# 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

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

- where  $K_r$  and  $K_z$  are the radial and vertical saturated hydraulic conductivities [L T<sup>-1</sup>],  $k_0$
- is the dimensionless isotropic relative hydraulic conductivity  $(0 < k_0 \le 1), \sigma = h_0 h = 0$
- $b + \psi_a h$  is drawdown in the vadose zone [L],  $h = \psi + z$  is hydraulic head [L],  $\psi$  is pressure
- head [L],  $\psi_a$  is air-entry pressure,  $C(\psi) = \frac{d\theta}{d\psi}$  is the dimensionless specific moisture capacity,
- and  $\theta$  is dimensionless volumetric water content. The unsaturated zone begins at the top of
- be 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

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$$\sigma(r,z,0)=0$$
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$$\sigma(\infty,z,t)=0$$
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$$\frac{\partial\sigma}{\partial z}=0 \qquad z=b+L$$
16 and 
$$\lim_{r\to 0}r\frac{\partial\sigma}{\partial r}=0 \qquad b\leq z\leq b+L.$$

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

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

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

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

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

where  $S_e$  is dimensionless effective saturation,  $\theta_r$  is dimensionless residual volumetric wa-

- 6 ter content,  $S_y = \theta_s \theta_r$  is dimensionless drainable porosity (specific yield), and  $\theta_s$  is
- <sup>7</sup> dimensionless saturated volumetric water content. The Gardner model for relative hydraulic
- s conductivity is used; the relative hydraulic conductivity is

$$k(\psi) = \begin{cases} e^{a_k(\psi - \psi_k)} & \psi \le \psi_k, \\ 1 & \psi < \psi_k \end{cases} \quad a_k \ge 0, \ \psi_k \le 0,$$

where  $\psi_k$  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

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

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

$$k_0(z_D) \frac{1}{r_D} \frac{\partial}{\partial r_D} \left( r_D \frac{\partial \sigma_D}{\partial r_D} \right) + \kappa \frac{\partial}{\partial z_D} \left( k_0(z_D) \frac{\partial \sigma_D}{\partial z_D} \right) = \gamma C_0(z_D) \frac{\partial \sigma_D}{\partial t_D}$$
(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,  $t_D = tK_r/(b^2S_S)$  is dimensionless time,  $\gamma = S_y a_c/S_S$ 

- is the dimensionless storage ratio, and  $S_S$  is the specific storage [L<sup>-</sup>1] in the saturated aquifer.
- 24 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

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

where  $a_{cD} = a_c b$ .

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#### 2 Unsaturated Zone Solution

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

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

4 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

$$-a^{2}\bar{\sigma}^{*} - \kappa a_{kD} \frac{d\bar{\sigma}_{D}^{*}}{dz_{D}} + \kappa \frac{d^{2}\bar{\sigma}_{D}^{*}}{dz_{D}^{2}} = p\gamma \bar{\sigma}_{D}^{*} e^{-a_{kD}\Psi_{D}} e^{(a_{kD} - a_{cD})(1 - z_{D})}$$
(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

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

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.

#### $_{\scriptscriptstyle 1}$ 2.1 Modified Solution Procedure #1

- <sub>2</sub> By further modifying the  $z_D$ -coordinate and performing an exponential substitution, (9)
- 3 can be simplified significantly and a solution can be found by integration. Using a scaled
- 4 dimensionless vertical coordinate

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

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

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

- we divide through by  $a_{kD}^2$  and performing the substitution  $\bar{\sigma}_D^*(\zeta) = e^{u(\zeta)}$  (e.g., see [BO78, p.
- 9 27] and [Zwi98, §60]). This exponential change of variables implies

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

11 and therefore

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

which changes (10) to

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

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

- 2 By further modifying the  $z_D$ -coordinate and performing a different exponential substitution,
- 3 (9) can be changed to the same form as the time-independent Schrödinger equation. Using
- 4 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

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

we multiply through by  $4/a_{kD}^2$  and performing the substitution  $\bar{\sigma}_D^* = H(\xi)e^{\xi}$ . This exponen-

stial change of variables (e.g., see [KW08]) implies

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

11 and therefore

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

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  $\xi$ -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  $(1/\xi, 1/\xi^2, e^{-\xi}, \text{etc.})$ .

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

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

6 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

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

$$\frac{\mathrm{d}\bar{s}_{UD}^*}{\mathrm{d}z_D} = \frac{\mathrm{d}\bar{\sigma}_D^*}{\mathrm{d}z_D} \longrightarrow \frac{\mathrm{d}\bar{s}_{UD}^*}{\mathrm{d}z_D} = \frac{\mathrm{d}u}{\mathrm{d}\zeta}e^u \qquad z_D = 1$$
(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  $A_2 \equiv 0$ .

### 3 4 Formulation of Finite Difference Solution

 $_{19}$  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

<sup>21</sup> 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  $\sigma$  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  $0 \le j \le N-1$ , 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
- 5 handling the boundary conditions, is

$$\begin{bmatrix}
\frac{1}{h^2} & \left(\frac{a_{kD}}{h} - \frac{2}{h^2} - \xi_0\right) & \frac{1}{h^2} - \frac{a_{kD}}{h} & 0 & 0 \\
0 & \frac{1}{h^2} & \left(\frac{a_{kD}}{h} - \frac{2}{h^2} - \xi_1\right) & \frac{1}{h^2} - \frac{a_{kD}}{h} & 0 \\
0 & 0 & \frac{1}{h^2} & \left(\frac{a_{kD}}{h} - \frac{2}{h^2} - \xi_2\right) & \frac{1}{h^2} - \frac{a_{kD}}{h}
\end{bmatrix}
\begin{bmatrix}
\sigma_{-1} \\
\sigma_{0} \\
\sigma_{1} \\
\sigma_{2} \\
\sigma_{3}
\end{bmatrix} = \begin{bmatrix}
0 \\
0 \\
0 \\
0
\end{bmatrix}$$
(18)

where  $\sigma_{-1}$  and  $\sigma_3$  are "ghost" nodes which will be used to represent boundary conditions,

- but do not physically exist; (18) is in the canonical form  $\mathbf{A}\mathbf{x} = \mathbf{b}$ . 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 **A** and
- eliminating  $\sigma_3$ .

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The node at the bottom of the vadose zone  $(\sigma_0)$  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  $\sigma_{-1}$  from **A**. Substituting  $\sigma_{-1} = \sigma_0 - hA_1\eta \sinh(\eta)$  into (18)

 $_{16}$  gives the following equation for the first row of  ${f A}$ 

$$\frac{1}{h^2} \left[ \sigma_0 - h A_1 \eta \sinh(\eta) \right] + \left( \frac{a_{kD}}{h} - \frac{2}{h^2} - \xi_0 \right) \sigma_0 + \left( \frac{1}{h^2} - \frac{a_{kD}}{h} \right) \sigma_1 = 0$$

Further using head continuity equation  $\sigma_0 = A_1 \cosh(\eta) + s_H(z_D = 1)$  to eliminate  $\sigma_0$  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  $\sigma_0$  into the second row of **A**, and regrouping to solve for  $A_1$ 

22 in place of the eliminated  $\sigma_0$  leads to

$$\begin{bmatrix} \cosh(\eta)\theta_{1} - \frac{\eta}{h}\sinh(\eta) & \frac{1}{h^{2}} - \frac{a_{kD}}{h} & 0\\ \frac{1}{h^{2}}\cosh(\eta) & \theta_{2} & \frac{1}{h^{2}} - \frac{a_{kD}}{h} \\ 0 & \frac{1}{h^{2}} & \theta_{2} + \frac{1}{h^{2}} - \frac{a_{kD}}{h} \end{bmatrix} \begin{bmatrix} A_{1} \\ \sigma_{1} \\ \sigma_{2} \end{bmatrix} = \begin{bmatrix} -\theta_{1}s_{H}(1) \\ -\frac{1}{h^{2}}s_{H}(1) \\ 0 \end{bmatrix}$$
(19)

- where  $\theta_1 = \frac{a_{kD}}{h} \frac{1}{h^2} \xi_j$  and  $\theta_2 = \frac{a_{kD}}{h} \frac{2}{h^2} \xi_j$ . This  $3 \times 3$  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 can-
- 4 cellation 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  $\sigma_j$ , where j = 1, 2, ..., n (not including  $\sigma_0$ ). Once  $A_1$  is found numerically, the solution
- 8 in the saturated zone is simply

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

- 10 This involves computing the Thomas algorithm in Laplace-Hankel space, for each com-
- bination of (a, p). The Thomas algorithm can be vectorized to compute many solutions
- 12 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

$$A_{1} = \left\{ -\frac{4\left(4 - 2a_{k}L_{D}\right)\left[4 + \left(C + Be^{-L_{D}\lambda_{D}}\right)L_{D}^{2}\right]}{L_{D}^{6}} + \left(B + C + \frac{4 - 2a_{k}L_{D}}{L_{D}^{2}}\right) \times \right.$$

$$\left[ \frac{8\left(-2 + a_{k}L_{D}\right)}{L_{D}^{4}} + \left(-C - Be^{-L_{D}\lambda_{D}} - \frac{4}{L_{D}^{2}}\right)\left(-C - Be^{-\frac{1}{2}L_{D}\lambda_{D}} + \frac{2\left(-4 + a_{k}L_{D}\right)}{L_{D}^{2}}\right)\right] \right\} s_{H} /$$

$$\left\{ \frac{4\cosh(\eta)\left(4 - 2a_{k}L_{D}\right)\left(4 + \left(C + Be^{-L_{D}\lambda_{D}}\right)L_{D}^{2}\right)}{L_{D}^{6}} + \left. (20) \right. \right.$$

$$\left. \frac{-4\cosh(\eta) + L_{D}\left(-2\eta\sinh(\eta) + 2\cosh(\eta)a_{k} - \left(B + C\right)\cosh(\eta)L_{D}\right)}{L_{D}^{2}} \right.$$

$$\left. \left[ \frac{8\left(-2 + a_{k}L_{D}\right)}{L_{D}^{4}} + \left(-C - Be^{-L_{D}\lambda_{D}} - \frac{4}{L_{D}^{2}}\right)\left(-C - Be^{-\frac{1}{2}L_{D}\lambda_{D}} + \frac{2\left(-4 + a_{k}L_{D}\right)}{L_{D}^{2}}\right)\right] \right\}$$

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

# 23 References

<sup>24</sup> [BO78] C.M. Bender and S.A. Orszag. Advanced mathematical methods for scientists and engineers: Asymptotic methods and perturbation theory. Springer, 1978.

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