A MATLAB function to determine the effective excess charge density under partial saturation from the van Genuchten parameters

Damien Jougnot[1], Niklas Linde[2]

December 28, 2021

(1) Sorbonne Université, CNRS, EPHE, UMR 7619 METIS, Paris, France
(2) University of Lausanne, Lausanne, Switzerland

Abstract

Modelling streaming potential generation in partially saturated porous media is of high interest for hydrological and reservoir studies as it allows to relate water fluxes to measurable electrical potential distributions. One key parameter to describe the electrokinetic coupling is the effective excess charge density. This document describes the Matlab function `fQeff_VG` to determine the effective excess charge density as a function of the saturation using the model described in Jougnot et al. (2012). This version of the code is based on the van Genuchten hydrodynamic parameters.

—-

Corresponding author: Damien Jougnot: damien.jougnot@upmc.fr

Description of the `fQeff_VG` function

This document briefly describes a Matlab function used in Jougnot et al. (2012) to determine the effective excess charge density from the hydrodynamic characteristics of porous media. For a complete description of the concept of effective excess charge density and its theoretical framework, we refer to Jougnot et al. (2020)[1].

The principle of the flux-averaging upscaling use in the model can be described by the sketch presented in Fig. 1. All the assumptions made for this model are described in Jougnot et al. (2012).

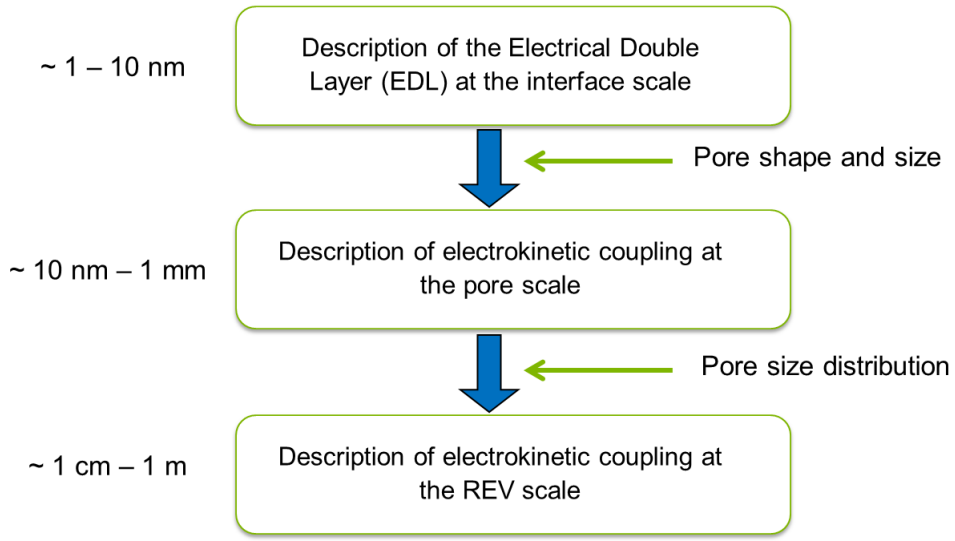

Figure 1: Sketch of the flux-averaging up-scaling procedure to obtain the effective excess charge density in a porous medium (Jougnot, 2020).

In this version of the model the solid-solution interface model that we used is based on the thin double layer and Debye-Hückel assumptions for a binary symetric electrolyte (e.g., NaCl). Then, we only consider cylindrical pores, for an analytical solution with irregular pores check Soldi et al. (2020). The pore size distribution is inferred from widely used hydrodynamic functions following two possible approaches as describe in Fig. 2: the WR approach which is based on the water retention curve and the RP approach that is based on the relative permeability curve. This model can be used with virtually any kind of hydrodynamic functions (e.g., Brooks and Corey, 1964; Van Genuchten, 1980). Nevertheless, we only provide the code using the closed form of Van Genuchten (1980) as it is the most widely used model in literature. For an analytical solution considering a fractal pore size distribution, we refer the reader to Soldi et al. (2019).

Input parameters

The input parameters used in the `fQeff_VG` function are defined in Jougnot et al. (2012). It includes: the porosity, the residual water content, the α and n parameter of Van Genuchten (1980), the saturated hydraulic conductivity, the NaCl concentration (or equivalent concentration), the ζ (Zeta) potential, and the temperature, with the units indicated in the code (see below). Note that the effect of the salinity (i.e., the NaCl concentration) has been studied in Jougnot et al. (2015) and Hu et al. (2020).

[1] In these two references, the effective excess charge density has a different notation but the same meaning: $\tilde{Q}_v^{eff} = \hat{Q}_v$.

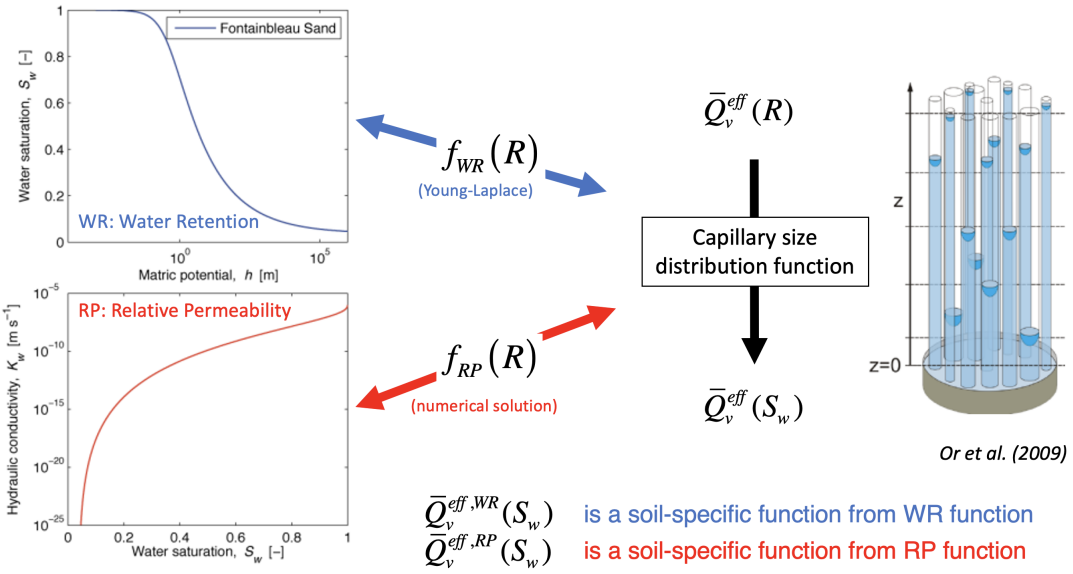

Figure 2: Sketch of the two approaches to infer the pore size distribution from hydrodynamic functions as proposed by Jougnot et al. (2012)

The input parameters can be recalled with the command `help fQeff_VG` which display the following text:

```
function [Sw, Qeff_WR, Qeff_RP] = fQeff_VG(Phi, theta_r, alpha, n, Ks, Cw, Zeta, T_C)
% Function [Sw, Qeff_WR, Qeff_RP] = fQeff_VG(Phi, theta_r, alpha, Ks, Cw, T_C, Zeta)
% Compute the effective excess charge density function using Jougnot et al. (2012)
% Authors: Niklas Linde & Damien Jougnot
% Input parameters
% Phi = Porosity [-]
% theta_r = residual water content [-]
% alpha = air entry matric pressure in van Genuchten (1980) [1/m]
% n = pore size disctribution in van Genuchten (1980) [-]
% Ks = saturated hydraulic conductivity [m/s]
% Cw = NaCl concentration [mol/L]
% Zeta = zeta potential [V]
% T_C = temperature [°C]
```

Output results

After running the function, one gets the evolution of the effective excess charge as a function of the saturation following the WR and the RP approach: `Sw, Qeff_WR, Qeff_RP`. To obtain the relative effective excess charge density function, one can simply divide this absolute value by the value at full saturation (i.e., $S_w = 1$).

Example with typical hydrodynamic functions from Carsel and Parrish (1988)

The present example can be obtained by running the file `Main_Example.m` that calls the `fQeff_VG` function. In this case, we use hydrodynamical parameters from Carsel and Parrish (1988). In their work, Carsel and Parrish (1988) perform a wide statistical analysis of typical Van Genuchten (1980) parameter values for 12 types of soils.

Figure 3 shows the results of the simulation when expressed in relative effective excess charge density as a function of the effective saturation (Fig. 3 in Jougnot et al., 2012).

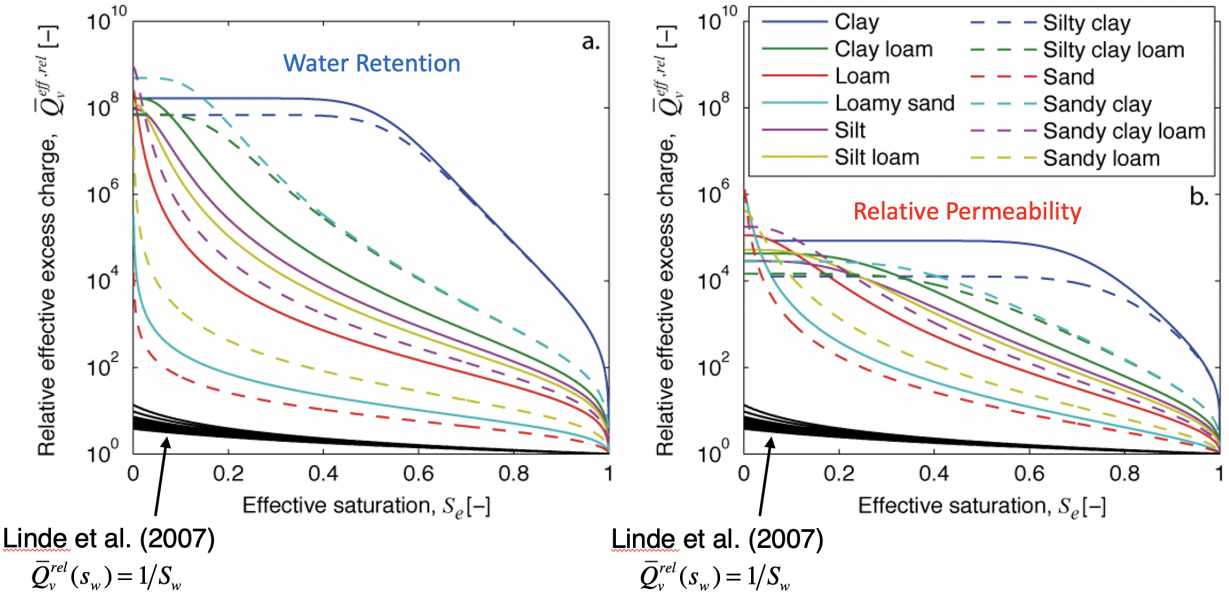

Figure 3: Relative effective excess charge density as a function of the saturation for the 12 soil types proposed by Carsel and Parrish (1988) using (a) the WR approach and (b) the RP approach of the flux-averaging model. Note that the black lines correspond to the volume-averaging model of Linde et al. (2007).

After running the file `Main_Example.m`, one obtains 5 text files with the calculations results. In these file, each column correspond to soil type while each row correspond to a saturation:

- Saturation values are in `Sw_Qeff.txt`.
- Effective excess charge densities from WR and RP approaches are in `Qeff_WR.txt` and `Qeff_RP.txt`, respectively.
- Relative effective excess charge densities from WR and RP approaches are in `Qeff_WR_rel.txt` and `Qeff_RP_rel.txt`, respectively.

How to cite

Please cite the corresponding paper:

Jougnot, D., Linde, N., Revil, A., Doussan, C. (2012). Derivation of soil-specific streaming potential electrical parameters from hydrodynamic characteristics of partially saturated soils. Vadose Zone Journal, 11(1).

References

Brooks, R., Corey, A.. Hydraulic properties of porous media. Hydrology Paper No 3, Colorado State University 1964;.

Carsel, R.F., Parrish, R.S.. Developing joint probability distributions of soil water retention characteristics. Water resources research 1988;24(5):755–769.

Hu, K., Jougnot, D., Huang, Q., Looms, M.C., Linde, N.. Advancing quantitative understanding of self-potential signatures in the critical zone through long-term monitoring. Journal of Hydrology 2020;585:124771.

Jougnot, D.. Developing hydrogeophysics for critical zone studies, importance of heterogeneities and processes at the mesoscopic scale. Ph.D. thesis; Sorbonne Université; 2020.

Jougnot, D., Linde, N., Haarder, E., Looms, M.. Monitoring of saline tracer movement with vertically distributed self-potential measurements at the HOBE agricultural test site, voulund, denmark. Journal of Hydrology 2015;521(0):314 – 327.

Jougnot, D., Linde, N., Revil, A., Doussan, C.. Derivation of soil-specific streaming potential electrical parameters from hydrodynamic characteristics of partially saturated soils. Vadose Zone Journal 2012;11(1).

Jougnot, D., Roubinet, D., Guarracino, L., Maineult, A.. Modeling streaming potential in porous and fractured media, description and benefits of the effective excess charge density approach. In: Advances in Modeling and Interpretation in Near Surface Geophysics. Springer; 2020. p. 61–96.

Linde, N., Jougnot, D., Revil, A., Matthäi, S., Arora, T., Renard, D., Doussan, C.. Streaming current generation in two-phase flow conditions. Geophysical Research Letters 2007;34(3):L03306.

Soldi, M., Guarracino, L., Jougnot, D.. An effective excess charge model to describe hysteresis effects on streaming potential. Journal of Hydrology 2020;588:124949.

Soldi, M., Jougnot, D., Guarracino, L.. An analytical effective excess charge density model to predict the streaming potential generated by unsaturated flow. Geophysical Journal International 2019;216(1):380–394.

Van Genuchten, M.T.. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil science society of America journal 1980;44(5):892–898.