nondimensional solute transport equation becomes:

$$\frac{d}{dz} \left[-\theta \left(\frac{|v|}{P_\alpha} + \frac{1}{P_m} \right) \frac{dc}{dz} + \theta v c \right] = 0 \quad (9)$$

where $P_\alpha = L^*/\alpha^*$ and $P_m = V^*L^*/D_m^*$ are Peclet numbers which represent relative magnitudes of mechanical dispersion and molecular diffusion, respectively, with respect to the advection. The ground water flow equation becomes:

$$\frac{d}{dz}(\rho \theta v) = 0. \quad (10)$$



The pore water velocity becomes:

$$v = -\frac{1}{\theta} \left(\frac{dp}{dz} + \rho \right) \quad (11)$$

where the dimensionless density is:

$$\rho = 1 + ac \quad (12)$$

in which the coefficient is

$$a = \hat{a}c_s^*/\rho_f^* \quad (13)$$

Governing and supplementary equations contain various transport related parameters each of which may be a function of aquifer material. Therefore, these parameters can be assumed constant within a layer of uniform soil material. However, across a layer interface there may be jump discontinuities in these values.

In this study we elect to set up a set of governing equations with constant parameter values for each layer. Then, solutions are derived for each layer along with boundary conditions specified independently. Clearly, boundary conditions specified at the layer interface are intermediate and can not be physical. These intermediate boundary conditions are removed using compatibility conditions. The last step would combine solutions derived independently into a complete solution for a layered soil column.

The first step is to write the governing equations with constant parameter values for each layer. Parameters that depend on aquifer material are: the Peclet number P_α , the intrinsic permeability k , and the porosity θ . These parameters in the new set of governing equations for each layer will have a subscript representing the layer number.

3 Boundary conditions

Solution procedures used herein requires a complete set of boundary conditions for each layer. First, for the solute equation, concentrations are specified at one end of a layer. More specifically, $c = c_i$ at $z = z_i$ for the first layer and $c = c_1$ at $z = 1$ for the second layer. Secondly, solute mass flux conditions are specified for both layers, i.e.,

$$\theta \left[-\left(\frac{|v|}{P_\alpha} + \frac{1}{P_m} \right) \frac{dc}{dz} + vc \right] = m_s \quad (14)$$

Likewise, pressures are specified at one end of a layer for the flow equation: $p = p_i$ at $z = z_i$ and $p = p_1$ at $z = 1$. The fluid mass flux conditions are specified for both layers:

$$\rho\theta v = m_f \quad (15)$$

Boundary conditions specified at the layer interface z_i are the intermediate conditions which are not known a priori. Therefore, c_i and p_i must be determined from compatibility conditions of concentration and pressure profiles. Furthermore, boundary conditions to be specified in actual problems at $z = 1$ may not be first types. If this is the case, c_1 and p_1 become additional intermediate boundary conditions that need to be determined.

4 Closed-form solutions

The governing ordinary differential equations are coupled through the density and the velocity. The integration of the equations would be easier when equations are decoupled. Decoupling is possible when unknown parameters can be expressed either with the spatial coordinate z or with the primary unknown of the equation. More specifically, if the density can be expressed with the primary unknown of the flow equation, namely the pressure, the flow equation is decoupled from the solute equation. Likewise, if the velocity can be written in terms of the concentration only, the solute equation can be separated from the flow equation.

Neither is possible for general multidimensional or unsteady state problems. However, for the case considered herein, the later is possible. The ground water velocity can be written in terms of the concentration only because

$$v = \frac{m_f}{\rho\theta} \quad (16)$$

where m_f is a constant and ρ is a simple function of concentration as it is given in (12).

Once the dependency upon the flow equation is removed, the solute equation can be integrated easily. For the layer 1, i.e., $0 \leq z \leq z_i (= L_1^*/L^*)$ the solute concentration profile becomes:

$$z - z_i = \frac{\theta_1}{P_m(am_s - m_f)} \left(\frac{1}{\beta_f} \ln \frac{1 + \beta_s c}{1 + \beta_s c_i} - a(c - c_i) \right) - \frac{1}{P_{\alpha_1} \beta'_f} \ln \frac{1 + \beta_s c}{1 + \beta_s c_i} \quad (17)$$

where $\beta_s = (am_s - m_f)/m_s$, $\beta_f = (am_s - m_f)/m_f$, and $\beta'_f = (am_s - m_f)/|m_f|$. Above equation displays clear dependence of the concentration distribution on the molecular diffusion and the mechanical dispersion.

Having obtained the concentration distribution, the density, which couples the flow equation with the solute equation, can be written in terms of the spatial coordinate, leaving the pressure the only unknown in the flow equation. But, writing the concentration as an explicit function of the spatial coordinate is possible only for special cases. For example, when molecular diffusion is neglected, writing $c = c(z)$ is possible. However,

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it may not even be desired. The integration of the pressure equation becomes simpler when the independent variable is switched from z to c via the chain rule of differentiation $dp/dz = (dp/dc)(dc/dz)$. The concentration gradient can be obtained directly from the solute transport equation (9). Then the pressure profile, in terms of the concentration, is for the first layer:

$$\begin{aligned}
 p &= p_i \\
 &+ \frac{1}{P_{\alpha_1} \beta_f'} \left[a(c - c_i) - \left(\frac{am_s - m_f}{k_1} + \frac{1}{\beta_f} \right) \ln \frac{1 + \beta_s c}{1 + \beta_s c_i} + \frac{am_s - m_f}{k_1} \ln \frac{1 + ac}{1 + ac_i} \right] \\
 &+ \frac{\theta_1}{P_m \beta_f} \left[\frac{a(c - c_i)}{m_f} \left(1 - \frac{1}{\beta_f} + \frac{a(c + c_i)}{2} \right) + \left(\frac{1}{k_1} + \frac{1}{m_f \beta_f^2} \right) \ln \frac{1 + \beta_s c}{1 + \beta_s c_i} \right]. \quad (18)
 \end{aligned}$$

For the second layer, i.e., $z_i \leq z \leq 1$ the concentration profile becomes:

$$z - 1 = \frac{\theta_2}{P_m(am_s - m_f)} \left(\frac{1}{\beta_f} \ln \frac{1 + \beta_s c}{1 + \beta_s c_1} - a(c - c_1) \right) - \frac{1}{P_{\alpha_2} \beta_f'} \ln \frac{1 + \beta_s c}{1 + \beta_s c_1} \quad (19)$$

and the pressure profile in terms of the concentration becomes

$$\begin{aligned}
 p &= p_1 \\
 &+ \frac{1}{P_{\alpha_2} \beta_f'} \left[a(c - c_1) - \left(\frac{am_s - m_f}{k_2} + \frac{1}{\beta_f} \right) \ln \frac{1 + \beta_s c}{1 + \beta_s c_1} + \frac{am_s - m_f}{k_2} \ln \frac{1 + ac}{1 + ac_1} \right] \\
 &+ \frac{\theta_2}{P_m \beta_f} \left[\frac{a(c - c_1)}{m_f} \left(1 - \frac{1}{\beta_f} + \frac{a(c + c_1)}{2} \right) + \left(\frac{1}{k_2} + \frac{1}{m_f \beta_f^2} \right) \ln \frac{1 + \beta_s c}{1 + \beta_s c_1} \right]. \quad (20)
 \end{aligned}$$

Equations (17) through (20) contain six parameters: c_1 , p_1 , c_i , p_i , m_s , and m_f . Four of these can be determined from four boundary conditions specified. Therefore, for closure we need two more conditions. The remaining two parameters are determined from the compatibility conditions for the pressure and concentration values at the layer interface. They can be stated as follows:

$$\lim_{\epsilon \rightarrow 0} c(z + \epsilon) = \lim_{\epsilon \rightarrow 0} c(z - \epsilon) \quad (21)$$

and

$$\lim_{\epsilon \rightarrow 0} p(z + \epsilon) = \lim_{\epsilon \rightarrow 0} p(z - \epsilon). \quad (22)$$

When actual boundary conditions specified for a particular problem differ from the boundary conditions used in deriving the solution, some of c_1 , p_1 , m_s , and m_f may become additional parameters to be determined. Since equations are nonlinear, iterative methods are required to compute these parameters.

5 Hydrostatic pressure distribution

A hydrostatic pressure distribution is obtained when the ground water flux in the vertical direction becomes zero. For this case the concentration profile becomes for a uniform soil column:

$$c = \frac{P_m m_s}{\theta} (1 - z) + c_1 \quad (23)$$

which depends only on the molecular diffusion. Note that the mechanical dispersion is absent since the ground water velocity is zero.

The corresponding hydrostatic pressure distribution becomes:

$$p = p_1 + \tilde{\rho}(1 - z) + \frac{a(c_0 - c_1)}{2} z(1 - z) \quad (24)$$

where c_0 is the concentration at $z = 0$ and $\tilde{\rho} = 1 + a\tilde{c}$ is the average ground water density in which $\tilde{c} = (c_0 + c_1)/2$ is the average concentration in the column. The first two terms in the right hand side of (24) represent hydrostatic pressure distribution when the ground water density is uniform at $\tilde{\rho}$. The last term is the parabolic correction term for nonuniform density distributions.

6 Concluding remarks

Closed-form analytical solutions are derived for steady-state ground water flow and solute transport phenomena in a layered soil column when the ground water density depends on the solute concentration. For brevity of presentation, only two layer systems was used. However, the methodology developed herein can be extended easily to a column of more than three layers. Solutions derived herein can be used to assess accuracies of numerical codes which simulate density-dependent ground water flow and solute transport. Comparisons made with various numerical models will be presented at the conference.

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