Physically-based model of soil hydraulic properties accounting for variable contact angle and its effect on hysteresis

Estathios Diamantopoulos & Wolfgang Durner  | e.diamantopoulos@tu-bs.de  | Phone +49 (0) 531 393-9931  | Technische Universität Braunschweig  | Institut für Geokolologie  | Langer Kamp 19c  | 38106 Braunschweig

Why do we need a new model?

Diamantopoulos et al. (2013). J. Hydrol, 468, 173-188. Aims to explore impact of drainage for the same soil using water and ethanol as liquids. The drainage curves for water were similar to those of ethanol, but the imbibition curves differed substantially. Thus, different hysteresis was observed for liquid saturation vs pressure head curves. Assuming that ethanol forms a zero contact angle with the soil grains, ethanol hysteresis was attributed to geometric factors alone. We hypothesize that the greater hysteresis of water is caused by a non-zero advancing contact angle. We develop a sample scale retention and hydraulic conductivity model taking into account the effect of the contact angle, based on theoretical considerations for retention and flow of liquid at the pore scale.

Model development in four steps

1. Calculate liquid retention Sw(h) in single angular pores
2. Compute pore side length l(h,a) at pore snap off
3. Derive permeability Kh(h) for single fully and partially saturated pores
4. Upscale to a gamma-density distribution of pores sizes

1. Liquid retention in angular pores

\[
\text{Sw}(h) = \frac{\text{Sw}_{\text{max}}}{\text{Sw}_{\text{max}}} \quad \text{where} \quad \text{Sw}_{\text{max}} = \tan(a) \left(\frac{\cos(e + \theta)}{\cos(e + \theta) - \frac{1}{2} \left(1 + \frac{\pi}{180}\right)}\right) \quad [\text{Ma et al., 1996}]
\]

Colloids and Surfaces, A, 112, 273-290 (and C(h) is the normalized meniscus curvature given by \[
C(h) = \frac{\text{C(h)}}{\text{C(h)_\text{max}}}
\]

Imbibition

Pore snap off when \(\text{C(h)_\text{max}} = \cos(\theta) - \tan(\theta) \leq 90^\circ\) (Ma et al., 1996).

Drainage

Pore snap off when \(\text{C(h)_\text{max}} = \cos(\theta) + \frac{\pi}{180} \leq 90^\circ\) (Masarik and Morrow, 1984). J. Colloid Interf. Sci., 141, 262-274.

2. Relationship between pressure head and pore side length at the pore snap off

For every regular polygon we can give a general relationship between the incircle radius and the polygon's side length \(l\):

\[
R_a = \frac{1}{2} \cdot \frac{l}{\cos(\frac{180}{n})}
\]

The relationship between pressure head \(h\) at the porous snap off in imbibition and the pore side length \(l\) is given by:

\[
L_{\text{im}}(h) = 2 \tan(\alpha) \frac{\cos(e) - \tan(\theta) \sin(\phi)}{\cos(e) + \tan(\theta) \sin(\phi)}
\]

and for drainage:

\[
L_{\text{dr}}(h) = 2 \tan(\alpha) \frac{\cos(e) + \tan(\theta) \sin(\phi)}{\cos(e) - \tan(\theta) \sin(\phi)}
\]

Permeabilities were derived for fully and partially saturated pores:

- For fully saturated pores: \(K_{\text{dr}} = \frac{\pi}{180} \quad \text{and} \quad K_{\text{im}} = \frac{\text{Sw}_{\text{max}}}{\text{Sw}_{\text{max}}}\).
- For partially saturated pores: \(K_{\text{dr}} = \frac{\pi}{180} \quad \text{and} \quad K_{\text{im}} = \frac{\text{Sw}_{\text{max}}}{\text{Sw}_{\text{max}}}\).

3. Hydraulieodynamics at the pore scale

Tuller and Or (2001) formulated Navier-Stokes equations for the two flow regimes and solved them for average flow velocity \(\mathbf{u}(\mathbf{r}, t)\):

- For full pores: \(\mathbf{u} = \frac{\Delta \rho}{\mu} \quad \text{and} \quad \mathbf{u} = \frac{\Delta \rho}{\mu}\).
- For partially saturated pores: \(\mathbf{u} = \frac{\Delta \rho}{\mu} \quad \text{and} \quad \mathbf{u} = \frac{\Delta \rho}{\mu}\).

4. Upscaling

We assumed the gamma density function for the pore side length \(l\) distribution given by:

\[
f(l) = \frac{\text{exp} \left( -\frac{1}{2} - \frac{l}{2} - l \right)}{\text{exp} \left( -\frac{1}{2} - \frac{l}{2} - l \right)} \quad \text{for} \quad l \geq 0, \xi \geq 2
\]

Parameter \(\xi(\cdot)\) and \(\xi(\cdot)\) are shape parameters and their values depend on the characteristics of each porous medium.

\[
\text{water saturation} \quad \text{Sw}(h) = \text{Sw}_{\text{max}} \cdot \text{f}(\text{Sw}) \quad \text{and} \quad \text{unsaturated hydraulic conductivity} \quad K(h) = K_1(h) + K_2(h)
\]

\[
K_1(h) = \frac{\text{Sw}_{\text{max}}}{\text{Sw}_{\text{max}}} \quad \text{and} \quad K_2(h) = \frac{\text{Sw}_{\text{max}}}{\text{Sw}_{\text{max}}} \quad \text{for} \quad \text{liquid-vapor interfacial area} \quad A(h) \quad \text{and} \quad \text{liquid-vapor interfacial area} \quad A(h) \quad \text{saturation} \quad \text{and} \quad \text{saturated hydraulic conductivity} \quad Ksat
\]

\[
A(h) = \frac{\text{Sw}_{\text{max}}}{\text{Sw}_{\text{max}}} \quad \text{and} \quad Ksat = \frac{\text{Sw}_{\text{max}}}{\text{Sw}_{\text{max}}} \quad \text{for} \quad \text{liquid-vapor interfacial area} \quad A(h) \quad \text{saturation} \quad \text{and} \quad \text{saturated hydraulic conductivity} \quad Ksat
\]

where \(A(h) = \text{f}(\text{Sw}) \quad \text{and} \quad \text{saturated hydraulic conductivity} \quad Ksat \quad \text{for} \quad \text{liquid-vapor interfacial area} \quad A(h) \quad \text{saturation} \quad \text{and} \quad \text{saturated hydraulic conductivity} \quad Ksat
\]

Further reading


Validation & predicted soil hydraulic properties

(a) Experimental data and fitted curve for the drainage of ethanol. Modeled curves is calculated using the Richards equation coupled with the new model.

(b) Observed and predicted imbibition of ethanol into initially dry material. The predicted curves were calculated using pore side length (i) distribution parameters estimated from the MSO experiment and conducting forward simulations using the Richards equation.

(c) same as (a) for water.

(d) same as (b) for water.

(e) Fitted (drainage) and predicted (imbibition) liquid saturation vs pF curves. Contact angle was assumed zero for both ethanol curves.

(f) Fitted (drainage) and predicted (imbibition) liquid conductivity vs pF curves.

(g) Predicted liquid vapor interfacial area vs Sw curves

(h) The pore side length distributions for the two soil columns analyzed in this study.

Conclusions

- Closed form expressions were derived for liquid retention, hydraulic conductivity and liquid-vapor interfacial area as a function of the pressure head.
- The new model is able to predict the ethanol and water imbibition dynamics based on the fitted pore side length distributions of the drainage experiments. Moreover, it describes successfully the different hysteresis for the two liquids assuming a similar pore side length distribution.

Acknowledgement

This work was financially supported by North Rhine-Westphalia through the project "Relating Hydromorphic Processes and Properties of Partially Hydromorphic Soils".

Further reading