

# RESolve – application to Johnstown Castle

Lennon Ó Náraigh, Saurabh Kumar\*

*School of Mathematics and Statistics,  
University College Dublin, Belfield, Dublin 4, Ireland*

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## I. INTRODUCTION

In this report we examine the time series data of tensiometer readings for Johnstown Castle, Co. Wexford, from January 1st 1998 – December 1st 2000, taken from the paper by Diamond and Sills [1]. We perform nonlinear optimization and fit the pressure-head readings at 15 cm depth to the data for the years 1998 – 1999 (two years). We use the year 2000 for validation. Meteorological inputs (daily rainfall, solar radiation and temperature) are taken from the available Met Éireann climate data [2] (Station number 915, open 1914, closed 2009) These are used to compute the top boundary condition (governed by rainfall) and the evapotranspiration (governed by wind speed and relative humidity).

## II. MATHEMATICAL MODEL

We use the 1D Richards Equation to model the flow of moisture in a soil column. The equation is given here as:

$$\frac{\partial \theta(h)}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} + 1 \right) \right] - \lambda(h, z, t), \quad z \in (0, L), \quad t > 0, \quad (1)$$

where

- $\theta(h)$  is the volumetric water content in notional units of  $\text{m}^3/\text{m}^3$ ;
- $h$  is the pressure head in units of m. The pressure head is negative in unsaturated conditions;  $h = 0$  indicates saturation;
- $K(h)$  is the hydraulic conductivity, in units of  $\text{m} \cdot \text{s}^{-1}$ ;
- $\lambda$  is a sink term representing evapo-transpiration (ET), in units of  $\text{s}^{-1}$ ;
- $z$  is the vertical coordinate, increasing upward with  $z = 0$  at the bottom and  $z = L$  at the soil surface.

This sign convention follows the Hydrus system. The same convention is used in the standard paper on the solution of the Richards equation by Dogan and Motz [3]. The gravity term therefore appears with a positive sign (as  $K(h)$ ) in the flux expression. For the avoidance of doubt, the flux is:

$$f = K(h) \left( \frac{\partial h}{\partial z} + 1 \right). \quad (2)$$

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\* Corresponding author. Email: onaraigh@maths.ucd.ie

### A. Numerical Solution Using PDEPE

We use Matlab's built-in PDE solver `pdepe` to solve the Richards Equation (1), as documented elsewhere.

### B. Soil Hydraulic Functions: van Genuchten model

To close the Richards equation, constitutive relationships are required for the soil the unsaturated hydraulic conductivity, among other things. We use the van Genuchten–Mualem (VG) model for this purpose. We first of all introduce the effective saturation:

$$S_e(h) = \begin{cases} \frac{\theta(h) - \theta_r}{\theta_s - \theta_r}, & h < 0, \\ 1, & h \geq 0, \end{cases} \quad (3)$$

where  $\theta_r$  and  $\theta_s$  are the residual and saturated water contents. Here,  $\theta_r$  and  $\theta_s$  are limiting values corresponding to a residual saturation under dry conditions, and a saturated condition. Hence,  $\theta_r \leq \theta \leq \theta_s$ . Correspondingly,  $0 \leq S_e \leq 1$ . For negative heads corresponding to unsaturated soils, the VG model links  $h$  to  $S_e$  via the relation:

$$S_e(h) = [1 + (\alpha|h|)^n]^{-m}, \quad (4)$$

Equation (4) describes the so-called **water-retention curve**. Here,  $\alpha$  is the air-entry pressure and is a parameter of the model. Also,

$$m = 1 - \frac{1}{n}, \quad \alpha > 0, \quad n > 1, \quad (5)$$

and  $n$  is a further model parameter. The volumetric water content then follows as

$$\theta(h) = \theta_r + S_e(\theta_s - \theta_r). \quad (6)$$

Finally, the permeability is given by:

$$K(h) = K_s S_e^\ell \left[ 1 - \left( 1 - S_e^{1/m} \right)^m \right]^2, \quad (7)$$

where  $K_s$  is the saturated hydraulic conductivity and  $\ell$  is the pore-connectivity parameter (commonly  $\ell = 0.5$ ).

In practice, it is better to solve the Richards Equation in the variable  $h$ . Therefore, Equation (1) is re-arranged. We have:

$$\frac{\partial \theta}{\partial t} = \frac{\partial \theta}{\partial h} \frac{\partial h}{\partial t}. \quad (8)$$

Here,  $\partial h / \partial \theta$  is computed analytically from Equation (6). In practice, we identify the capacity  $C(h)$ :

$$C(h) = (\theta_s - \theta_r) \frac{dS_e}{dh} + \theta \rho g (c_r + c_w), \quad (9)$$

and we solve the following PDE in place of Equation (1):

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} + 1 \right) \right] - \lambda(h, z, t), \quad z \in (0, L), \quad t > 0, \quad (10)$$

Here, following Mathis et al. [4],  $\rho g (c_r + c_w)$  is taken to be  $9.81 \times 10^{-7} \text{ m}^{-1}$ .

### C. Sink Term for Evapotranspiration

The sink term  $\lambda(h, z, t)$  accounts for water removal due to plant root uptake and/or soil surface evaporation. We follow the work by Mathias et al. [4] and use a Feddes-type reduction function, whereby

$$\lambda(z, t) = E_p(t)\phi_1(z)\phi_2(h) \quad (11)$$

Here,  $E_p(t)$  is the potential evaporation, which is obtained from meteorological conditions. The term  $\phi_1$  is the root function, which describes the distribution of roots in the soil column. We use:

$$\phi_1(z) = \begin{cases} \frac{a}{L_r} \left[ \frac{e^{-a} - e^{-az_M/L_r}}{(1+a)e^{-a} - 1} \right], & 0 \leq z_M \leq L_r, \\ 0, & z_M > L_r. \end{cases} \quad (12)$$

Here, we have momentarily used the Mathias convention for the vertical coordinate, with  $z_M = L - z$ , such that  $z_M = 0$  corresponds to the surface. The parameters  $a$  (dimensionless) and  $L_r$  (units of m) characterize the root distribution. We use values characteristic of grass:  $a = 1.55$  and  $L_r = 0.25$  m.

In this work, we use a simplified version of the plant stress function, loosely inspired by Feddes et al. [5]. Hence, we look at the range  $\theta_s - \theta_r$ , and we divide the range into intervals of length  $\Delta\theta = (\theta_s - \theta_r)/5$ . We introduce  $\theta_i = i\Delta\theta$ , where  $i \in \{1, 2, 3, 4\}$ . We write down the plant stress function in the  $\theta$  space:

$$\phi_2(\theta) = \begin{cases} 0, & \theta \leq \theta_1, \\ \frac{\theta - \theta_1}{\theta_2 - \theta_1}, & \theta \leq \theta_2, \\ 1, & \theta \leq \theta_3, \\ 1 - \frac{\theta - \theta_3}{\theta_4 - \theta_3}, & \theta \leq \theta_4, \\ 0, & \text{otherwise.} \end{cases} \quad (13)$$

This simplifies the analysis, and prevents parameter mismatch whereby the plant stress function could potentially be non-zero for values of  $\theta$  less than  $\theta_r$ , which would be unphysical, and could lead to code blow-up. This is an important factor when performing optimization, in which case the code samples unknown regions of parameter space, where such a parameter mismatch could occur.

### D. Boundary Conditions

For Johnstown Castle, the tensiometer readings reveal that the soil remains close to saturation year round at a depth 1.2 m. Consequently, we apply a **saturation boundary condition** at the bottom, which we set as  $L = 1.2$  m. Thus, we have:

$$h = h_{ref}, \quad z = 0. \quad (14)$$

Here,  $h_{ref}$  is a constant reference level. To describe a saturated soil at  $z = 0$ , in principle we would take  $h_{ref} = 0$ . However, we define ‘numerical saturation’ slightly differently from  $h = 0$  as Equation (10) may have trouble handling the extreme cases  $\theta = \theta_s$  (corresponding to  $h = 0$ ) and  $\theta = \theta_r$  (corresponding to  $h = -\infty$ ). Consequently, we introduce a ‘numerical saturation level’  $h_{ref}$ , such that:

$$\theta(h_{ref}) = 0.999\theta_s. \quad (15)$$

Here,  $\theta(h_{ref})$  is evaluated using Equation (6) Because Matlab's `pdepe` cannot handle a true ponding condition, for the top, we look at a **pseudo-ponding condition**:

$$f(L, t) = f_{rain}(t), \text{ if } f_{rain}(t) < f_{max}, \quad (16a)$$

$$h(L, t) = h_{ref}, \text{ otherwise.} \quad (16b)$$

where  $f_{max}$  is a fixed maximum infiltration flux, which is viewed as a model paramter, to be set *ab initio*. We take  $f_{max}$  as:

$$f_{max} = 8 \times 10^{-8} \text{ m} \cdot \text{s}^{-1}, \quad (17)$$

hence  $f_{max} = 6.9 \text{ mm} \cdot \text{day}^{-1}$ . This value is chosen because it leads to saturation at the top for around 75 days per year, consistent with observations at Johnstown Castle [1] (Table 7 and Table 9 therein).

### E. Initial Conditions

The initial pressure head distribution is specified as

$$h(z, 0) = h_{ref}, \quad (18)$$

corresponding to saturation throughout the soil layer. Initial conditions are set on January 1st 1997 and correspond to full saturation of the soil column. The first year of simulation time (all of 1997) is used for ‘burn-in’ so that the simulation effectively ‘forgets’ this arbitrary initial condition.

## III. OPTIMIZATION

We have digitized the tensiometer data for Johnstown Castle from Reference [1]. We single out dates on and after Jan 1st 1998 for special study. We break up the simulation as follows:

- One year (1997) for ‘burn-in’, so that the simulation ‘forgets’ the arbitrary initial condition. In this period, the model neither uses nor references the tensiometer data. However, meteorological data is used in this period, for the top BC and the evapotranspiration model.
- Two years (1998,1999) for training, where the model is fitted to the data.
- Subsequent years (e.g. 2000) for testing, to compare the model’s prediction with the data.

Rainfall data for these days are obtained from the Johnstown Castle weather station, together with solar radiation and temperature [2]. Potential evapotranspiration  $E_p$  is modelled using the Hargreaves–Samani equation, a temperature-based method that provides reliable PET predictions when limited meteorological data are available. The formulation relates PET to the extraterrestrial solar radiation  $R_a$  and the daily temperature range, and is expressed as

$$E_p = 0.0023 R_a (T_{\text{mean}} + 17.8) (T_{\text{max}} - T_{\text{min}})^{0.5}, \quad (19)$$

TABLE I. Estimated van Genuchten Parameters for Johnstown Castle

Parameter	Symbol	Value
Residual water content	$\theta_r$	0.08
Saturated water content	$\theta_s$	0.4
VG parameter	$n$	1.4
Pore-connectivity parameter	$\ell$	0.5

where  $T_{\text{mean}}$ ,  $T_{\text{max}}$ , and  $T_{\text{min}}$  are the mean, maximum, and minimum air temperatures ( $^{\circ}\text{C}$ ), respectively. Also,  $R_a$  is the solar radiation in units of  $\text{MJ} \cdot \text{m}^{-2} \cdot \text{day}^{-1}$  meaning that overall,  $E_p$  has units of  $\text{mm} \cdot \text{day}^{-1}$ .

We estimate the VG parameters  $n$ ,  $\theta_r$ , and  $\theta_s$  using ROSETTA and the characterization of the soil given in Diamond and Sills [1]. We also take  $\ell = 0.5$  which is standard. Values are given in Table I. We allow for uncertainty in the values of  $K_{\text{sat}}$  and  $\alpha$  by taking these in the range  $[10^{-6}, 5 \times 10^{-6}] \text{m} \cdot \text{s}^{-1}$  and  $[0.7, 1] \text{m}^{-1}$ , respectively. We then perform a nonlinear least-squares fitting in these parameters using the cost function

$$J(K_{\text{sat}}, \alpha) = \frac{1}{2 \text{ years}} \int_{\text{Jan 1st 1998}}^{\text{Dec 31st 1999}} [h_{\text{model}}(15 \text{ cm depth}, t) - h_{\text{obs}}(15 \text{ cm depth}, t)]^2 dt. \quad (20)$$

We use Matlab's `surrogateopt` surrogate optimization function to pick out a minimum. Cost-function evaluations are done in parallel by passing appropriate options to `surrogateopt`:

```
opts = optimoptions('surrogateopt', ...
    'UseParallel', true, ...
    'Display', 'iter', ...           % Show iteration info
    'MaxFunctionEvaluations', 50); % Limit costly PDE calls for test runs
```

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