Supplementary Material

Open-source high-performance toolbox for direct and inverse solving of horizontal infiltration equation

Gabriel S. Gerlero[1], Claudio L. A. Berli[2], and Pablo A. Kler[1,3]

[1]Centro de Investigación de Métodos Computacionales (CIMEC, UNL–CONICET), Colectora RN 168 km 472, (3000) Santa Fe, Argentina

[2]Instituto de Desarrollo Tecnológico para la Industria Química (INTEC, UNL–CONICET), Colectora RN 168 km 472, (3000) Santa Fe, Argentina

[3]Departamento de Ingeniería en Sistemas de Información, Facultad Regional Santa Fe, Universidad Tecnológica Nacional, Lavaisse 610, (3000) Santa Fe, Argentina

1 Porous media fluid flow models

In this section, the expressions that were used to implement the various unsaturated flow models in *Fronts* are presented.

1.1 Brooks and Corey

The Brooks and Corey model defines the following correlation between pressure head h and moisture content θ [1]:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{|\alpha h|^n}, \tag{1}$$

and, for hydraulic conductivity K:

$$K = K_s \left(\frac{1}{|\alpha h|^n} \right)^{\frac{2}{n}+l+2}, \tag{2}$$

so that the moisture diffusivity function D for capillary flow is:

$$D(\theta) = K\frac{dh}{d\theta} = \frac{K_s}{\alpha} \frac{1}{n(\theta_s - \theta_r)} \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{\frac{1}{n}+l+1}. \tag{3}$$

1.2 Van Genuchten

The Van Genuchten model defines [1]:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{(1 + |\alpha h|^n)^m}, \tag{4}$$

and:

$$K = K_s \Theta^l \left(1 - \left(1 - \Theta^{\frac{1}{m}} \right)^m \right)^2, \tag{5}$$

both with $m = 1 - 1/n$ and $\Theta = (\theta - \theta_r)/(\theta_s - \theta_r)$, so that:

$$D(\theta) = \frac{Ks}{\alpha} \frac{(1-m)}{m(\theta_s - \theta_r)} \Theta^{l-\frac{1}{m}} \left(\left(1 - \Theta^{\frac{1}{m}} \right)^{-m} + \left(1 - \Theta^{\frac{1}{m}} \right)^m - 2 \right). \tag{6}$$

1.3 LET

For the model that uses the LET correlations, we define hydraulic conductivity with the LETx formula [2] as:

$$K = K_s \frac{S_{wp}^{L_w}}{S_{wp}^{L_w} + E_w(1 - S_{wp})^{T_w}}, \tag{7}$$

where S_{wp} depends on the saturation S_w (or moisture content θ) via:

$$S_{wp} = \frac{S_w - S_{wir}}{1 - S_{wir}} = \frac{\theta - \theta_r}{\theta_s - \theta_r}. \tag{8}$$

Additionally, we can use a LETs function [2], which relates saturation and pressure under spontaneous imbibition:

$$P_c = P_{cir} \frac{(1 - S_{ws})^{L_s}}{(1 - S_{ws})^{L_s} + E_s S_{ws}^{T_s}} \tag{9}$$

In order to combine both expressions, we first assume that $S_{ws} = S_{wp}$. Then, considering that the pressure head is $h = \gamma P_c$ (with γ the specific weight of the fluid), and defining $\alpha \equiv \gamma / P_{cir}$, we obtain the expression for the moisture diffusivity [3]:

$$D(\theta) = \frac{K_s}{\alpha} \frac{E_s S_{wp}^{L_w} S_{wp}^{T_s} (1 - S_{wp})^{L_s} (L_s S_{wp} - S_{wp} T_s + T_s)}{\theta_s S_{wp} (S_{wir} - 1)(S_{wp} - 1) \left(E_s S_{wp}^{T_s} + (1 - S_{wp})^{L_s}\right)^2 \left(E_w (1 - S_{wp})^{T_w} + S_{wp}^{L_w}\right)}. \tag{10}$$

1.4 LETd

The simplified LETd model uses the following expression for capillary flow [3]:

$$D(\theta) = D_{wt} \frac{S_{wp}^{L}}{S_{wp}^{L} + E(1 - S_{wp})^{T}}, \tag{11}$$

with S_{wp} defined as in Eq. (8).

2 Alternative formulations of Boltzmann-transformed equations

The general form of the transient nonlinear diffusion equation as presented in the main paper is:

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \left[D(\theta) \frac{\partial \theta}{\partial r} \hat{\mathbf{r}} \right] \tag{12}$$

which, where $\hat{\mathbf{r}}$ is a Cartesian coordinate unit vector (or the axial coordinate unit vector in a cylindrical coordinate system), is equivalent to:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial r} \left(D(\theta) \frac{\partial \theta}{\partial r} \right) \tag{13}$$

and can be converted by applying the Boltzmann transformation into the ordinary differential form shown in the main text.

2.1 Radial coordinates

Eq. (12) is also susceptible to the Boltzmann transformation when $\hat{\mathbf{r}}$ is a radial coordinate unit vector in a cylindrical or spherical coordinate system. In these cases, the expression is equivalent to:

$$\frac{\partial \theta}{\partial t} = \frac{1}{r^{m-1}} \frac{\partial}{\partial r} \left(r^{m-1} D(\theta) \frac{\partial \theta}{\partial r} \right) \tag{14}$$

with $m = 2$ in cylindrical coordinates and $m = 3$ in spherical coordinates. These transform into the ordinary differential expression:

$$-\frac{\phi}{2} \frac{d\theta}{d\phi} = \frac{m-1}{\phi} D(\theta) \frac{d\theta}{d\phi} + D(\theta) \frac{d^2\theta}{d\phi^2} + \frac{dD}{d\theta} \left(\frac{d\theta}{d\phi} \right)^2 \tag{15}$$

The radial forms have been implemented in *Fronts*, even though they are not as versatile due to being more restricted in terms of which boundary conditions are applicable in practice (see Section 3.2), including the fact that they are singular at $\phi = 0$. However, the radial–cylindrical ($m = 2$) case is of special interest insofar it can support a fixed-flowrate boundary condition, which will be described in Section 3.2.2.

2.2 Integral expression for the diffusivity

The integral expression that is the basis of the “inverse” feature of *Fronts* is derived here. For this, we start with Eq. (13) and use the product rule in reverse to obtain:

$$-\frac{\phi}{2} \frac{d\theta}{d\phi} = \frac{d}{d\phi} \left(D(\theta) \frac{d\theta}{d\phi} \right) \tag{16}$$

Subsequently, a mathematical procedure known as Bolztmann–Matano analysis may be applied [4]. The previous equation is multiplied by $d\phi/d\theta$:

$$-\frac{\phi}{2} = \frac{d}{d\theta} \left(D(\theta) \frac{d\theta}{d\phi} \right) \tag{17}$$

Integrating both sides in θ from the initial value θ_i gives:

$$-\frac{1}{2} \int_{\theta_i}^{\theta} \phi \, d\theta = D(\theta) \frac{d\theta}{d\phi} - D(\theta_i) \frac{d\theta}{d\phi} \bigg|_{\theta_i} \tag{18}$$

where the rightmost term is neglected given that $d\theta/d\phi \to 0$ as $\theta \to \theta_i$ (see Section 3.1), so that solving for D yields the final expression:

$$D(\theta) = -\frac{1}{2} \frac{d\phi}{d\theta} \int_{\theta_i}^{\theta} \phi \, d\theta \tag{19}$$

2.3 Pressure-based Richards equation

The moisture diffusivity equation is in fact a special case of the Richards equation for flow in unsaturated porous media [5]. While the moisture diffusivity equation can only describe spontaneous capillary-driven flow as explained by a moisture content–dependent diffusivity, the Richards equation distinguishes between the effect of hydraulic conductivity and that of pressure in accounting for the motion of the fluid. The segregation of the pressure field allows for modeling external pressure–driven flow concurrent with capillary flow. The horizontal (i.e., gravity neglected) case of such equation, which can be expressed as:

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial r} \left(K(h) \frac{\partial h}{\partial r} \right) \tag{20}$$

is also compatible with the Boltzmann transformation, susceptible to being rewritten as:

$$-C(h) \frac{\phi}{2} \frac{dh}{d\phi} = K(h) \frac{d^2 h}{d\phi^2} + \frac{dK}{dh} \left(\frac{dh}{d\phi} \right)^2 \tag{21}$$

where h is the pressure head field, $K(h)$ the hydraulic conductivity function that accounts for shifting medium permeabilities under changes in saturation or pressure, and $C(h) \equiv dh/d\theta$ the hydraulic "capacity" function that relates moisture content and pressure. Eq. (13) can be recovered from this formulation by defining $D \equiv K/C$.

The Julia version of *Fronts* implements functionality to solve problems of this equation too, using the same solvers and boundary conditions and with $C(h)$ and $K(h)$ as arbitrary functions, possibly obtained from the built-in porous models as described in Section 1. The analogous radial forms of Eq. (20) (c.f. Section 2.1) are also compatible with the Boltzmann transformation and have been implemented as well.

3 Initial and boundary conditions

3.1 Initial condition

Application of the Boltzmann transformation to the initial condition is covered in the main paper. We note that the limit of $\theta \to \theta_i$ as $\phi \to \infty$ also implies that $d\theta/d\phi \to 0$ at the same limit.

3.2 Boundary conditions

For more generality when dealing with boundary conditions, we shall define a boundary position function r_b, parameterized by a constant ϕ_b:

$$r_b(t) = \phi_b \sqrt{t} \tag{22}$$

The main purpose of this function is to accommodate the radial equations (Section 2.1), which are otherwise singular at $r = 0$. In non-radial coordinates, the obvious case of a boundary fixed at $r = 0$ appears as a special case when $\phi_b = 0$. On the other hand, $\phi_b \neq 0$ implies the existence of a moving boundary, its movement controlled by the value of ϕ_b.

3.2.1 Dirichlet boundary condition

The general form of a Dirichlet condition with value θ_b at the boundary:

$$\theta(r_b(t), t) = \theta_b \tag{23}$$

transforms into the following condition for the univariate function at $\phi = \phi_b$:

$$\theta(\phi = \phi_b) = \theta_b \tag{24}$$

This form of the Dirichlet boundary condition is usable with both radial and non-radial forms; however, in actual scenarios the practicality of imposing a fixed θ value is mostly limited to non-radial cases with $\phi_b = 0$.

3.2.2 Flowrate boundary condition

In a radial–cylindrical case in particular, a fixed-flowrate condition that prescribes a rate of flow Q_b at the boundary:

$$Q(r_b(t), t) = Q_b \tag{25}$$

is also compatible with the Boltzmann transformation, as it transforms into:

$$-D(\theta(\phi_b))\ \phi_b \left.\frac{d\theta}{d\phi}\right|_{\phi_b} = \frac{Q_b}{\Delta\varphi \Delta z} \tag{26}$$

where $0 < \Delta\varphi \leq 2\pi$ is the central angle and Δz the axial height. If $\phi_b \to 0$, this boundary condition can in effect model a line source or sink at $r = 0$ [6]. In practice, the line source/sink scenario with this boundary condition is implemented in *Fronts* by allowing ϕ_b to take on some small value (10^{-6} by default).

3.2.3 Cauchy boundary condition

A different type of boundary condition is that which prescribes the values of both θ and $d\theta/d\phi$ at the boundary (with no specification of an initial condition, as that would result in an overdetermined problem). This constitutes a Cauchy boundary condition and is used internally as part of the shooting algorithm in the solvers (every iteration consisting of an attempt to solve a Cauchy problem). It is exposed as an accessible problem type in the Julia implementation of *Fronts*, as it may be used as an optimization in parameter estimation runs where the initial condition is unknown in order to sidestep the shooting algorithm where it is not strictly necessary.

References

[1] Qi Li, Kazumasa Ito, Zhishen Wu, Christopher S Lowry, and Steven P Loheide II. COMSOL Multiphysics: A novel approach to ground water modeling. *Groundwater*, 47(4):480–487, 2009.

[2] Frode Lomeland. Overview of the LET family of versatile correlations for flow functions. In *Proceedings of the International Symposium of the Society of Core Analysts*, pages SCA2018–056, 2018.

[3] Gabriel S Gerlero, Andrés R Valdez, Raúl Urteaga, and Pablo A Kler. Validity of capillary imbibition models in paper-based microfluidic applications. *Transport in Porous Media*, 141 (2):359–378, 2022.

[4] P J Tumidajski and G W Chan. Boltzmann-Matano analysis of chloride diffusion into blended cement concrete. *Journal of Materials in Civil Engineering*, 8(4):195–200, 1996.

[5] Jacob Bear and Alexander H-D Cheng. *Modeling groundwater flow and contaminant transport*, volume 23. Dordrecht, Netherlands, Springer Science & Business Media, 2010.

[6] Arthur L Ruoff, Denver L Prince, J Calvin Giddings, and George H Stewart. The diffusion analogy for solvent flow in paper. *Kolloid-Zeitschrift*, 166(2):144–151, 1959.