RICHARDS' EQUATION AND ITS CONSTITUTIVE RELATIONS AS A SYSTEM OF DIFFERENTIAL-ALGEBRAIC EQUATIONS

by

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The thesis presented by *Shannon K. Murray* entitled *Richards' Equation and its Constitutive Relations as a System of Differential-Algebraic Equations* is hereby approved.

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Chapter 1

INTRODUCTION

1.1 Basic Flow Equation

Fluid flow through an unsaturated porous media is an important consideration for many problems in science and engineering. In particular, infiltration of water through unsaturated soil is of concern for watershed simulation models, with applications in soil science, agricultural engineering, groundwater hydrology, and environmental engineering.

The traditional equation for saturated fluid flow in a homogenous porous media is given by Darcy's Law

$$q = -K\nabla H, \tag{1.1}$$

where q [L/T] is the flux, or the volume of fluid flowing though a unit cross-sectional area per unit time, H [L] is the total hydraulic head, and K [L/T] is the hydraulic conductivity of the media [6]. The total hydraulic head is the sum of the gravitational head, z and the pressure head ψ, i.e.,

$$H = \psi + z. \tag{1.2}$$

The gravitational head is determined by the distance from some reference point called a datum. Darcy's Law can be rewritten as

$$q = -K\nabla\left(\psi + z\right). \tag{1.3}$$

This equation describes flow under saturated conditions.

1.2 Richards' Equation and its Constitutive Relations

To understand unsaturated flow, we apply the continuity equation, or conservation of mass. This principle states that the amount of water entering a given body of soil minus the amount exiting said soil is the same as the change in water content. In unsaturated conditions (i.e. pores partially filled with a mixture of air and water), the portion of pores that are filled with water is known as the soil moisture water content, θ. Thus the continuity equation in mathematical form is written as

$$\frac{\partial\theta}{\partial t} = -\nabla \cdot q. \tag{1.4}$$

Combining this concept with Darcy's law, it becomes

$$\frac{\partial\theta}{\partial t} = -\nabla \cdot q = \nabla \cdot \left[K(\psi)\nabla\left(\psi + z\right)\right]. \tag{1.5}$$

Because of surface tension effects at the air-water and water-soil interfaces within

unsaturated pores, water is under tension, and ψ is negative. Further, tension within pores creates interdependence between θ, K, and ψ. For instance, the higher the soil moisture content, the better the soil will conduct, hence more movement of water will occur. In essence, K is the ease with which water moves through the soil. Since ψ depends on space and time the hydraulic conductivity K and the volumetric soil moisture θ depend on space and time, i.e.

$$\begin{aligned} \theta(\psi) &= \theta(\psi(x, y, z, t)), \\ K(\psi) &= K(\psi(x, y, z, t)). \end{aligned} \tag{1.6}$$

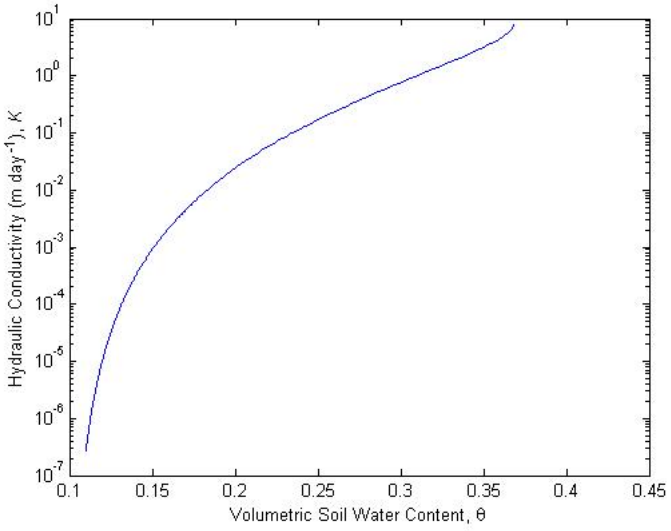

Figure 1.1. Example of the $K(\theta)$ curve for a sandy soil.

Figure 1.1 is an example of how the hydraulic conductivity increases as the soil moisture content increases in a typical sandy soil. Now since the soil moisture content θ varies in response to the pressure ψ, the hydraulic conductivity may also be written

as a function of ψ. Figure 1.2 is an example of how the pressure head affects the soil

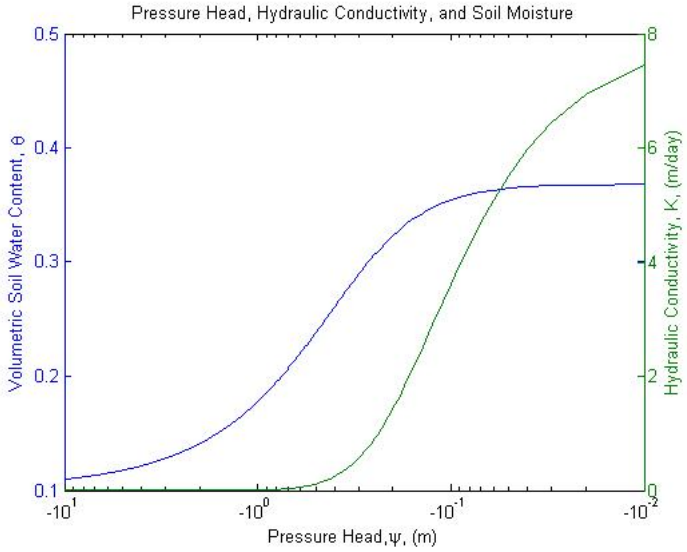

Figure 1.2.: Typical relationship between the tension and both the volumetric soil moisture content and the hydraulic conductivity

moisture content and the hydraulic conductivity.

To apply this information to the continuity equation 1.5, we consider θ as a function of the pressure hear ψ. Having determined that both the soil moisture content and hydraulic conductivity vary with space and time for unsaturated flow, and noting that the gravitational head varies only in the vertical direction, we see that equation

1.5, in three dimensions, becomes

$$\begin{aligned}
\frac{\partial\theta}{\partial t} &= \nabla\cdot\left[K\nabla\left(\psi+z\right)\right] \\
&= \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{bmatrix} \cdot \begin{bmatrix} K(\psi)\left(\frac{\partial}{\partial x}(\psi+z)\right) \\ K(\psi)\left(\frac{\partial}{\partial y}(\psi+z)\right) \\ K(\psi)\left(\frac{\partial}{\partial z}(\psi+z)\right) \end{bmatrix} \\
&= \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{bmatrix} \cdot \begin{bmatrix} K(\psi)\left(\frac{\partial\psi}{\partial x}\right) \\ K(\psi)\left(\frac{\partial\psi}{\partial y}\right) \\ K(\psi)\left(\frac{\partial\psi}{\partial z}+1\right) \end{bmatrix} \\
&= \frac{\partial}{\partial x}\left[K(\psi)\left(\frac{\partial\psi}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[K(\psi)\left(\frac{\partial\psi}{\partial y}\right)\right] + \frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial\psi}{\partial z}+1\right)\right].
\end{aligned} \tag{1.7}$$

This equation is known as the Richards' equation (RE) [15] and is the most commonly used model in unsaturated flow. There are several different forms [3]; the form above is called the mixed form since it uses both the pressure head ψ and the soil moisture content θ as independent variables.

By noting that

$$\frac{\partial\theta}{\partial t} = \frac{\partial\theta}{\partial\psi}\frac{\partial\psi}{\partial t}, \tag{1.8}$$

we get the pressure head form

$$C(\psi)\frac{\partial\psi}{\partial t} = \frac{\partial}{\partial x}\left[K(\psi)\left(\frac{\partial\psi}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[K(\psi)\left(\frac{\partial\psi}{\partial y}\right)\right] + \frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial\psi}{\partial z}+1\right)\right], \tag{1.9}$$

where

$$C(\psi) = \frac{\partial \theta}{\partial \psi} \tag{1.10}$$

is known as the specific moisture capacity [1/L].

Richards' equation in mixed form 1.7 and in pressure head form 1.9 are analytically equivalent, however, the mixed form is typically used in applications. Since this work is intended to align closely with findings in hydrology and soil sciences, we have chosen to restrict our attention to the mixed form, which has been more widely used in these disciplines.

There are many empirical models which describe the relationship between θ, K and ψ [2, 12, 18]. For this work, however, we will restrict our discussions to the van Genuchten and Mualem equations for $\theta(\psi)$ and $K(\psi)$, respectively. [12, 18]. The van Genuchten equation describes how soil moisture content varies with pressure head and is given by

$$\begin{aligned} \theta(\psi) &= \theta_r + (\theta_s - \theta_r) S_e(\psi) \\ S_e(\psi) &= (1 + (\alpha|\psi|)^n)^{-m} \end{aligned} \tag{1.11}$$

where θ_r [L^3/L^{-3}] is the residual soil moisture content, θ_s [L^3/L^{-3}] is the saturated soil moisture content, and α [1/L], n (unitless), and m (unitless) are empirical parameters with no physical meaning. Typically we set $m = 1 - 1/n$. Some scientists also consider θ_r as a fitting parameter as well, since its value changes depending on how it is measured (ref Molly). The empirical equation S_e is defined as the effective

saturation.

Coupling van Genuchten's equation with Mualem's equation yields

$$\begin{aligned} K(\psi) &= K_s S_e^{1/2}(1-(1-S_e^{1/m})^m)^2 \\ &= K_s \frac{\{1-(\alpha|\psi|)^{n-1}[1+(\alpha|\psi|)^n]^{-m}\}^2}{[1+(\alpha|\psi|)^n]^{m/2}} \end{aligned} \tag{1.12}$$

where K_s [L/T] is the saturated hydraulic conductivity.

1.2.1 Summary of Numerical Techniques

Richards' equation and its constitutive relations form a system of differential-algebraic equations. Exact solutions can be found if (1.7), (1.9), (1.11) or (1.12) are simplified. However, this requires certain assumptions about the physical system. In this work, we solve (1.7), (1.11) and (1.12) numerically, for which there are no analytical solutions. Numerical solutions for the pressure head form (1.9) are discussed in [3, 17], and for the mixed form in [4, 5, 7, 10, 11, 14, 16].

In [3] it was shown that the pressure head form of RE has large mass balance errors, which means the numerical solution does not conserve mass, and that the same numerical scheme conserves mass in the mixed form much better. However, more recent studies show that the pressure head form of RE does conserve mass if it is discretized together with its constitutive relations as a differential-algebraic equation (DAE) [17].

The mixed form can be solved linearly [16] or nonlinearly [4, 5, 7, 10, 11]. Picard

iterations are used in the linear formulations while Newton's method is used in the nonlinear formulations. Linear and nonlinear techniques have been compared with the general conclusion that the nonlinear formulations are more robust, i.e. iterations of the nonlinear system converge more quickly and with less chance of failure to the solution [10, 11]. Richards' Equation and its constitutive relations will be solved both linearly and nonlinearly in this work.

The spatial discretization of Richards' equation has remained consistent throughout all numerical solution techniques in the literature [7, 10, 11, 14, 16, 17], and the same discretization is used in this work. Temporal discretizations in the literature vary, with some using higher order methods [5, 7, 10]. This leads to a more efficient method, however, accuracy is usually not improved since lower order methods are usually needed to compute the initial conditions for higher order methods [5, 7, 10]. The most accurate and efficient approach is to use variable order methods with an adaptive time stepping scheme [5, 7, 10, 11]. In this work we will apply this technique to both the linear and nonlinear formulations. Additionally, we will compare linear formulations using the full DAE structure with the analogous nonlinear DAE.

The focus of this work is on the numerical solution of the forward problem, i.e. finding solutions ψ, θ, and K of (1.11), (1.12), (1.7). However, in order to solve these equations, measured data must be used to find parameters α, n ,m, θ_r, θ_s, and K_s in an inversion or data assimilation scheme. An open problem is the question of how to incorporate model and data error in this process. We propose to solve (1.11), (1.12),

(1.7) simultaneously, where each of ψ, θ and K are independent variables, so that error can easily be incorporated. Typically Eq. (1.12) is substituted into Eq. (1.7), and the variable K is eliminated in the DAE structure. This approach would appear to make the solution process more efficient, but does not alow the incorporation of uncertainty. Since the hydraulic conductivity K cannot be measure directly, it is actually the most uncertain variable. Viewing the problem in this manner implies that we solve (1.11), (1.12), (1.7) as a system of differential-algebraic equations.

In this work, we compare four different analytic DAE formulations. There are two linear formulations and two nonlinear formulations. The first linear formulation is a modification of a commonly used software package called HYDRUS [16]. It is of the form

$$f(\theta, \psi) = A \begin{bmatrix} \theta \\ \\ \psi \end{bmatrix} - \overrightarrow{b} = 0, \tag{1.13}$$

and we refer to it as HYDRUS FE.

The second DAE formulation is also linear, but includes the hydraulic conductivity, K, in the solution scheme. It is of the form

$$f(\theta, \psi, K) = A \begin{bmatrix} \theta \\ \\ \psi \\ \\ K \end{bmatrix} - \overrightarrow{b} = 0, \tag{1.14}$$

and we refer to it as PLDAE.

The nonlinear DAE formulation found in [7, 10, 11] is similar to HYDRUS in that

it does not include the hydraulic conductivity as an independent variable. It is of the form

$$f(\theta,\psi) = \begin{bmatrix} \frac{\partial\theta}{\partial t} - \frac{\partial}{\partial z}\left[K\left(\frac{\partial\psi}{\partial z}+1\right)\right] \\ \theta(\psi) - \theta_r + (\theta_s - \theta_r)S_e(\psi) \end{bmatrix} = 0, \tag{1.15}$$

and we refer to it as NDAE The final DAE formulation is also nonlinear, but includes hydraulic conductivity, he hydraulic conductivity, K, in the solution scheme. It is of the form

$$f(\theta,\psi,K) = \begin{bmatrix} \frac{\partial\theta}{\partial t} - \frac{\partial}{\partial z}\left[K\left(\frac{\partial\psi}{\partial z}+1\right)\right] \\ \theta(\psi) - \theta_r + (\theta_s - \theta_r)S_e(\psi) \\ K(\psi) - K_s S_e(\psi)^{1/2}\left[1-(1-S_e(\psi)^{1/m})^m\right]^2 \end{bmatrix} = 0, \tag{1.16}$$

and we refer to it as PNDAE.

The linear and nonlinear formulations, PLDAE and PNDAE, respectively, have not been studied in the literature. We would expect them to be less efficient, but possibly more accurate than HYDRUS FE and NDAE. The main motivation for these new formulations, however, is that they allow us to explicitly incorporate model and data error for hydraulic conductivity into the numerical solutions.

In Chapter 2 we discuss the numerical discretizations for Richards' equation used in the literature and in this work. In Chapter 3 we develop Richards' equation and its constitutive relations analytically as a system of DAEs and determine its index. In Chapter 4, we apply the discretizations presented in Chapter 2 to the DAEs formulated in Chapter 3. In Chapter 5 we show the results of solving two test

problems found in the literature [8, 11, 10, 14, 17], as well as our conclusions and future work.

Chapter 2

DISCRETIZATION OF RICHARDS' EQUATION

The majority of water movement in the unsaturated zone is attributed to gravity, so we also restrict our attention to one spatial variable, namely the vertical direction, which accounts for the effects of gravity. For the remainder of this work, the term RE refers to the mixed form of RE restricted to the vertical space dimension:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z} + 1\right)\right] \tag{2.1}$$

with initial and boundary condition

$$\begin{aligned} \psi(z, t = 0) &= \psi_0(z) \\ \psi(z = 0, t > 0) &= \psi_{LB}(t) \\ \psi(z = Z, t > 0) &= \psi_{RB}(t) \end{aligned} \tag{2.2}$$

where Z is the length of the spatial domain. Initial and boundary conditions for θ and K are found by using the initial and boundary conditions of ψ in van Genuchten and Mualem's equations.

The goal of the work is to compare and contrast the linear and nonlinear DAE

formulations (1.13) - (1.16). To this end, we keep the spatial and temporal approximation methods fixed, as described below. Though there are many ways to define numerical methods, we found the following was a common approach used throughout the literature.

2.1 The Spatial Discretization

The standard approach in the literature is to apply a finite difference scheme [7, 10, 11, 14, 16, 17]. The finite element approach has also been constructed but, it has been shown to reduce to the finite difference scheme presented here [3, 14, 16].

Assume the spatial domain is $[0, L]$, and divide this interval into J subintervals of length Δz. Let $z_j = j\Delta z$ with $j = 0, \ldots, J$. Then the pressure head is evaluated at the grid points $\psi_j = \psi(z_j)$, while the hydraulic conductivity K is evaluated exactly halfway between each subinterval. This leads to the spatial discretization of the RHS of (2.1)

$$\frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z}+1\right)\right] = \frac{1}{\Delta z}\left[\frac{K_{j+1/2}(\psi_{j+1}-\psi_j)}{\Delta z} - \frac{K_{j-1/2}(\psi_j-\psi_{j-1})}{\Delta z} + K_{j+1/2} - K_{j-1/2}\right]. \tag{2.3}$$

A full derivation of the scheme is presented in Appendix I. In practice, we may not

be able to evaluate K at the half interval, so we approximate it by

$$\begin{aligned} K_{j+1/2} &= \frac{K_{j+1} + K_j}{2} \\ K_{j-1/2} &= \frac{K_j + K_{j-1}}{2} \end{aligned} \tag{2.4}$$

This is the spatial discretization used for HYDRUS FE, PLDAE, NDAE, and PNDAE.

2.2 The Temporal Discretization

The temporal derivative of the LHS of (2.1) is approximated using the backward differentiation formulae (BDF) methods, which are a subclass of the multistep methods [1]. After applying the spatial discretization we are left with a system of ODEs of the form

$$\frac{d\theta_j}{dt} = \frac{1}{\Delta z}\left[\frac{K_{j+1/2}(\psi_{j+1} - \psi_j)}{\Delta z} - \frac{K_{j-1/2}(\psi_j - \psi_{j-1})}{\Delta z} + K_{j+1/2} - K_{j-1/2}\right]. \tag{2.5}$$

Assume the temporal domain is $[0, T]$, and divide this interval into N_t subintervals, each of length Δt. Let $z^{n_t} = n_t \Delta t$, with $n_t = 0, \ldots, N_t$. Then we can approximate $\frac{d\theta_j}{dt}$ by

$$\frac{d\theta_j}{dt} \approx \frac{1}{\Delta t} \sum_{i=0}^{p} \lambda_i \theta_j^{n_t+1-i}, \tag{2.6}$$

where λ_i and p are given in Table 2.2 [1]. Note that p is the order of the method [1], which is allowed to vary in variable order experiments. For example, the first order

p	λ_0	λ_1	λ_2	λ_3	λ_4
1	1	-1			
2	$\frac{3}{2}$	-2	$\frac{1}{2}$		
3	$\frac{11}{6}$	-3	$\frac{3}{2}$	$-\frac{1}{3}$	
4	$\frac{25}{12}$	-4	3	$-\frac{4}{3}$	$\frac{1}{4}$

TABLE 2.1 Coefficients of BDF methods up to order 4

BDF method is equivalent to the backward Euler scheme

$$\frac{d\theta_j}{dt} \approx \frac{\theta_j^{n_t+1} - \theta_j^{n_t}}{\Delta t}. \tag{2.7}$$

The solution is assumed to be unknown at time steps $n_t + 1$, and known at time step n_t. From (2.2), we can see that for an order p method, we need p initial conditions. If these additional initial conditions are not known, they can be computed using a lower order method. However, this technique limits the overall order to the lowest order needed to compute the required initial conditions.

Variable order, variable time step methods allow the method to vary based on the history of the numerical solution. In a truly adaptive scheme, the order of the method and the length of Δt are chosen so that the numerical solution at each time step satisfies some error condition. However, for this work, we imposed the order of the method and the length of Δt based on the results of numerical simulations for fixed Δt. The details are given in Chapter 5.

Chapter 3

DIFFERENTIAL ALGEBRAIC EQUATIONS

In this chapter, we discuss some of the basic theory of DAEs and show how this theory applies to RE. We show that RE and its constitutive relations form an semi-explicit index 1 DAE. This implies that traditional methods can be used and there are some freely available codes in Matlab and fortran. In this work we use the BDF and finite difference methods discussed in the previous chapter to solve the DAE..

3.1 Theory

A differential-algebraic equation (DAE) is defined as a differential equation which is constrained by algebraic equations. A DAE has the general form

$$\begin{aligned} 0 &= \mathbf{f}(t, \mathbf{x}', \mathbf{x}, \mathbf{z}) \\ 0 &= \mathbf{g}(t, \mathbf{x}, \mathbf{z}) \end{aligned} \tag{3.1}$$

where $\mathbf{x}(t)$ are the differential variables, and $\mathbf{z}(t)$ are the algebraic variables.

If we define

$$\mathbf{F}(t, \mathbf{x}', \mathbf{x}, \mathbf{z}) \equiv \begin{bmatrix} \mathbf{f}(t, \mathbf{x}, \mathbf{z}) \\ \\ \mathbf{g}(t, \mathbf{x}, \mathbf{z}) \end{bmatrix}, \tag{3.2}$$

and define

$$\mathbf{y} \equiv \begin{bmatrix} \mathbf{x} \\ \\ \mathbf{z} \end{bmatrix}, \tag{3.3}$$

then the Jacobian $\frac{\partial \mathbf{F}}{\partial \mathbf{y}}$ is singular. Thus we cannot simply apply numerical methods for differential equations to a DAE system. In order to formulate adequate numerical methods for DAEs, we must first have an understanding of some of the theory behind them.

One property of DAEs that affects the numerical solution is the index. The index of a solvable DAE [13] is the smallest nonnegative integer m such that $\mathbf{F}$ has m continuous derivatives and the nonlinear system

$$\begin{aligned} &\mathbf{F}(t, \mathbf{y}, \mathbf{y}') = 0 \\ &\frac{d\mathbf{F}}{dt}(t, \mathbf{y}, \mathbf{y}', \mathbf{y}'') = \frac{\partial \mathbf{F}}{\partial \mathbf{y}}\mathbf{y}' + \frac{\partial \mathbf{F}}{\partial \mathbf{y}'}\mathbf{y}'' + \frac{\partial \mathbf{F}}{\partial t} = 0 \\ &\vdots \\ &\frac{d^m\mathbf{F}}{dt^m}(t, \mathbf{y}, \mathbf{y}', \mathbf{y}'', \ldots, \mathbf{y}^{(m+1)}) = 0 \end{aligned} \tag{3.4}$$

can be solved for $\mathbf{y}'$ uniquely in terms of $\mathbf{y}$ and t. An index 1 DAE can be solved numerically using ODE methods for stiff problems. Higher index systems must first undergo an index reduction and them solved [1].

A common numerical method for solving index 1 or index 0 systems is by backward differentiation formulae (BDF) [1]. Analogous to Chapter 2, the BDF method for the

DAE

$$\mathbf{F}(t, \mathbf{y}, \mathbf{y}') = 0 \tag{3.5}$$

is given by

$$\mathbf{F}(t^{n_t+1}, \mathbf{y}^{n_t+1}, \frac{1}{\Delta t} \sum_{i=0}^{p} \lambda_i \mathbf{y}^{n_t+1-i}) = 0. \tag{3.6}$$

It has been shown that for nonlinear index 1 DAEs, the BDF method converges with order p, as noted in Chapter 2 [1, 9].

The next section shows that RE together with the constitutive relations discussed in Chapter 1 is an index 1 system. Thus, we can employ the BDF method.

3.2 Richards' Equation and its Constitutive Relations as a DAE

First, we align the notation of the previous section with our notation for RE. The mixed form of RE has two differential variables, namely ψ and θ, and one algebraic variable, K. Thus

$$\mathbf{y} = \begin{bmatrix} \theta \\ \psi \\ K \end{bmatrix} \tag{3.7}$$

and

$$\mathbf{F}(t,z,\theta,\psi,K,\theta_t,\psi_{zz}) = \begin{bmatrix} \frac{\partial\theta}{\partial t} - \frac{\partial}{\partial z}\left[K\left(\frac{\partial\psi}{\partial z}+1\right)\right] \\ \theta(\psi) - \theta_r + (\theta_s-\theta_r)S_e(\psi) \\ K(\psi) - K_s S_e(\psi)^{1/2}\left[1-(1-S_e(\psi)^{1/m})^m\right]^2 \end{bmatrix} = 0. \quad (3.8)$$

We apply our spatial discretization to get

$$\mathbf{F}_j(t,\theta,\psi,\mathbf{K},\theta') = \begin{bmatrix} f_j(t,\theta,\psi,\mathbf{K},\theta') \\ g_j(t,\theta,\psi) \\ h_j(t,\psi,\mathbf{K}) \end{bmatrix} \quad (3.9)$$

where

$$\begin{aligned} f_j(t,\theta,\psi,\mathbf{K},\theta') = \theta'_j - \frac{1}{\Delta z}\Bigg[&\left(\frac{K_{j+1}+K_j}{2}\right)\left(\frac{\psi_{j+1}-\psi_j}{\Delta z}\right) \\ &-\left(\frac{K_j+K_{j-1}}{2}\right)\left(\frac{\psi_j-\psi_{j-1}}{\Delta z}\right)+\frac{K_{j+1}-K_{j-1}}{2}\Bigg], \end{aligned} \quad (3.10)$$

$$g_j(t,\theta,\psi) = \theta_j - \theta_r + (\theta_s-\theta_r)(1+(\alpha|\psi_j|)^n)^{-m}, \quad (3.11)$$

and

$$h_j(t,\psi,\mathbf{K}) = K_j - K_s\frac{\{1-(\alpha|\psi_j|)^{n-1}[1+(\alpha|\psi_j|)^n]^{-m}\}^2}{[1+(\alpha|\psi_j|)^n]^{m/2}} \quad (3.12)$$

for $j = 0,\ldots,J$.

3.2.1 Index

Theorem: The mixed form of Richards' Equation given in Eq. (2.3) is a semi-explicit (or Hessenburg) index 1 DAE.

Proof. Begin with the system

$$\begin{aligned}
\theta_j' &= \frac{1}{\Delta z}\left[\left(\frac{K_{j+1}+K_j}{2}\right)\left(\frac{\psi_{j+1}-\psi_j}{\Delta z}\right) - \left(\frac{K_j+K_{j-1}}{2}\right)\left(\frac{\psi_j-\psi_{j-1}}{\Delta z}\right)\right. \\
&\qquad \left. + \frac{K_{j+1}-K_{j-1}}{2}\right], \\
\theta_j &= \theta_r + (\theta_s-\theta_r)(1+(\alpha|\psi_j|)^n)^{-m}, \\
K_j &= K_s \frac{\{1-(\alpha|\psi_j|)^{n-1}[1+(\alpha|\psi_j|)^n]^{-m}\}^2}{[1+(\alpha|\psi_j|)^n]^{m/2}}.
\end{aligned} \tag{3.13}$$

If we differentiate the algebraic constraints, for van Genuchten's equation we have

$$\theta_j' = (\theta_s-\theta_r)mn\alpha(1+(\alpha|\psi_j|)^n)^{-m-1}(\alpha|\psi_j|)^{n-1}\psi_j' \tag{3.14}$$

and the derivative of Mualem's equation follows similarly, however, for ease of presentation, we write it more generally as

$$K_j' = q(\psi_j, \psi_j'). \tag{3.15}$$

We can now substitute Richards' equation into the differentiated van Genuchten equa-

tion to get

$$(\theta_s - \theta_r)mn\alpha(1 + (\alpha|\psi_j|)^n)^{-m-1}(\alpha|\psi_j|)^{n-1}\psi_j' = \frac{1}{\Delta z}\left[\left(\frac{K_{j+1} + K_j}{2}\right)\left(\frac{\psi_{j+1} - \psi_j}{\Delta z}\right) - \left(\frac{K_j + K_{j-1}}{2}\right)\left(\frac{\psi_j - \psi_{j-1}}{\Delta z}\right) + \frac{K_{j+1} - K_{j-1}}{2}\right] \tag{3.16}$$

We now solve for ψ_j':

$$\psi_j' = \frac{\left(\frac{K_{j+1}+K_j}{2}\right)\left(\frac{\psi_{j+1}-\psi_j}{\Delta z}\right) - \left(\frac{K_j+K_{j-1}}{2}\right)\left(\frac{\psi_j-\psi_{j-1}}{\Delta z}\right) + \frac{K_{j+1}-K_{j-1}}{2}}{\Delta z(\theta_s - \theta_r)mn\alpha(1 + (\alpha|\psi_j|)^n)^{-m-1}(\alpha|\psi_j|)^{n-1}}, \tag{3.17}$$

and insert this functional representation into K_j':

$$K_j' = q\left(\psi_j, \frac{\left(\frac{K_{j+1}+K_j}{2}\right)\left(\frac{\psi_{j+1}-\psi_j}{\Delta z}\right) - \left(\frac{K_j+K_{j-1}}{2}\right)\left(\frac{\psi_j-\psi_{j-1}}{\Delta z}\right) + \frac{K_{j+1}-K_{j-1}}{2}}{\Delta z(\theta_s - \theta_r)mn\alpha(1 + (\alpha|\psi_j|)^n)^{-m-1}(\alpha|\psi_j|)^{n-1}}\right). \tag{3.18}$$

We now have an explicit ODE system. Since we differentiated the algebraic constraints once, we have an index 1 DAE, and the system (3.13) is an ODE with algebraic constraints it is in semi-explicit form. □

This theorem refers to the nonlinear form of RE and its constitutive relations, PNDAE. The linear formulations, PLDAE, is also index 1 and the proof follows similarly. The other formulations, HYDRUS FE and NDAE are index 0 since they can be written in explicit form without any differentiation of the algebraic constraints.

Index 0 DAEs are explicit differential equations. Since all 4 formulations are index 0 or index 1 we are able to apply the same numerical approximation in each case, as described in Chapter 2.

Chapter 4

DAE FORMULATIONS

In this Chapter we apply the discretizations in Chapter 2 to the four different formulations of RE and its constitutive relations as a DAE, Eqs. (1.13) – (1.16).

4.1 Linear Formulations

The linear formulations (1.13) and (1.14) are derived by applying Taylor series expansions to $f(\theta, \psi)$ or $f(\theta, \psi, K)$ about a previous estimate θ^ν, ψ^ν, and K^ν. For example

$$f(\psi^{\nu+1}) = f(\psi^\nu) + \left(\left. \frac{\partial f}{\partial \psi} \right|_{\psi^\nu} \right) (\psi^{\nu+1} - \psi^\nu). \tag{4.1}$$

This is called a Picard iteration scheme [3]. The basic idea is that it will converge, given good initial estimates θ^0, ψ^0 and K^0. Once in linear form, the spatial and temporal discretizations are applied.

4.1.1 HYDRUS and HYDRUS FE

HYDRUS is a common tool used by many scientists [16] to solve RE and its constitutive equations both as a forward model and for inversion. The discretization in

HYDRUS was derived by (*Celia et al*, 1990) and is given there as

$$\frac{\theta_j^{n_t+1,\nu+1}-\theta_j^{n_t}}{\Delta t}=\frac{1}{\Delta z}\left[\frac{K_{j+1/2}^{n_t+1,\nu}(\psi_{j+1}^{n_t+1,\nu+1}-\psi_j^{n_t+1,\nu+1})}{\Delta z}-\frac{K_{j-1/2}^{n_t+1,\nu}(\psi_j^{n_t+1,\nu+1}-\psi_{j-1}^{n_t+1,\nu+1})}{\Delta z}\right.$$
$$\left.+K_{j+1/2}^{n_t+1,\nu}-K_{j-1/2}^{n_t+1,\nu}\right], \tag{4.2}$$

where θ and K are found by interpolation, using a table of values generated by the van Genuchten-Mualem model. By evaluating θ and K and then inserting these values into RE, HYDRUS is index 0 DAE form of RE and its constitutive relations.

In HYDRUS the derivative $\frac{\partial\theta}{\partial t}$ is approximated using the first order BDF method, as indicated in (4.2). Note that the nonlinear coefficient K is evaluated at the previous iterate, ν, and that θ is evaluated at the new iterate, $\nu+1$. This value of θ, $\theta_j^{n_t+1,\nu+1}$, is found by linearizing $\theta_j^{n_t+1,\nu+1}$ about the point $\psi_j^{n_t+1,\nu}$ using a first order Taylor Series expansion,

$$\begin{aligned}\theta_j^{n_t+1,\nu+1}&=\theta(\psi_j^{n_t+1,\nu+1})\approx\theta(\psi_j^{n_t+1,\nu})+\left.\frac{\partial\theta}{\partial\psi}\right|_{\psi_j^{n_t+1,\nu}}\left(\psi_j^{n_t+1,\nu+1}-\psi_j^{n_t+1,\nu}\right)\\&=\theta_j^{n_t+1,\nu}+C_j^{n_t+1,\nu}\left(\psi_j^{n_t+1,\nu+1}-\psi_j^{n_t+1,\nu}\right)\end{aligned} \tag{4.3}$$

To effectively compare this formulation with the proposed linear formulation and nonlinear formulations, we introduce a series of modifications to the original HYDRUS formulation: First, θ and K are found by evaluating van Genuchten's and Mualem's equations (1.11) - (1.12) explicitly instead of interpolating a table values

of these functions. Secondly, the temporal derivative $\frac{\partial \theta}{\partial t}$ is approximated by the BDF scheme discussed in Chapter 3. Although the first order BDF method is equivalent to HYDRUS, we also employed higher order methods, as well as VOVT methods. We denote this formulation as HYDRUS FE. Using BDF methods leads to to following matrix equation,

$$A_H \psi^{n_t+1,\nu+1} = \mathbf{b}_H. \tag{4.4}$$

This matrix equation is similar to the matrix equation solved in HYDRUS, with the main differences occurring in the diagonal entries of the matrix A_H and the vector $\mathbf{b}$. The matrix A_H is symmetric and tridiagonal, with diagonal entries a_j, $j = 1, \ldots, J-1$, given by

$$a_j = \frac{\Delta z}{\Delta t}\lambda_0 C_j^{n_t+1,\nu} + \frac{K_{j+1}^{n_t+1,\nu} + 2K_j^{n_t+1,\nu} + K_{j-1}^{n_t+1,\nu}}{2\Delta z}, \tag{4.5}$$

and subdiagonal entries d_j, $j = 1, \ldots, J-2$, given by

$$d_j = -\frac{K_j^{n_t+1,\nu} + K_{j+1}^{n_t+1,\nu}}{2\Delta z}. \tag{4.6}$$

The values b_j, $j = 1, \ldots, J-1$, of the vector $\mathbf{b}_H$ are given by

$$b_j = \frac{K_{j+1}^{n_t+1,\nu} - K_{j-1}^{n_t+1,\nu}}{2\Delta z} + \frac{\Delta z}{\Delta t}\lambda_0 C_j^{n_t+1,\nu}\psi_j^{n_t+1,\nu} - \frac{\Delta z}{\Delta t}\sum_{i=0}^{p}\lambda_i \theta_j^{n_t+1-i}. \tag{4.7}$$

HYDRUS can be recovered from (4.5) - (4.7) by $p = 1$, $\lambda_0 = 1$, $\lambda_1 = -1$. Note that the values of a_1, d_1, b_1 and a_{J-1}, d_{J-2}, b_{J-1} are dependent on the boundary

conditions and

$$b_1 = \frac{K_2^{n_t+1,\nu} - K_0^{n_t+1}}{2\Delta z} + \frac{\Delta z}{\Delta t}\lambda_0 C_1^{n_t+1,\nu}\psi_1^{n_t+1,\nu} - \frac{\Delta z}{\Delta t}\sum_{i=0}^{p}\lambda_i\theta_1^{n_t+1-i} + \left(\frac{K_0^{n_t+1} + K_1^{n_t+1,\nu}}{2\Delta z}\right)\psi_0^{n_t+1}$$
$$b_{J-1} = \frac{K_J^{n_t+1} - K_{J-2}^{n_t+1,\nu}}{2\Delta z} + \frac{\Delta z}{\Delta t}\lambda_0 C_{J-1}^{n_t+1,\nu}\psi_{J-1}^{n_t+1,\nu} - \frac{\Delta z}{\Delta t}\sum_{i=0}^{p}\lambda_i\theta_{J-1}^{n_t+1-i} + \left(\frac{K_{J-1}^{n_t+1,\nu} + K_J^{n_t+1}}{2\Delta z}\right)\psi_J^{n_t+1} \tag{4.8}$$

We implemented this alternate form of HYDRUS, HYDRUS FE, in Matlab and the results are given in Chapter 5. We found HYDRUS FE to a more efficient and accurate method than HYDRUS. In addition it is a better formulation to compare with our other DAE formulations.

4.1.2 Proposed Linear Formulation (PLDAE)

In the modified HYDRUS formulation above, HYDRUS FE, the hydraulic conductivity K is evaulated at the previous linear iterate, ν. PLDAE is a formulation where K is evaluated at the current linear iterate, $\nu + 1$. Just as $\theta^{n_t+1,\nu+1}$ is linearized about $\psi^{n_t+1,\nu}$ in HYDRUS, we can linearize $K^{n_t+1,\nu+1}$ about $\psi^{n_t+1,\nu}$ in order to approximate the most current value of K. This allows us to explicitly include K in the linear DAE, rather than first reducing the index and solving the explicit differential equation.

Recall Richards' Equation is given by

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left[K\left(\frac{\partial\psi}{\partial z} + 1\right)\right]. \tag{4.9}$$

Consider

$$f_R = K(\psi_z + 1). \tag{4.10}$$

The first order Taylor series expansion of $f_R(K^{\nu+1}, \psi_z^{\nu+1})$ about the point (K^ν, ψ_z^ν) is given by

$$\begin{aligned} K^{\nu+1}(\psi_z^{\nu+1} + 1) &\approx K^\nu(\psi_z^\nu + 1) + (\psi_z^\nu + 1)(K^{\nu+1} - K^\nu) + K^\nu(\psi_z^{\nu+1} - \psi_z^\nu) \\ &= K^{\nu+1}(\psi_z^\nu + 1) + K^\nu\psi_z^{\nu+1} - K^\nu\psi_z^\nu. \end{aligned} \tag{4.11}$$

Thus the linear form of Richards' Equation which approximates the most current iterate of K is given by

$$\frac{\partial\theta^{\nu+1}}{\partial t} = \frac{\partial}{\partial z}\left[K^{\nu+1}(\psi_z^\nu + 1) + K^\nu\psi_z^{\nu+1} - K^\nu\psi_z^\nu\right]. \tag{4.12}$$

If we apply our BDF scheme in time and the centered finite difference scheme in space

we have

$$\begin{aligned}
&\left(\frac{\Delta z}{\Delta t}\right)\lambda_0\theta_j^{n_t+1,\nu+1} - \left(\frac{\psi_{j+1}^{n_t+1,\nu} - \psi_j^{n_t+1,\nu}}{2\Delta z} + \frac{1}{2}\right)K_{j+1}^{n_t+1,\nu+1} \\
&\quad - \left(\frac{\psi_{j+1}^{n_t+1,\nu} - 2\psi_j^{n_t+1,\nu} + \psi_{j-1}^{n_t+1,\nu}}{2\Delta z}\right)K_j^{n_t+1,\nu+1} + \left(\frac{\psi_j^{n_t+1,\nu} - \psi_{j-1}^{n_t+1,\nu}}{2\Delta z} + \frac{1}{2}\right)K_{j-1}^{n_t+1,\nu+1} \\
&\quad - \left(\frac{K_{j+1}^{n_t+1,\nu} + K_j^{n_t+1,\nu}}{2\Delta z}\right)\psi_{j+1}^{n_t+1,\nu+1} + \left(\frac{K_{j+1}^{n_t+1,\nu} + 2K_j^{n_t+1,\nu} + K_{j-1}^{n_t+1,\nu}}{2\Delta z}\right)\psi_j^{n_t+1,\nu+1} \\
&\quad - \left(\frac{K_j^{n_t+1,\nu} + K_{j-1}^{n_t+1,\nu}}{2\Delta z}\right)\psi_{j-1}^{n_t+1,\nu+1} \\
&= -\left(\frac{\Delta z}{\Delta t}\right)\sum_{i=1}^{p}\theta_j^{n_t+1-i} - \left(\frac{K_{j+1}^{n_t+1,\nu} + K_j^{n_t+1,\nu}}{2}\right)\left(\frac{\psi_{j+1}^{n_t+1,\nu} - \psi_j^{n_t+1,\nu}}{\Delta z}\right) \\
&\quad + \left(\frac{K_j^{n_t+1,\nu} + K_{j-1}^{n_t+1,\nu}}{2}\right)\left(\frac{\psi_j^{n_t+1,\nu} - \psi_{j-1}^{n_t+1,\nu}}{\Delta z}\right).
\end{aligned} \tag{4.13}$$

Van Genuchten's Equation is given by

$$\theta = \theta_r + (\theta_s - \theta_r)S_e(\psi), \tag{4.14}$$

where

$$S_e(\psi) = (1 + (\alpha|\psi|)^n)^{-m}. \tag{4.15}$$

Since $S_e(\psi)$ is nonlinear in ψ we linearize $S_e(\psi^{\nu+1})$ using the first order Taylor series

expansion about the point ψ^{ν} and apply the discretizations to get

$$\theta_j^{n_t+1,\nu+1}+(\theta_r-\theta_s)\left(\left.\frac{\partial S_e}{\partial\psi}\right|_{\psi_j^{n_t+1,\nu}}\right)\psi_j^{n_t+1,\nu+1}=\theta_r+(\theta_s-\theta_r)\left[S_e(\psi_j^{n_t+1,\nu})-\left(\left.\frac{\partial S_e}{\partial\psi}\right|_{\psi_j^{n_t+1,\nu}}\right)\psi_j^{n_t+1,\nu}\right] \tag{4.16}$$

We employ the same technique to Mualem's Equation, which is given by

$$K=K_sS_e(\psi)^{1/2}\left[1-(1-S_e(\psi)^{1/m})^m\right]^2. \tag{4.17}$$

Since K is nonlinear, we linearize $K(\psi^{\nu+1})$ about the point ψ^{ν}, and apply the discretizations to get

$$\begin{aligned}K_j^{n_t+1,\nu+1}-\left(\left.\frac{\partial K}{\partial\psi}\right|_{\psi_j^{n_t+1,\nu}}\right)\psi_j^{n_t+1,\nu+1}&=K_sS_e(\psi_j^{n_t+1,\nu})^{1/2}[1-(1-S_e(\psi_j^{n_t+1,\nu})^{1/m})^m]^2\\&\quad-\left(\left.\frac{\partial K}{\partial\psi}\right|_{\psi_j^{n_t+1,\nu}}\right)\psi_j^{n_t+1,\nu}\end{aligned} \tag{4.18}$$

A full derivation of the linearizations (4.13), (4.16) and (4.18) is given in Appendix II.

For each time step n_t+1 we iterate the linear system

$$A\mathbf{y}=\mathbf{b}, \tag{4.19}$$

where A consists of block matrices

$$A = \begin{bmatrix} A_{f\theta} & A_{f\psi} & A_{fK} \\ A_{g\theta} & A_{g\psi} & A_{gK} \\ A_{h\theta} & A_{h\psi} & A_{hK} \end{bmatrix} \tag{4.20}$$

where $A_{f\theta}$ is a $J-1 \times J-1$ diagonal matrix whose diagonal entries are the constant $\frac{\Delta z}{\Delta t}\lambda_0$, $A_{g\theta}$ and A_{hK} are $J-1 \times J-1$ identity matrices, $A_{h\theta}$ and A_{gK} are $J-1 \times J-1$ zero matrices, $A_{g\psi}$ and $A_{h\psi}$ are $J-1 \times J-1$ diagonal matrices with entries $a_{g\psi_j}$ and $a_{h\psi_j}$, respectively, given by

$$a_{g\psi_j} = (\theta_r - \theta_s)\left(\left.\frac{\partial S_e}{\partial \psi}\right|_{\psi_j^{n_t+1,\nu}}\right), \tag{4.21}$$

$$a_{h\psi_j} = -\left(\left.\frac{\partial K}{\partial \psi}\right|_{\psi_j^{n_t+1,\nu}}\right), \tag{4.22}$$

and $A_{f\psi}$ and A_{fK} are $J-1 \times J-1$ tridiagonal matrices. The subdiagonal and superdiagonal entries, $a_{f\psi_{sj}}$, of $A_{f\psi}$ are given by

$$a_{f\psi_{sj}} = -\left(\frac{K_{j+1}^{n_t+1,\nu} + K_j^{n_t+1,\nu}}{2\Delta z}\right), \tag{4.23}$$

and the diagonal entries, $a_{f\psi_{dj}}$, of $A_{f\psi}$ are given by

$$a_{f\psi_{dj}} = \left(\frac{K_{j+1}^{n_t+1,\nu} + 2K_j^{n_t+1,\nu} + K_{j-1}^{n_t+1,\nu}}{2\Delta z}\right). \tag{4.24}$$

The subdiagonal and superdiagonal entries, $a_{fK_{sj}}$, of A_{fK} are given by

$$a_{fK_{sj}} = \pm \left(\frac{\psi_{j+1}^{n_t+1,\nu} - \psi_j^{n_t+1,\nu}}{2\Delta z} + \frac{1}{2} \right), \tag{4.25}$$

where the entries are negative along the superdiagonal and positive along the subdiagonal. The diagonal entries, $a_{fK_{dj}}$, of $A_{f\psi}$ are given by

$$a_{f\psi_{dj}} = - \left(\frac{\psi_{j+1}^{n_t+1,\nu} - 2\psi_j^{n_t+1,\nu} + \psi_{j-1}^{n_t+1,\nu}}{2\Delta z} \right). \tag{4.26}$$

We implemented PLDAE in Matlab and the results are given in Chapter 5. In general, PLDAE gave equivalent accuracy results, though it was less efficient than HYDRUS FE, NDAE, and PNDAE.

4.2 Nonlinear Formulations

In this section we consider solving the nonlinear form of RE (1.15) and (1.16). A common approach to solving nonlinear systems is by applying Newton iterations **??**. Even though Newton's method is a nonlinear method, Newton iterations effectively use a linearized version of the system at each iterate. The method proceeds as follows.

Given a nonlinear system of the form

$$\mathbf{F}(\mathbf{y}) = \mathbf{0} \tag{4.27}$$

and an initial estimate $\mathbf{y}^0$, then the new iterate using Newton's method is given by

$$\begin{aligned} \left(\frac{\partial \mathbf{F}}{\partial \mathbf{y}}\right)^{\nu} \delta &= -\mathbf{F}(\mathbf{y}^{\nu}) \\ \mathbf{y}^{\nu+1} &= \mathbf{y}^{\nu} + \delta. \end{aligned} \tag{4.28}$$

Most of the work associated with the nonlinear formulations is in computing the Jacobian. This will become more apparent as we compare the nonlinear formulations and see how the Jacobian for each formulation differs. Though many sophisticated techniques for reducing the computational cost for computing the Jacobian have been studied for RE, we defer this analysis to later work and concentrate on the subtle differences associated the formulations.

4.3 Nonlinear DAE formulation by Kees and Miller (2002) (NDAE)

In the Kees and Miller (2002) formulation, only θ and ψ are considered independent variables. Thus we let

$$\mathbf{y} = \begin{bmatrix} \theta_1 & \dots & \theta_{J-1} & \psi_1 & \dots & \psi_{J-1} \end{bmatrix}^T. \tag{4.29}$$

Then the nonlinear system is

$$\mathbf{F}(\mathbf{y}, \mathbf{y}') = \begin{bmatrix} \mathbf{f} \\ \\ \mathbf{g} \end{bmatrix} = \mathbf{0}, \tag{4.30}$$

where

$$\begin{aligned} f_j &= \frac{\Delta z}{\Delta t} \sum_{i=0}^{p} \lambda_j \theta_j^{n_t+1-i} - \left(\frac{K(\psi_{j+1}^{n_t+1}) + K(\psi_j^{n_t+1})}{2} \right) \left(\frac{\psi_{j+1}^{n_t+1} - \psi_j^{n_t+1}}{\Delta z} \right) \\ &\quad + \left(\frac{K(\psi_j^{n_t+1}) + K(\psi_{j-1}^{n_t+1})}{2} \right) \left(\frac{\psi_j^{n_t+1} - \psi_{j-1}^{n_t+1}}{\Delta z} \right) - \frac{K(\psi_{j+1}^{n_t+1}) - K(\psi_{j-1}^{n_t+1})}{2}, \\ g_j &= \theta_j^{n_t+1} - \theta_r + (\theta_r - \theta_s) S_e(\psi_j^{n_t+1}). \end{aligned} \tag{4.31}$$

Since we now have a system of nonlinear equations for which we would like to find roots, we apply Newton's method. The Jacobian for this system of equations is given by

$$J = \frac{\partial \mathbf{F}}{\partial \mathbf{y}^{n_t+1}} = \begin{bmatrix} \frac{\partial \mathbf{f}}{\partial \theta} & \frac{\partial \mathbf{f}}{\partial \psi} \\ \\ \frac{\partial \mathbf{g}}{\partial \theta} & \frac{\partial \mathbf{g}}{\partial \psi} \end{bmatrix}^{n_t+1} \tag{4.32}$$

where

$$\left[\frac{\partial \mathbf{f}}{\partial \theta} \right]^{n_t+1} = \begin{bmatrix} \frac{\lambda_0 \Delta z}{\Delta t} & 0 & \cdots & 0 \\ 0 & \ddots & & \\ \vdots & & & \\ 0 & 0 & \cdots & \frac{\lambda_0 \Delta z}{\Delta t} \end{bmatrix}, \tag{4.33}$$

$$\left[\frac{\partial \mathbf{g}}{\partial \theta}\right]^{n_t+1} = I \tag{4.34}$$

$$\left[\frac{\partial \mathbf{f}}{\partial \psi}\right]^{n_t+1} = \begin{bmatrix} \frac{\partial f_1}{\partial \psi_1^{n_t+1}} & \frac{\partial f_1}{\partial \psi_2^{n_t+1}} & 0 & \cdots & 0 \\ \frac{\partial f_2}{\partial \psi_1^{n_t+1}} & \frac{\partial f_2}{\partial \psi_2^{n_t+1}} & \frac{\partial f_2}{\partial \psi_3^{n_t+1}} & \cdots & 0 \\ \vdots & & & & \\ 0 & \cdots & & \frac{\partial f_{J-1}}{\partial \psi_{J-2}^{n_t+1}} & \frac{\partial f_{J-1}}{\partial \psi_{J-1}^{n_t+1}} \end{bmatrix}, \tag{4.35}$$

$$\left[\frac{\partial \mathbf{g}}{\partial \psi}\right]^{n_t+1} = \begin{bmatrix} \frac{\partial g_1}{\partial \psi_1^{n_t+1}} & 0 & \cdots & 0 \\ 0 & \frac{\partial g_2}{\partial \psi_2^{n_t+1}} & \cdots & 0 \\ \vdots & & \ddots & \\ 0 & 0 & \cdots & \frac{\partial g_{J-1}}{\partial \psi_{J-1}^{n_t+1}} \end{bmatrix}, \tag{4.36}$$

where

$$\frac{\partial f_j}{\partial \psi_{j-1}^{n_t+1}} = \frac{1}{2}\left(\frac{\partial K}{\partial \psi}(\psi_{j-1}^{n_t+1})\right)\left(\frac{\psi_j^{n_t+1} - \psi_{j-1}^{n_t+1}}{\Delta z}\right) - \left(\frac{K(\psi_j^{n_t+1}) + K(\psi_{j-1}^{n_t+1})}{2\Delta z}\right) + \frac{1}{2}\left(\frac{\partial K}{\partial \psi}(\psi_{j-1}^{n_t+1})\right), \tag{4.37}$$

$$\frac{\partial f_j}{\partial \psi_j^{n_t+1}} = \frac{1}{2}\left(\frac{\partial K}{\partial \psi}(\psi_j^{n_t+1})\right)\left(\frac{\psi_{j+1}^{n_t+1} - \psi_j^{n_t+1}}{\Delta z}\right) + \left(\frac{K(\psi_{j+1}^{n_t+1}) + K(\psi_j^{n_t+1})}{2\Delta z}\right) + \frac{1}{2}\left(\frac{\partial K}{\partial \psi}(\psi_j^{n_t+1})\right)\left(\frac{\psi_j^{n_t+1} - \psi_{j-1}^{n_t+1}}{\Delta z}\right) + \left(\frac{K(\psi_j^{n_t+1}) + K(\psi_{j-1}^{n_t+1})}{2\Delta z}\right), \tag{4.38}$$

$$\frac{\partial f_j}{\partial \psi_{j+1}^{n_t+1}} = -\frac{1}{2}\left(\frac{\partial K}{\partial \psi}(\psi_{j+1}^{n_t+1})\right)\left(\frac{\psi_{j+1}^{n_t+1} - \psi_j^{n_t+1}}{\Delta z}\right) - \left(\frac{K(\psi_{j+1}^{n_t+1}) + K(\psi_j^{n_t+1})}{2\Delta z}\right) - \frac{1}{2}\left(\frac{\partial K}{\partial \psi}(\psi_{j+1}^{n_t+1})\right), \tag{4.39}$$

and

$$\frac{\partial g_j}{\partial \psi_j^{n_t+1}} = (\theta_r - \theta_s)\left(\frac{\partial S_e}{\partial \psi}(\psi_j^{n_t+1})\right). \tag{4.40}$$

Recall that

$$\frac{\partial S_e}{\partial \psi} = \begin{cases} -mn\alpha(1+(\alpha|\psi|)^n)^{-m-1}(\alpha|\psi|)^{n-1} & \psi > 0; \\ mn\alpha(1+(\alpha|\psi|)^n)^{-m-1}(\alpha|\psi|)^{n-1} & \psi \leq 0 \end{cases} \tag{4.41}$$

and

$$\begin{aligned} \frac{\partial K}{\partial \psi} = K_s \Bigg[& \frac{1}{2} S_e(\psi)^{-1/2} \frac{\partial S_e}{\partial \psi}(1-(1-S_e(\psi)^{1/m})^m)^2 \\ & +2S_e(\psi)^{1/2}(1-(1-S_e(\psi)^{1/m})^m)(1-S_e(\psi)^{1/m})^{m-1} S_e(\psi)^{1/m-1} \frac{\partial S_e}{\partial \psi} \Bigg] \end{aligned} \tag{4.42}$$

We denote this formulation as NDAE. Note that the Jacobian is expensive to compute because of the nonlinear coefficient K. In [5, 7, 10] they use techniques such as quasi-Newton methods, which approximate the Jacobian using the previous iterate, reusing the Jacobian from the previous iterate, and inexact Newton methods with preconditioned Krylov iterations, that can reduce the computational expense of computing the Jacobian. The results shown in this work for NDAE do not include these sophisticated numerical techniques.

4.4 Proposed Nonlinear DAE (PNDAE)

In this section, we propose a formulation where θ, ψ and K are independent variables.

Thus,

$$\mathbf{y} = \begin{bmatrix} \theta_1 & \dots & \theta_{J-1} & \psi_1 & \dots & \psi_{J-1} & K_1 & \dots & K_{J-1} \end{bmatrix}^T. \tag{4.43}$$

Then we have

$$\mathbf{F}(\mathbf{y}, \mathbf{y}') = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \\ \mathbf{h} \end{bmatrix} = \mathbf{0}, \tag{4.44}$$

where

$$\begin{aligned} f_j &= \frac{\Delta z}{\Delta t} \sum_{i=0}^{p} \lambda_j \theta_j^{n_t+1-i} - \left(\frac{K_{j+1}^{n_t+1} + K_j^{n_t+1}}{2} \right) \left(\frac{\psi_{j+1}^{n_t+1} - \psi_j^{n_t+1}}{\Delta z} \right) \\ &\quad + \left(\frac{K_j^{n_t+1} + K_{j-1}^{n_t+1}}{2} \right) \left(\frac{\psi_j^{n_t+1} - \psi_{j-1}^{n_t+1}}{\Delta z} \right) - \frac{K_{j+1}^{n_t+1} - K_{j-1}^{n_t+1}}{2}, \\ g_j &= \theta_j^{n_t+1} - \theta_r + (\theta_r - \theta_s) S_e(\psi_j^{n_t+1}), \\ h_j &= K_j^{n_t+1} - K_s S_e(\psi_j^{n_t+1})^{1/2} (1 - (1 - S_e(\psi_j^{n_t+1})^{1/m})^m)^2. \end{aligned} \tag{4.45}$$

Next we apply Newton's method. We must first determine the Jacobian

$$J = \frac{\partial \mathbf{F}}{\partial \mathbf{y}^{n_t+1}} = \begin{bmatrix} \frac{\partial \mathbf{f}}{\partial \theta} & \frac{\partial \mathbf{f}}{\partial \psi} & \frac{\partial \mathbf{f}}{\partial \mathbf{K}} \\ \frac{\partial \mathbf{g}}{\partial \theta} & \frac{\partial \mathbf{g}}{\partial \psi} & \frac{\partial \mathbf{g}}{\partial \mathbf{K}} \\ \frac{\partial \mathbf{h}}{\partial \theta} & \frac{\partial \mathbf{h}}{\partial \psi} & \frac{\partial \mathbf{h}}{\partial \mathbf{K}} \end{bmatrix}^{n_t+1} \tag{4.46}$$

where $\frac{\partial \mathbf{f}}{\partial \theta^{n_t+1}}$ is a $J-1 \times J-1$ diagonal matrix with $\frac{\lambda_0 dz}{dt}$ along the main diagonal, $\frac{\partial \mathbf{g}}{\partial \theta^{n_t+1}}$

and $\frac{\partial \mathbf{h}}{\partial \mathbf{K}^{n_t+1}}$ are $J-1 \times J-1$ identity matrices, $\frac{\partial \mathbf{g}}{\partial \mathbf{K}^{n_t+1}}$ and $\frac{\partial \mathbf{h}}{\partial \theta^{n_t+1}}$ are $J-1 \times J-1$ zero matrices, and $\frac{\partial \mathbf{f}}{\partial \psi^{n_t+1}}$ and $\frac{\partial \mathbf{f}}{\partial \mathbf{K}^{n_t+1}}$ are tridiagonal matrices. For $\frac{\partial \mathbf{f}}{\partial \psi^{n_t+1}}$, the subdiagonal is

$$\frac{\partial f_j}{\partial \psi_{j-1}^{n_t+1}} = -\frac{K_j^{n_t+1} + K_{j-1}^{n_t+1}}{2\Delta z}, \tag{4.47}$$

the superdiagonal is given by

$$\frac{\partial f_j}{\partial \psi_{j+1}^{n_t+1}} = -\frac{K_{j+1}^{n_t+1} + K_j^{n_t+1}}{2\Delta z}, \tag{4.48}$$

and the main diagonal is

$$\frac{\partial f_j}{\partial \psi_j^{n_t+1}} = \frac{K_{j+1}^{n_t+1} + 2K_j^{n_t+1} + K_{j-1}^{n_t+1}}{2\Delta z}. \tag{4.49}$$

For $\frac{\partial \mathbf{f}}{\partial \mathbf{K}^{n_t+1}}$, the subdiagonal is

$$\frac{\partial f_j}{\partial K_{j-1}^{n_t+1}} = \frac{h_j^{n_t+1} - h_{j-1}^{n_t+1}}{2\Delta z} + \frac{1}{2}, \tag{4.50}$$

the superdiagonal is

$$\frac{\partial f_j}{\partial K_{j+1}^{n_t+1}} = -\frac{h_{j+1}^{n_t+1} - h_j^{n_t+1}}{2\Delta z} - \frac{1}{2}, \tag{4.51}$$

and the main diagonal is

$$\frac{\partial f_j}{\partial K_j^{n_t+1}} = -\frac{h_{j+1}^{n_t+1} - 2h_j^{n_t+1} + h_{j-1}^{k+1}}{2\Delta z}. \tag{4.52}$$

We denote this formulation as PNDAE. While the Jacobian in PNDAE is much larger in dimension than NDAE, many of its elements remain constant throughout the numerical simulation. In addition, those element which must be computed for each iteration are easy computations and do not rely on function evaluations. Since most of the work comes from computing the Jacobian, this method is extremely efficient in the sense that it does not require much work to run a complete simulation.

Observations from the analytical formulation combined with results presented in Chapter 5 show that PNDAE is much more efficient than NDAE. The numerical techniques presented by Kees and Miller (2002), included sophisticated ways to increase the efficiency of computing the Jacobian. We expect that we could also apply these techniques to PNDAE with an analogous improvement in efficiency.

In this chapter we have shown both linear and nonlinear formulations from the literature which do not include the hydraulic conductivity K as an independent variable in the DAE structure. For the linear formulations, the only advantage of including K is that we can then incorporate model and data error of hydraulic conductivity into the numerical simulation. For the nonlinear formulations, including K as an independent variable in the DAE structure not only allows us to incorporate model and data error of hydraulic conductivity, it also significantly reduces the computational cost of computing the Jacobian.

Chapter 5

RESULTS AND DISCUSSION

5.1 Test Problems

To test our formulations, we use two problems which are commonly used in the literature as a standard test problems [11, **?**, 14, 10, 17]. Both problems represent a sharp front close to saturation, though Problem A never achieves saturated conditions, whereas Problem B does. Thus, Problem B represents a more difficult problem. We use problem A to illustrate various aspects of the numerical formulations and solve problem B using only the most efficient techniques found for problem A. The simulation conditions for both problems are given in Table 5.1

Note that Δt is computed as

$$\Delta t = \frac{t_{N_t} - t_0}{N} \tag{5.1}$$

where the temporal domain is $[t_0, t_{N_t}]$ and N is the number of time steps. For most formulations, we keep Δz constant and allow Δt to vary in order to examine the efficiency of each formulation.

Figure 5.1 is a representative solution of problem A which shows ψ as a function of z for $t = 0.25$ days. Similarly, Figure 5.1 is a representative solution of problem B which shows ψ as a function of z for $t = 0.2$ days.

Variable	Problem A	Problem B
θ_r	0.102	0.0930
θ_s	0.368	0.301
α (m^{-1})	3.35	5.47
n	2.0	4.26
K_s (m/day)	7.97	5.04
z (m)	[0,0.3]	[0,10]
t (days)	[0,0.25]	[0,0.2]
ψ_0 (m)	-0.1	$-z$
$\psi_{LB}(m)$	-0.1	0
$\psi_{RB}(m)$	-0.75	0.1
Δz (m)	0.0025	0.0125

TABLE 5.1 Simulation Conditions for Test Problems

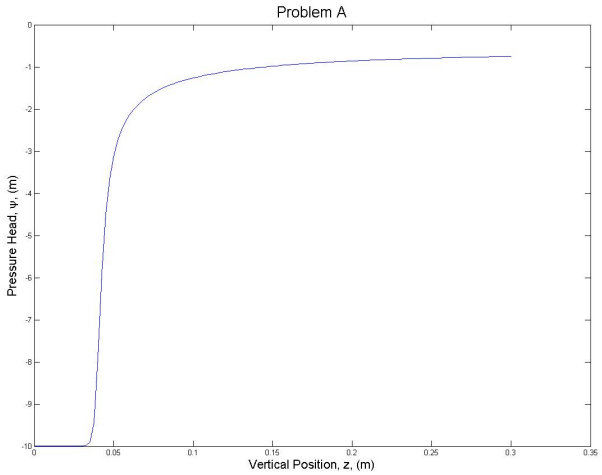

Figure 5.1. Problem A solution of ψ as a function of z for $t = 0.25$ days

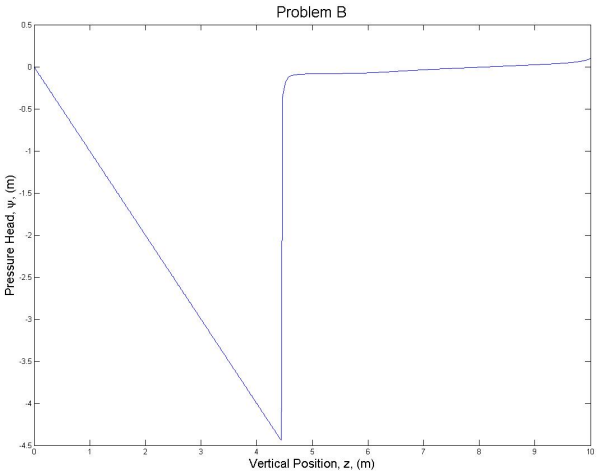

Figure 5.2. Problem B solution of ψ as a function of z for $t = 0.2$ days

5.2 Accuracy

Since no analytical solutions of the test problems exist, we must rely on our numerical models using a dense grid to formulate an "accurate" approximation. This dense

grid consists of 3841 spatial nodes for problem A, which corresponds to $\Delta z/32$. For comparison with the linear formulations, this accurate approximation, denote it by $\hat{\psi}$, is found using the modified HYDRUS formulation with variable time steps and variable order imposed. For comparison of the nonlinear formulations it is found by using the proposed nonlinear formulation, again with variable order, variable time step. The local error for each time step $n_t = 1, \ldots, N_t$ is then computed by

$$||\epsilon||_2 = \left[\frac{1}{J} \sum_{j=1}^{J+1} \left(\hat{\psi}_j^{n_t} - \psi_j^{n_t} \right)^2 \right]^{1/2} . \tag{5.2}$$

Initial numerical experiments suggested that the both Picard and Newton iterations were likely to fail during the early time steps if Δt was not chosen small enough, though often converged in later time steps using a larger Δt, given that the solutions to previous time steps converged. Thus a very small Δt and the first order method was chosen for approximations during the initial time steps. Increasing order methods and increasing Δt where then used. The details for the variable step size, variable order method for HYDRUS FE, PLDAE and NDAE for Problem A are given in Table 5.2.

Temporal Range	[0, 0.000125]	[0.000125, 0.0012]	[0.0012,0.0325]	[0.0325,0.0975]	[0.0975, 0.25]
Δt	1.0417×10^{-5}	4.1667×10^{-5}	1.6667×10^{-4}	8.3333×10^{-4}	2.5×10^{-3}
Method Order	1	2	3	4	4

TABLE 5.2: Variable Order, Variable Time Step for HYDRUS FE, PLDAE, NDAE Formulations of Problem A.

Interestingly, this variable step size, variable order technique was not helpful for the PNDAE. In fact, a constant step size of $\Delta t = 5 \times 10^{-4}$ was the most accurate

	HYDRUS FE		PLDAE		NDAE		PNDAE	
Δt (m)	Run Time(s)	Max Error	Run Time(s)	Max Error	Run Time(s)	Max Error	Run Time(s)	Max Error
2.5×10^{-3}	69	1.4475	NC	NC	NC	NC	36	1.9934
5.0×10^{-4}	313	0.8061	NC	NC	NC	NC	184	0.3188
2.5×10^{-4}	636	0.6982	NC	NC	2276	0.4363	367	0.4671
1.67×10^{-4}	1031	0.6473	NC	NC	4270	0.5077	658	0.5212
1.04×10^{-5}	run	run	4696	0.609	need	need	NC	NC

TABLE 5.3: Error and run time results for constant step size and first order BDF methods for HYDRUS FE and the nonlinear formulations NDAE and PNDAE. NC means that the method does not converge for the given Δt.

	HYDRUS FE		PLDAE		NDAE		PNDAE	
N	Run Time (s)	Max Error	Run Time (s)	Max Error	Run Time (s)	Max Error	Run Time (s)	Max Error
363	264.528	0.6137	272.580	0.6111	912.39	0.6134	NC	NC

TABLE 5.4: VOVT as given in Table 5.2 for the linear formulations HYDRUS FE and PLDAE, and the nonlinear formulation NDAE. N represents the number of time steps taken to complete the simulation. NC means the method is not convergent.

numerical solution when compared with the fine grid solution from HYDRUS FE described above. Results for constant step size using the first order BDF method and VOVT for the different formulations are shown in Tables 5.2 and 5.2. From these tables, the superiority of the VOVT is easily noted.

All of the maximum errors occurred within the range $t \in [0.0025, .025]$. This indicates that more refinement may still be needed during the initial time steps, and that an adaptive time stepping method would be useful. Such methods for RE have been studied [7]& others, although not used to generate results for this work.

5.3 Efficiency

An efficient formulation solves the test problems within a fair degree of accuracy as quickly as possible. Figures **??** and **??** show how the run time vs. the error for each formulation. From these figures we can see that the PNDAE appears to be the most efficient method.

5.4 Problem B

5.5 Conclusions

The goal of this work was to compare four different formulations of RE as its constitutive relations as a DAE. From these comparisons we can draw several conclusions for the two sharp front problems.

- By referring to Table 5.2 and Figure **??**, we see that the PLDAE is as efficient and accurate as HYDRUS FE under variable order and variable time steps.
- The PLDAE is not efficient using a constant step size. This is because the Δt required for convergence during the initial time steps is very small.
- From Table 5.2 and Figure **??**, it is clear that the PNDAE is the most efficient formulation. In general, it has already been shown that Newton iterations are more efficient than Picard iterations. Our formulations reflect this observation.
- VOVT increases the efficiency and accuracy of HYDRUS FE, PLDAE, and NDAE.

5.6 Future Work

Chapter 6

APPENDICES

6.1 Appendix I - Derivation of the Spatial Discretization

Assume the spatial domain is $[0, L]$. We divide this interval into J subintervals of length Δz. Let $z_j = j\Delta z$, $j = 0, \ldots, J$ and $\psi_j = \psi(z_j)$. By evaluating the nonlinear coefficient K exactly halfway between each interval, we can approximate the spatial

derivative (i.e. the RHS of 2.1) by

$$
\begin{aligned}
\frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z}+1\right)\right] &= \frac{\partial}{\partial z}\left[K\frac{\partial \psi}{\partial z}+K\right] \\
&= \left(\frac{\partial K}{\partial z}\right)\left(\frac{\partial \psi}{\partial z}\right)+K\left(\frac{\partial^2 \psi}{\partial z^2}\right)+\frac{\partial K}{\partial z} \\
&\approx \left(\frac{K_{j+1/2}-K_{j-1/2}}{\Delta z}\right)\left(\frac{\psi_{j+1}-\psi_{j-1}}{2\Delta z}\right) \\
&\quad +\left(\frac{K_{j+1/2}+K_{j-1/2}}{2}\right)\left(\frac{\psi_{j+1}-2\psi_j+\psi_{j-1}}{(\Delta z)^2}\right) \\
&\quad +\frac{K_{j+1/2}-K_{j-1/2}}{\Delta z} \\
&= \left(\frac{K_{j+1/2}-K_{j-1/2}}{\Delta z}\right)\left(\frac{(\psi_{j+1}-\psi_j)+(\psi_j-\psi_{j-1})}{2\Delta z}\right) \\
&\quad +\left(\frac{K_{j+1/2}+K_{j-1/2}}{2}\right)\left(\frac{(\psi_{j+1}-\psi_j)-(\psi_j-\psi_{j-1})}{(\Delta z)^2}\right) \\
&\quad +\frac{K_{j+1/2}-K_{j-1/2}}{\Delta z} \\
&= \frac{1}{\Delta z}\left[\left(\frac{K_{j+1/2}}{2}\right)\left(\frac{\psi_{j+1}-\psi_j}{\Delta z}\right)+\left(\frac{K_{j+1/2}}{2}\right)\left(\frac{\psi_j-\psi_{j-1}}{\Delta z}\right)\right. \\
&\quad -\left(\frac{K_{j-1/2}}{2}\right)\left(\frac{\psi_{j+1}-\psi_j}{\Delta z}\right)-\left(\frac{K_{j-1/2}}{2}\right)\left(\frac{\psi_j-\psi_{j-1}}{\Delta z}\right) \\
&\quad +\left(\frac{K_{j+1/2}}{2}\right)\left(\frac{\psi_{j+1}-\psi_j}{\Delta z}\right)-\left(\frac{K_{j+1/2}}{2}\right)\left(\frac{\psi_j-\psi_{j-1}}{\Delta z}\right) \\
&\quad +\left(\frac{K_{j-1/2}}{2}\right)\left(\frac{\psi_{j+1}-\psi_j}{\Delta z}\right)-\left(\frac{K_{j-1/2}}{2}\right)\left(\frac{\psi_j-\psi_{j-1}}{\Delta z}\right) \\
&\quad \left.+K_{j+1/2}-K_{j-1/2}\right] \\
&= \frac{1}{\Delta z}\left[\frac{K_{j+1/2}(\psi_{j+1}-\psi_j)}{\Delta z}-\frac{K_{j-1/2}(\psi_j-\psi_{j-1})}{\Delta z}+K_{j+1/2}-K_{j-1/2}\right].
\end{aligned}
\tag{6.1}
$$

In practice, we may not be able to evaluate K at the half interval, so we approx-

imate it by

$$K_{j+1/2} = \frac{K_{j+1} + K_j}{2}$$
$$K_{j-1/2} = \frac{K_j + K_{j-1}}{2} \tag{6.2}$$

6.2 Appendix II - Derivation of the Proposed Linear DAE (PLDAE)

The linear form of Richards' Equation which approximates the most current iterate of K is given by

$$\frac{\partial \theta^{\nu+1}}{\partial t} = \frac{\partial}{\partial z}\left[K^{\nu+1}(\psi_z^{\nu}+1) + K^{\nu}\psi_z^{\nu+1} - K^{\nu}\psi_z^{\nu}\right]. \tag{6.3}$$

If we apply our BDF scheme in time and the centered finite difference scheme in space we have

$$\begin{aligned}
\frac{\lambda_0\theta_j^{n_t+1,\nu+1}}{\Delta t} + \frac{1}{\Delta t}\sum_{i=1}^{p}\lambda_i\theta_j^{n_t+1-i} = \frac{1}{\Delta z}\Bigg[& \left(\frac{K_{j+1}^{n_t+1,\nu+1}+K_j^{n_t+1,\nu+1}}{2}\right)\left(\frac{\psi_{j+1}^{n_t+1,\nu}-\psi_j^{n_t+1,\nu}}{\Delta z}\right) \\
& - \left(\frac{K_j^{n_t+1,\nu+1}+K_{j-1}^{n_t+1,\nu+1}}{2}\right)\left(\frac{\psi_j^{n_t+1,\nu}-\psi_{j-1}^{n_t+1,\nu}}{\Delta z}\right) \\
& + \frac{K_{j+1}^{n_t+1,\nu+1}-K_{j-1}^{n_t+1,\nu+1}}{2} \\
& + \left(\frac{K_{j+1}^{n_t+1,\nu}+K_j^{n_t+1,\nu}}{2}\right)\left(\frac{\psi_{j+1}^{n_t+1,\nu+1}-\psi_j^{n_t+1,\nu+1}}{\Delta z}\right) \\
& - \left(\frac{K_j^{n_t+1,\nu}+K_{j-1}^{n_t+1,\nu}}{2}\right)\left(\frac{\psi_j^{n_t+1,\nu+1}-\psi_{j-1}^{n_t+1,\nu+1}}{\Delta z}\right) \\
& - \left(\frac{K_{j+1}^{n_t+1,\nu}+K_j^{n_t+1,\nu}}{2}\right)\left(\frac{\psi_{j+1}^{n_t+1,\nu}-\psi_j^{n_t+1,\nu}}{\Delta z}\right) \\
& + \left(\frac{K_j^{n_t+1,\nu}+K_{j-1}^{n_t+1,\nu}}{2}\right)\left(\frac{\psi_j^{n_t+1,\nu}-\psi_{j-1}^{n_t+1,\nu}}{\Delta z}\right)\Bigg].
\end{aligned} \tag{6.4}$$

Next, we expand about the unknown variables, namely the $\nu + 1$ terms:

$$\begin{aligned}
\frac{\lambda_0 \theta_j^{n_t+1,\nu+1}}{\Delta t} + \frac{1}{\Delta t}\sum_{i=1}^{p} \lambda_i \theta_j^{n_t+1-i} = \frac{1}{\Delta z}\Bigg[& \left(\frac{\psi_{j+1}^{n_t+1,\nu} - \psi_j^{n_t+1,\nu}}{2\Delta z}\right) K_{j+1}^{n_t+1,\nu+1} \\
& + \left(\frac{\psi_{j+1}^{n_t+1,\nu} - \psi_j^{n_t+1,\nu}}{2\Delta z}\right) K_j^{n_t+1,\nu+1} \\
& - \left(\frac{\psi_j^{n_t+1,\nu} - \psi_{j-1}^{n_t+1,\nu}}{2\Delta z}\right) K_j^{n_t+1,\nu+1} \\
& - \left(\frac{\psi_j^{n_t+1,\nu} - \psi_{j-1}^{n_t+1,\nu}}{2\Delta z}\right) K_{j-1}^{n_t+1,\nu+1} \\
& + \frac{1}{2} K_{j+1}^{n_t+1,\nu+1} - \frac{1}{2} K_{j-1}^{n_t+1,\nu+1} \\
& + \left(\frac{K_{j+1}^{n_t+1,\nu} + K_j^{n_t+1,\nu}}{2\Delta z}\right) \psi_{j+1}^{n_t+1,\nu+1} \\
& - \left(\frac{K_{j+1}^{n_t+1,\nu} + K_j^{n_t+1,\nu}}{2\Delta z}\right) \psi_j^{n_t+1,\nu+1} \\
& - \left(\frac{K_j^{n_t+1,\nu} + K_{j-1}^{n_t+1,\nu}}{2\Delta z}\right) \psi_j^{n_t+1,\nu+1} \\
& + \left(\frac{K_j^{n_t+1,\nu} + K_{j-1}^{n_t+1,\nu}}{2\Delta z}\right) \psi_{j-1}^{n_t+1,\nu+1} \\
& - \left(\frac{K_{j+1}^{n_t+1,\nu} + K_j^{n_t+1,\nu}}{2}\right)\left(\frac{\psi_{j+1}^{n_t+1,\nu} - \psi_j^{n_t+1,\nu}}{\Delta z}\right) \\
& + \left(\frac{K_j^{n_t+1,\nu} + K_{j-1}^{n_t+1,\nu}}{2}\right)\left(\frac{\psi_j^{n_t+1,\nu} - \psi_{j-1}^{n_t+1,\nu}}{\Delta z}\right)\Bigg].
\end{aligned} \tag{6.5}$$

Grouping like terms:

$$\begin{aligned}
\frac{\lambda_0\theta_j^{n_t+1,\nu+1}}{\Delta t}+\frac{1}{\Delta t}\sum_{i=1}^{p}\lambda_i\theta_j^{n_t+1-i} = \frac{1}{\Delta z}\Bigg[&\left(\frac{\psi_{j+1}^{n_t+1,\nu}-\psi_j^{n_t+1,\nu}}{2\Delta z}+\frac{1}{2}\right)K_{j+1}^{n_t+1,\nu+1}\\
&+\left(\frac{\psi_{j+1}^{n_t+1,\nu}-2\psi_j^{n_t+1,\nu}+\psi_{j-1}^{n_t+1,\nu}}{2\Delta z}\right)K_j^{n_t+1,\nu+1}\\
&-\left(\frac{\psi_j^{n_t+1,\nu}-\psi_{j-1}^{n_t+1,\nu}}{2\Delta z}+\frac{1}{2}\right)K_{j-1}^{n_t+1,\nu+1}\\
&+\left(\frac{K_{j+1}^{n_t+1,\nu}+K_j^{n_t+1,\nu}}{2\Delta z}\right)\psi_{j+1}^{n_t+1,\nu+1}\\
&-\left(\frac{K_{j+1}^{n_t+1,\nu}+2K_j^{n_t+1,\nu}+K_{j-1}^{n_t+1,\nu}}{2\Delta z}\right)\psi_j^{n_t+1,\nu+1}\\
&+\left(\frac{K_j^{n_t+1,\nu}+K_{j-1}^{n_t+1,\nu}}{2\Delta z}\right)\psi_{j-1}^{n_t+1,\nu+1}\\
&-\left(\frac{K_{j+1}^{n_t+1,\nu}+K_j^{n_t+1,\nu}}{2}\right)\left(frac\psi_{j+1}^{n_t+1,\nu}-\psi_j^{n_t+1,\nu}\Delta z\right)\\
&+\left(\frac{K_j^{n_t+1,\nu}+K_{j-1}^{n_t+1,\nu}}{2}\right)\left(\frac{\psi_j^{n_t+1,\nu}-\psi_{j-1}^{n_t+1,\nu}}{\Delta z}\right)\Bigg].
\end{aligned} \tag{6.6}$$

$$
\begin{aligned}
&\left(\frac{\Delta z}{\Delta t}\right)\lambda_0\theta_j^{n_t+1,\nu+1} - \left(\frac{\psi_{j+1}^{n_t+1,\nu} - \psi_j^{n_t+1,\nu}}{2\Delta z} + \frac{1}{2}\right)K_{j+1}^{n_t+1,\nu+1} \\
&\quad - \left(\frac{\psi_{j+1}^{n_t+1,\nu} - 2\psi_j^{n_t+1,\nu} + \psi_{j-1}^{n_t+1,\nu}}{2\Delta z}\right)K_j^{n_t+1,\nu+1} + \left(\frac{\psi_j^{n_t+1,\nu} - \psi_{j-1}^{n_t+1,\nu}}{2\Delta z} + \frac{1}{2}\right)K_{j-1}^{n_t+1,\nu+1} \\
&\quad - \left(\frac{K_{j+1}^{n_t+1,\nu} + K_j^{n_t+1,\nu}}{2\Delta z}\right)\psi_{j+1}^{n_t+1,\nu+1} + \left(\frac{K_{j+1}^{n_t+1,\nu} + 2K_j^{n_t+1,\nu} + K_{j-1}^{n_t+1,\nu}}{2\Delta z}\right)\psi_j^{n_t+1,\nu+1} \\
&\quad - \left(\frac{K_j^{n_t+1,\nu} + K_{j-1}^{n_t+1,\nu}}{2\Delta z}\right)\psi_{j-1}^{n_t+1,\nu+1} \\
&= -\left(\frac{\Delta z}{\Delta t}\right)\sum_{i=1}^{p}\theta_j^{n_t+1-i} - \left(\frac{K_{j+1}^{n_t+1,\nu} + K_j^{n_t+1,\nu}}{2}\right)\left(\frac{\psi_{j+1}^{n_t+1,\nu} - \psi_j^{n_t+1,\nu}}{\Delta z}\right) \\
&\quad + \left(\frac{K_j^{n_t+1,\nu} + K_{j-1}^{n_t+1,\nu}}{2}\right)\left(\frac{\psi_j^{n_t+1,\nu} - \psi_{j-1}^{n_t+1,\nu}}{\Delta z}\right).
\end{aligned}
\tag{6.7}
$$

Van Genuchten's Equation is given by

$$
\theta = \theta_r + (\theta_s - \theta_r)S_e(\psi), \tag{6.8}
$$

where

$$
S_e(\psi) = (1 + (\alpha|\psi|)^n)^{-m}. \tag{6.9}
$$

Since $S_e(\psi)$ is nonlinear in ψ we linearize $S_e(\psi^{\nu+1})$ using the first order Taylor series expansion about the point ψ^{ν}:

$$
\begin{aligned}
S_e(\psi^{\nu+1}) &\approx S_e(\psi^{\nu}) + \left(\left.\frac{\partial S_e}{\partial \psi}\right|_{\psi^{\nu}}\right)(\psi^{\nu+1} - \psi^{\nu}) \\
&= S_e(\psi^{\nu}) + \left(\left.\frac{\partial S_e}{\partial \psi}\right|_{\psi^{\nu}}\right)\psi^{\nu+1} - \left(\left.\frac{\partial S_e}{\partial \psi}\right|_{\psi^{\nu}}\right)\psi^{\nu},
\end{aligned}
\tag{6.10}
$$

where

$$\frac{\partial S_e}{\partial \psi} = \begin{cases} -mn\alpha \left(1 + (\alpha|\psi|)^n\right)^{-m-1} (\alpha|\psi|)^{n-1} & \psi \geq 0 \\ mn\alpha \left(1 + (\alpha|\psi|)^n\right)^{-m-1} (\alpha|\psi|)^{n-1} & \psi < 0 \end{cases} \tag{6.11}$$

The linear form of Van Genuchten's Equation is given by

$$\theta^{\nu+1} = \theta_r + (\theta_s - \theta_r) \left[S_e(\psi^\nu) + \left(\frac{\partial S_e}{\partial \psi}\bigg|_{\psi^\nu} \right) \psi^{\nu+1} - \left(\frac{\partial S_e}{\partial \psi}\bigg|_{\psi^\nu} \right) \psi^\nu \right]. \tag{6.12}$$

Applying the temporal and spatial discretization and regrouping gives

$$\theta_j^{n_t+1,\nu+1} + (\theta_r - \theta_s) \left(\frac{\partial S_e}{\partial \psi}\bigg|_{\psi_j^{n_t+1,\nu}} \right) \psi_j^{n_t+1,\nu+1} = \theta_r + (\theta_s - \theta_r) \left[S_e(\psi_j^{n_t+1,\nu}) - \left(\frac{\partial S_e}{\partial \psi}\bigg|_{\psi_j^{n_t+1,\nu}} \right) \psi_j^{n_t+1,\nu} \right] \tag{6.13}$$

We employ the same technique to Mualem's Equation, which is given by

$$K = K_s S_e(\psi)^{1/2} \left[1 - (1 - S_e(\psi)^{1/m})^m \right]^2. \tag{6.14}$$

Since K is nonlinear, we linearize $K_s S_e(\psi^{\nu+1})^{1/2} \left[1 - (1 - S_e(\psi^{\nu+1})^{1/m})^m \right]^2$ about

the point ψ^ν:

$$\begin{aligned} K_s S_e(\psi^{\nu+1})^{1/2}\left[1-(1-S_e(\psi^{\nu+1})^{1/m})^m\right]^2 \approx K_s S_e(\psi^\nu)^{1/2}\left[1-(1-S_e(\psi^\nu)^{1/m})^m\right]^2 \\ \left.\frac{\partial K}{\partial \psi}\right|_{\psi^\nu}(\psi^{\nu+1}-\psi^\nu) \\ = K_s S_e(\psi^\nu)^{1/2}\left[1-(1-S_e(\psi^\nu)^{1/m})^m\right]^2 \\ \left.\frac{\partial K}{\partial \psi}\right|_{\psi^\nu}\psi^{\nu+1} - \left.\frac{\partial K}{\partial \psi}\right|_{\psi^\nu}\psi^\nu), \end{aligned} \tag{6.15}$$

where

$$\begin{aligned} \frac{\partial K}{\partial \psi} = K_s\Bigg[&\frac{1}{2}S_e(\psi)^{-1/2}\frac{\partial S_e}{\partial \psi}(1-(1-S_e(\psi)^{1/m})^m)^2 \\ &+2S_e(\psi)^{1/2}(1-(1-S_e(\psi)^{1/m})^m)(1-S_e(\psi)^{1/m})^{m-1}S_e(\psi)^{1/m-1}\frac{\partial S_e}{\partial \psi}\Bigg] \end{aligned} \tag{6.16}$$

If we apply the spatial and temporal discretizations, we get

$$\begin{aligned} K_j^{n_t+1,\nu+1} - \left(\left.\frac{\partial K}{\partial \psi}\right|_{\psi_j^{n_t+1,\nu}}\right)\psi_j^{n_t+1,\nu+1} = K_s S_e(\psi_j^{n_t+1,\nu})^{1/2}[1-(1-S_e(\psi_j^{n_t+1,\nu})^{1/m})^m]^2 \\ - \left(\left.\frac{\partial K}{\partial \psi}\right|_{\psi_j^{n_t+1,\nu}}\right)\psi_j^{n_t+1,\nu} \end{aligned} \tag{6.17}$$

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