Alternate Potential Formulations for Mishra-Neuman (2010) Solution

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1 Unsaturated Zone Governing Equations

The governing equation in the unsaturated zone, as used by [MN10] and [TN07], is

$$K_r k_0(\psi)\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \sigma}{\partial r}\right)+K_z\frac{\partial}{\partial z}\left(k_0(z)\frac{\partial \sigma}{\partial z}\right)=C(\psi)\frac{\partial \sigma}{\partial t} \tag{1}$$

where K_r and K_z are the radial and vertical saturated hydraulic conductivities [L T^{-1}], k_0 is the dimensionless isotropic relative hydraulic conductivity ($0 < k_0 \leq 1$), $\sigma = h_0 - h = b + \psi_a - h$ is drawdown in the vadose zone [L], $h = \psi + z$ is hydraulic head [L], ψ is pressure head [L], ψ_a is air-entry pressure, $C(\psi) = \frac{d\theta}{d\psi}$ is the dimensionless specific moisture capacity, and θ is dimensionless volumetric water content. The unsaturated zone begins at the top of the aquifer, $b \leq z \leq b + L$. Further, the unsaturated parameters are assumed to only be functions of z. The initial and boundary conditions for the unsaturated zone are

$$\sigma(r,z,0)=0$$

$$\sigma(\infty,z,t)=0$$

$$\frac{\partial \sigma}{\partial z}=0 \qquad z=b+L$$

and

$$\lim_{r\to 0} r\frac{\partial \sigma}{\partial r}=0 \qquad b\leq z\leq b+L.$$

Drawdown in the aquifer (s) and the vadose zone are connected using compatibility conditions at the water table ($z = b$), namely

$$s=\sigma \qquad z=b$$

$$\frac{\partial s}{\partial z} = \frac{\partial \sigma}{\partial z} \qquad z = b.$$

The moisture retention curve in the vadose zone is modeled as an exponential function

$$S_e = \frac{\theta(\psi) - \theta_r}{S_y} = e^{a_c(\psi - \psi_a)} \qquad a_c \geq 0$$

where S_e is dimensionless effective saturation, θ_r is dimensionless residual volumetric water content, $S_y = \theta_s - \theta_r$ is dimensionless drainable porosity (specific yield), and θ_s is dimensionless saturated volumetric water content. The Gardner model for relative hydraulic conductivity is used; the relative hydraulic conductivity is

$$k(\psi) = \begin{cases} e^{a_k(\psi - \psi_k)} & \psi \leq \psi_k, \\ 1 & \psi < \psi_k \end{cases} \qquad a_k \geq 0,\ \psi_k \leq 0,$$

where ψ_k is the pressure head beyond which the hydraulic conductivity is essentially saturated.

The four-parameter exponential model for hydraulic conductivity used in the vadose zone is

$$k_0(z) = e^{a_k(\Psi + b - z)} \qquad \Psi = \psi_a - \psi_k \tag{2}$$

and the exponential model use for moisture capacity is

$$C_0(z) = S_y a_c e^{a_c(b-z)}. \tag{3}$$

The governing equation will be non-dimensionalized before proceeding further with the solution. Equation (1) can be written in dimensionless form as

$$k_0(z_D)\frac{1}{r_D}\frac{\partial}{\partial r_D}\left(r_D \frac{\partial \sigma_D}{\partial r_D}\right) + \kappa \frac{\partial}{\partial z_D}\left(k_0(z_D)\frac{\partial \sigma_D}{\partial z_D}\right) = \gamma C_0(z_D)\frac{\partial \sigma_D}{\partial t_D} \tag{4}$$

where $r_D = r/b$ is the dimensionless radial coordinate, $z_D = z/b$ is the dimensionless vertical coordinate, $\kappa = K_z/K_r$ is the anisotropy ratio, $\sigma_D = \sigma/H_c$ is dimensionless vadose zone drawdown, H_C is a characteristic head, $t_D = tK_r/(b^2 S_S)$ is dimensionless time, $\gamma = S_y a_c / S_S$ is the dimensionless storage ratio, and S_S is the specific storage [L^-1] in the saturated aquifer. The hydraulic conductivity constitutive model is non-dimensionalized as

$$k_0(z_D) = e^{a_{kD}(\Psi_D + 1 - z_D)}, \tag{5}$$

where $a_{kD} = a_k b$ and $\Psi_D = \Psi/b$, and the moisture capacity model is non-dimensionalized as

$$C_0(z_D) = e^{a_{cD}(1 - z_D)}, \tag{6}$$

where $a_{cD} = a_c b$.

2 Unsaturated Zone Solution

The dimensionless Laplace transformation (over-bar and p) of (4) results in

$$k_0(z_D)\frac{1}{r_D}\frac{\partial}{\partial r_D}\left(r_D\frac{\partial\bar{\sigma}_D}{\partial r_D}\right)+\kappa\frac{\partial}{\partial z_D}\left(k_0(z_D)\frac{\partial\bar{\sigma}_D}{\partial z_D}\right)=p\gamma C_0(z_D)\bar{\sigma}_D. \tag{7}$$

The associated transformed dimensionless boundary and initial conditions of

$$\bar{\sigma}_D(\infty, z_D, p) = 0$$

$$\frac{\partial\bar{\sigma}_D}{\partial z_D}=0 \qquad z_D = 1+L_D$$

$$\lim_{r_D\to 0} r_D\frac{\partial\bar{\sigma}_D}{\partial r_D}=0 \qquad 1\le z_D\le 1+L_D,$$

where $L_D = L/b$ is the dimensionless vadose zone thickness.

Further applying the dimensionless Hankel transformation (superscript $*$ and a) to (7), followed by substitution of the dimensionless constitutive models (5) and (6) results in the ordinary differential equation

$$-a^2\bar{\sigma}^* - \kappa a_{kD}\frac{\mathrm{d}\bar{\sigma}^*_D}{\mathrm{d}z_D}+\kappa\frac{\mathrm{d}^2\bar{\sigma}^*_D}{\mathrm{d}z_D^2}=p\gamma\bar{\sigma}^*_D e^{-a_{kD}\Psi_D}e^{(a_{kD}-a_{cD})(1-z_D)} \tag{8}$$

and the no-flow condition at the top of the vadose zone,

$$\frac{\mathrm{d}\bar{\sigma}^*_D}{\mathrm{d}z_D}=0 \qquad z_D = 1+L_D$$

Equation 8 can be rearranged and regrouped as

$$\frac{\mathrm{d}^2\bar{\sigma}^*_D}{\mathrm{d}z_D^2}-a_{kD}\frac{\mathrm{d}\bar{\sigma}^*_D}{\mathrm{d}z_D}-\left[Be^{\lambda_D(1-z_D)}+C\right]\bar{\sigma}^*=0 \tag{9}$$

where $\lambda_D = a_{kD} - a_{cD}$, $B=\frac{p\gamma}{\kappa}e^{-a_{kD}\Psi_D}$, and $C=\frac{a^2}{\kappa}$.

The dimensional form of (9) was solved in [MN10] using a general solution from a reference book on differential equations. The solution given in terms of two types of Bessel functions of complex argument and non-integer order is non-trivial to evaluate numerically.

2.1 Modified Solution Procedure #1

By further modifying the z_D-coordinate and performing an exponential substitution, (9) can be simplified significantly and a solution can be found by integration. Using a scaled dimensionless vertical coordinate

$$\zeta = a_{kD} z_D \qquad z_D = \frac{\zeta}{a_{kD}}$$

the transformed differential equation representing drawdown in the vadose zone (9) becomes

$$a_{kD}^2 \frac{\mathrm{d}^2 \bar{\sigma}_D^*}{\mathrm{d}\zeta^2} - a_{kD}^2 \frac{\mathrm{d}\bar{\sigma}_D^*}{\mathrm{d}\zeta} - \left[B e^{\lambda_D (1-\zeta/a_{kD})} + C \right] \bar{\sigma}_D^* = 0 \tag{10}$$

we divide through by a_{kD}^2 and performing the substitution $\bar{\sigma}_D^*(\zeta) = e^{u(\zeta)}$ (e.g., see [BO78, p. 27] and [Zwi98, §60]). This exponential change of variables implies

$$\frac{\mathrm{d}\bar{\sigma}_D^*}{\mathrm{d}\zeta} = \frac{\mathrm{d}u}{\mathrm{d}\zeta} e^u$$

and therefore

$$\frac{\mathrm{d}^2 \bar{\sigma}_D^*}{\mathrm{d}\zeta^2} = \left[\frac{\mathrm{d}^2 u}{\mathrm{d}\zeta^2} + \left(\frac{\mathrm{d}u}{\mathrm{d}\zeta} \right)^2 \right] e^u$$

which changes (10) to

$$\left[\frac{\mathrm{d}^2 u}{\mathrm{d}\zeta^2} + \left(\frac{\mathrm{d}u}{\mathrm{d}\zeta} \right)^2 \right] e^u - \left[\frac{\mathrm{d}u}{\mathrm{d}\zeta} e^u \right] - \left[B e^{\lambda_D (1-\zeta/a_{kD})} + C \right] \frac{e^u}{a_{kD}^2} = 0.$$

Multiplying this by e^{-u} and simplifying results in

$$\frac{\mathrm{d}v}{\mathrm{d}\zeta} + v^2 - v = \left[\frac{B}{a_{kD}^2} e^{\lambda_D (1-\zeta/a_{kD})} + \frac{C}{a_{kD}^2} \right], \tag{11}$$

which is known as the Riccati equation, where $v = u'$. This would only be solvable if a solution could first be guessed, then reducing (11) to a Bernoulli equation, which are always solvable.

A simple solution, that is not a Bessel function, might be guessed but I tried a few things and made no progress.

2.2 Modified Solution Procedure #2

By further modifying the z_D-coordinate and performing a different exponential substitution, (9) can be changed to the same form as the time-independent Schrödinger equation. Using a slightly different scaled dimensionless vertical coordinate

$$\xi = \frac{a_{kD}}{2} z_D \qquad z_D = \frac{2\xi}{a_{kD}}$$

the transformed differential equation representing drawdown in the vadose zone (9) becomes

$$\frac{a_{kD}^2}{4}\frac{\mathrm{d}^2\bar{\sigma}_D^*}{\mathrm{d}\xi^2} - \frac{a_{kD}^2}{2}\frac{\mathrm{d}\bar{\sigma}_D^*}{\mathrm{d}\xi} - \left[Be^{\lambda_D(1-2\xi/a_{kD})} + C\right]\bar{\sigma}_D^* = 0 \tag{12}$$

we multiply through by $4/a_{kD}^2$ and performing the substitution $\bar{\sigma}_D^* = H(\xi)e^{\xi}$. This exponential change of variables (e.g., see [KW08]) implies

$$\frac{\mathrm{d}\bar{\sigma}_D^*}{\mathrm{d}\xi} = \frac{\mathrm{d}H}{\mathrm{d}\xi}e^{\xi} + He^{\xi}$$

and therefore

$$\frac{\mathrm{d}^2\bar{\sigma}_D^*}{\mathrm{d}\xi^2} = \frac{\mathrm{d}^2H}{\mathrm{d}\xi^2}e^{\xi} + 2\frac{\mathrm{d}H}{\mathrm{d}\xi}e^{\xi} + He^{\xi}$$

which changes (12) to the form

$$\frac{d^2H}{d\xi^2} - \left[B'e^{\lambda_D(1-2\xi/kD)} + C'\right]H = 0 \tag{13}$$

where $B' = 4B/a_{kD}^2$ and $C' = 4C/a_{kD}^2 + 1$. (13) is in the form of the time-independent Schrödinger equation. The ξ-dependent coefficient in brackets is referred to as the potential function in the quantum-mechanics literature. Closed-form solutions have been derived for different potential functions ($1/\xi$, $1/\xi^2$, $e^{-\xi}$, etc.).

A common solution technique is to transform (13) into Bessel's equation and express the solution in terms of Bessel functions (*no help here*).

3 Saturated Zone Unconfined Solution

Following [MN10], we decompose the saturated zone solution into two solutions: 1) the Hantush solution s_H for a confined aquifer and a partially penetrating well; 2) an unconfined solution s_U with no well but continuity conditions with the vadose zone solution just derived.

The solution for s_H is given elsewhere, either in terms of a finite cosine transform, or a multi-layer fully penetrating solution.

The governing ordinary differential equation in Laplace-Hankel transform space for the saturated unconfined $\bar{s}^*_{UD}$ is

$$\frac{\mathrm{d}^2 \bar{s}^*_{UD}}{\mathrm{d}z_D^2} - \left(\frac{p+a^2}{\kappa}\right)\bar{s}^*_U = 0 \qquad 0 \leq z_D \leq 1 \tag{14}$$

with the no-flow boundary condition at the base of the aquifer

$$\frac{\mathrm{d}\bar{s}^*_{UD}}{\mathrm{d}z_D} = 0 \qquad z_D = 0$$

and the following continuity equations at the water table

$$\bar{s}^*_{UD} + \bar{s}^*_{HD} = \bar{\sigma}^*_D \qquad z_D = 1 \tag{15}$$

$$\frac{\mathrm{d}\bar{s}^*_{UD}}{\mathrm{d}z_D} = \frac{\mathrm{d}\bar{\sigma}^*_D}{\mathrm{d}z_D} \qquad \rightarrow \qquad \frac{\mathrm{d}\bar{s}^*_{UD}}{\mathrm{d}z_D} = \frac{\mathrm{d}u}{\mathrm{d}\zeta}e^u \qquad z_D = 1 \tag{16}$$

note the vertical flux of $\bar{s}^*_{HD}$ is defined as zero at the top and bottom of the aquifer, so it is not included in the continuity condition (16).

The general solution to (14) is

$$\bar{s}^*_{UD} = A_1 \cosh(\eta z_D) + A_2 \sinh(\eta z_D) \tag{17}$$

where A_i are constants to determine and $\eta^2 = \frac{p+a^2}{\kappa}$. The no-flow boundary condition at the bottom of the aquifer forces $A_2 \equiv 0$.

4 Formulation of Finite Difference Solution

The ordinary differential equation in the vadose zone can be solved via finite differences in space, while still within Laplace-Hankel space. This is done mostly as a check of the other derivation, and partly because of inspiration derived from a pithy remark by a co-worker.

Substituting finite difference approximations for the z_D derivatives in (9) gives

$$\frac{1}{h^2}\left(\sigma_{j+1} - 2\sigma_j + \sigma_{j+1}\right) - \frac{a_{kD}}{h}\left(\sigma_{j+1} - \sigma_j\right) - \left(Be^{-\lambda_D jh} + C\right)\sigma_j = 0$$

where the bar, star, and D decorators on σ are left out for simplicity, h is the dimensionless inter-node spacing (assumed constant), and the subscript indicates the current node j and the node one above $j+1$ and below $j-1$. The node index run $0 \leq j \leq N-1$, where there are N nodes and $h = L_D/(N-1)$.

In the following $\xi_j = Be^{-\lambda_D jh} + C$. Explicitly writing out the finite-difference matrix for a 3-node problem with node 1 at $z_D = 1$ and node 3 at $z_D = 1 + L/b$, without explicitly handling the boundary conditions, is

$$\begin{bmatrix} \frac{1}{h^2} & \left(\frac{a_{kD}}{h} - \frac{2}{h^2} - \xi_0\right) & \frac{1}{h^2} - \frac{a_{kD}}{h} & 0 & 0 \\ 0 & \frac{1}{h^2} & \left(\frac{a_{kD}}{h} - \frac{2}{h^2} - \xi_1\right) & \frac{1}{h^2} - \frac{a_{kD}}{h} & 0 \\ 0 & 0 & \frac{1}{h^2} & \left(\frac{a_{kD}}{h} - \frac{2}{h^2} - \xi_2\right) & \frac{1}{h^2} - \frac{a_{kD}}{h} \end{bmatrix} \begin{bmatrix} \sigma_{-1} \\ \sigma_0 \\ \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{18}$$

where σ_{-1} and σ_3 are "ghost" nodes which will be used to represent boundary conditions, but do not physically exist; (18) is in the canonical form $\mathbf{Ax} = \mathbf{b}$. Because $\partial\sigma/\partial z = 0$ at $z = b + L$, we can set $\sigma_2 = \sigma_3$, which means adding the two rightmost columns of $\mathbf{A}$ and eliminating σ_3.

The node at the bottom of the vadose zone (σ_0) appears in two boundary conditions, the head and flux continuity conditions with the aquifer. The flux continuity condition can be written in finite-difference form as

$$\lim_{h \to 0} \frac{\sigma_0 - \sigma_{-1}}{h} = A_1 \eta \sinh(\eta)$$

which can be used to eliminate σ_{-1} from $\mathbf{A}$. Substituting $\sigma_{-1} = \sigma_0 - hA_1\eta\sinh(\eta)$ into (18) gives the following equation for the first row of $\mathbf{A}$

$$\frac{1}{h^2}\left[\sigma_0 - hA_1\eta\sinh(\eta)\right] + \left(\frac{a_{kD}}{h} - \frac{2}{h^2} - \xi_0\right)\sigma_0 + \left(\frac{1}{h^2} - \frac{a_{kD}}{h}\right)\sigma_1 = 0$$

Further using head continuity equation $\sigma_0 = A_1\cosh(\eta) + s_H(z_D = 1)$ to eliminate σ_0 from this first row leads to

$$\frac{A_1}{h}\eta\sinh(\eta) + \left(\frac{a_{kD}}{h} - \frac{1}{h^2} + -\xi_0\right)\left[A_1\cosh(\eta) + s_H(1)\right] + \left(\frac{1}{h^2} - \frac{a_{kD}}{h}\right)\sigma_1 = 0.$$

Performing the substitution for σ_0 into the second row of $\mathbf{A}$, and regrouping to solve for A_1 in place of the eliminated σ_0 leads to

$$\begin{bmatrix} \cosh(\eta)\theta_1 - \frac{\eta}{h}\sinh(\eta) & \frac{1}{h^2} - \frac{a_{kD}}{h} & 0 \\ \frac{1}{h^2}\cosh(\eta) & \theta_2 & \frac{1}{h^2} - \frac{a_{kD}}{h} \\ 0 & \frac{1}{h^2} & \theta_2 + \frac{1}{h^2} - \frac{a_{kD}}{h} \end{bmatrix} \begin{bmatrix} A_1 \\ \sigma_1 \\ \sigma_2 \end{bmatrix} = \begin{bmatrix} -\theta_1 s_H(1) \\ -\frac{1}{h^2}s_H(1) \\ 0 \end{bmatrix} \tag{19}$$

where $\theta_1 = \frac{a_k D}{h} - \frac{1}{h^2} - \xi_j$ and $\theta_2 = \frac{a_k D}{h} - \frac{2}{h^2} - \xi_j$. This 3×3 case illustrates all the entries in a general $n \times n$ problem; including boundary nodes and an interior node.

The upper–left coefficient $\cosh(\eta)\theta_1 - \frac{\eta}{h}\sinh(\eta)$ in (19) may be problematic due to cancellation between large quantities, so it can be re-written in terms of exponentials as

$$\frac{1}{2}\left[e^{\eta}\left(\theta_1 - \frac{\eta}{h}\right) + e^{-\eta}\left(\theta_1 + \frac{\eta}{h}\right)\right].$$

The Thomas algorithm for tri-diagonal matrices can be used to numerically solve for A_1 and σ_j, where $j = 1, 2, \ldots, n$ (not including σ_0). Once A_1 is found numerically, the solution in the saturated zone is simply

$$\bar{\sigma}^*_D(z_D) = \bar{\sigma}^*_{HD}(z_D) + A_1 \cosh(\eta z_D).$$

This involves computing the Thomas algorithm in Laplace-Hankel space, for each combination of (a, p). The Thomas algorithm can be vectorized to compute many solutions simultaneously.

For small problems ($n \leq 5$) the finite difference matrix above can be solved algebraically using Cramer's rule, or equivalently using Mathematica. For example, the matrix (19) for three nodes ($h = L_D/2$) can be solved for A_1 analytically as

$$\begin{aligned} A_1 = &\left\{-\frac{4\left(4-2a_kL_D\right)\left[4+\left(C+Be^{-L_D\lambda_D}\right)L_D^2\right]}{L_D^6} + \left(B + C + \frac{4-2a_kL_D}{L_D^2}\right) \times \right. \\ &\left.\left[\frac{8\left(-2+a_kL_D\right)}{L_D^4} + \left(-C - Be^{-L_D\lambda_D} - \frac{4}{L_D^2}\right)\left(-C - Be^{-\frac{1}{2}L_D\lambda_D} + \frac{2\left(-4+a_kL_D\right)}{L_D^2}\right)\right]\right\} s_H \Bigg/ \\ &\left\{\frac{4\cosh(\eta)\left(4-2a_kL_D\right)\left(4+\left(C+Be^{-L_D\lambda_D}\right)L_D^2\right)}{L_D^6} + \right. \\ &\frac{-4\cosh(\eta) + L_D\left(-2\eta\sinh(\eta) + 2\cosh(\eta)a_k - (B+C)\cosh(\eta)L_D\right)}{L_D^2} \\ &\left.\left[\frac{8\left(-2+a_kL_D\right)}{L_D^4} + \left(-C - Be^{-L_D\lambda_D} - \frac{4}{L_D^2}\right)\left(-C - Be^{-\frac{1}{2}L_D\lambda_D} + \frac{2\left(-4+a_kL_D\right)}{L_D^2}\right)\right]\right\} \end{aligned} \tag{20}$$

which would only be accurate if the vadose zone was small, so that $L_D/2 \ll 1$.

References

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