Splintex 2.0: A computer program for estimating the parameters of soil hydraulic equations by the principle of physically-based pedotransfer functions

built by:

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SUMMARY

1. General

The quantification of soil hydraulic properties is of great importance in the modeling of hydrological processes. The relations between water content (θ) and matric potential (h) (the soil water retention function [$\theta(h)$]) and between hydraulic conductivity (K) and θ (the hydraulic conductivity function [$K(\theta)$]), expressed by mathematical functions, are essential tools for modeling flow in unsaturated soils and to comprehend issues related to crop water availability, irrigation, and internal drainage within soil profiles (Rahmati et al., 2018) or to many other processes that occur in the vadose zone and the low atmosphere (Vereecken et al., 2016; Elhakeem et al., 2018).

High labor costs are involved in measuring $\theta(h)$ and $K(\theta)$ functions and the estimation of hydraulic properties from other available data is often an alternative. The wide range of scales applied in modeling is essential for different applications, such as precision agriculture, irrigation management, crop available water and hydrology.

To reduce the limitations of simulating mass and energy transport in the vadose zone imposed by the lack of soil hydraulic properties, some computer programs based on statistical and empirical (regression) principles and on other process-based models have been developed (Silva et al., 2017a; Zhang and Schaap, 2017). These programs apply pedotransfer functions (PTFs) that predict parameters of hydraulic equations (e.g., water retention, hydraulic conductivity, specific water capacity, and hydraulic diffusivity) from other basic soil physical data, such as texture, bulk density, particle density and total porosity (Silva et al., 2017a; Silva et al., 2017b). Splintex 2.0 is a physically-based PTF computer model that estimates parameters used to build the soil water retention curve (SWRC) and the soil hydraulic conductivity curve (SHCC). Silva et al. (2020a) presented the second version of Splintex (Splintex 2.0), which was improved having its code written in C++ language and a user-friendly interface. After that, Silva et al. (2020b) analyzed the performance of Splintex 2.0 to estimate the vGM parameters of the SHCC (Silva et al., 2021).

2. Downloading and installing Splintex 2.0

To install Splintex 2.0, please follow these steps:

- Download "Splintex_2.0.exe" (approximately 900 KB) along with the application extensions *wxmsw30u_gcc_custom.dll* and *wxmsw30u_gl_gcc_custom.dll*. Put all these files in the same folder.

- Open the folder and run Splintex_2.0.EXE by double-clicking. Splintex 2.0 requires less than 20 MB of disk space when installed.

3. *Splintex 2.0 program*

The Splintex 2.0 (Silva et al., 2020a) was developed based on its precursor (Splintex 1.0), written in BASIC language by Prevedello and Loyola (2002) and evaluated by Dos Reis et al. (2018), Silva et al. (2020a), Silva et al. (2020b), and Silva et al. (2021).

Splintex 2.0 consists of a computer algorithm developed in C ++, compiled in an Integrated Programming Environment (IPE) CodeBlocks, structured with data input, mathematical interactions, and data output. Splintex 2.0 is built in a Windows 10 environment to estimate unsaturated hydraulic properties from soil data (inputs) such as particle diameters and the corresponding particle size fraction (%), bulk density (ρ_b), particle density (ρ_p), saturated soil water content (θ_s) or total porosity (ϕ), and any other measured $\theta(h)$ pair-value. Splintex 2.0 can be used to estimate the parameters of the following equations (Silva et al. 2020a and b):

- Soil water retention curve [$\theta(h)$], according to the van Genuchten (1980) equation, given by:

$$\theta(\mathrm{h}) = \theta_\mathrm{r} + \frac{\theta_\mathrm{s} - \theta_\mathrm{r}}{\left[1 + \left(\alpha \cdot |\mathrm{h}|\right)^\mathrm{n}\right]^\mathrm{m}} \tag{1}$$

in which θ is the volumetric soil water content as a function of the matric potential (h), θ_r and θ_s are, respectively, the residual and saturated water content, α, n and m (m = 1–1/n) are fitting curve shape parameters. In this program, h is expressed in units of energy per weight (e.g., $m = J/N$).

- Soil hydraulic conductivity curve [$K(\theta)$], according to the van Genuchten (1980) equation. Taking use of Mualem's (1976) equation, van Genuchten (1980) derived the following closed-form expression for $K(\theta)$:

$$\mathrm{K}(\theta) = \mathrm{K}_\mathrm{s}\left(\frac{\theta - \theta_\mathrm{r}}{\theta_\mathrm{s} - \theta_\mathrm{r}}\right)^{\lambda}\left\{1 - \left[1 - \left(\frac{\theta - \theta_\mathrm{r}}{\theta_\mathrm{s} - \theta_\mathrm{r}}\right)^{1/\mathrm{m}}\right]^{\mathrm{m}}\right\}^{2} \tag{2}$$

in which K is the unsaturated hydraulic conductivity as a function of the volumetric soil water content (θ). K_S is the saturated soil hydraulic conductivity as a matching point at saturation), θ_r

and θ_s are, respectively, the residual and saturated water content, and λ and m ($m=1-1/n$) are fitting parameters related with the connectivity of pores and shape of the $\theta(h)$ function.

4. Internal structure of the Splintex 2.0 program

The development of the Splintex pedotransfer functions was based on a compilation of the models described by Arya and Paris (1981), Arya et al. (1999b), and Arya and Heitman (2015) to estimate the parameters of equations (1) and (2). The Arya and Paris (1981) model present in its structure a set of physical equations to quantify pairs of $\theta(h)$ data. The calculation of θ is based on the particle size distribution (PSD), as the contribution of each fraction to soil wetting, according to:

$$\theta_i \approx \phi S_w \sum_{j=0}^{j=1} w_j \qquad i=1, 2, \; ....,n \tag{3}$$

in which ϕ is the total porosity of the soil sample ($m^3\ m^{-3}$), S_w is the ratio of measured saturated water content to theoretical porosity and w_i is the solid mass of the i-th fraction ($kg\ kg^{-1}$).

The second principle is the capillarity equation that relates h to the radius of the largest pore filled with water (R_i). The value of R_i is estimated using the particle size class and a scale factor (β) for correcting the non-sphericity of the soil particles (Arya et al., 1999b; Arya and Paris, 1981). The combination of R_i and h results in:

$$h_i \approx \frac{2\sigma\, cos(\omega)}{\rho_w g \mu_i \sqrt{\frac{2(\rho_p-\rho_b)}{3\rho_b}\left(\frac{3w_i}{4\pi\mu_i^3\rho_p}\right)^{1-\beta}}} \qquad i=1, 2, \; ....,n \tag{4}$$

in which σ is the surface tension at the air-water interface ($J\ m^{-2} = kg\ s^{-2}$), μ is the soil particle radius considering packing of spherical particles (m), ω is the contact angle in the largest water-filled pore (AP model considers ω = 0), wi is the solid mass of the i-th fraction ($kg\ kg^{-1}$), g is gravity ($m\ s^{-2}$), ρ_w is the density of water ($kg\ m^{-3}$), ρ_b and ρ_p are the soil bulk and particle density ($kg\ m^{-3}$), respectively. A more complete description to obtain equation (4) is given in Arya and Paris (1981) and Silva et al. (2020a).

The value of β = 1.38 suggested by AP model performs well for some soils, but not for all particle size distribution. Arya et al. (1982) analyzed 181 soil samples from New Jersey and found values of $1.26 \leq \beta \leq 2.10$. Vaz et al. (2005) reported an average value of β = 0.977 for 104 soil samples obtained from south and southeast Brazil. Because the aim is the size and distribution of pores and not the size and distribution of particles, some deviations may occur in this estimation. They can be minimized if the user provides one (θ_s) or two measured SWRC points [θ_s and any other $\theta(h)$ value]. Otherwise, an automatic correction to estimate $\theta(3.3\ m)$ is accomplished with another PTF, presented by Arruda et al. (1987). A more complete description to obtain the value of β is given in Arya and Paris (1981) and Silva et al. (2020a).

Regarding the SHCC, a compilation of the methodologies proposed by Arya et al. (1999a), Arya and Heitman (2015), and Arya and Paris (1981) was applied to estimate the parameters of equation (2). Splintex 2.0 is built under the assumption that soil pores can be represented by equivalent capillary tubes and that the flow rate (q) is a function of pore size distribution (Arya et al., 1999a). Therefore, $K(\theta)$ may be computed by

$$K(\theta_i) = \frac{1}{A_b}\sum_{j=1}^{j=i}\left(cR_j^x\right)N_j \qquad i = 1, 2, \ ...., N$$

$$R_i = \sqrt{\frac{0.0717\phi\, w_i}{\tau^{4/3}\mu_i\, \rho_b}} \tag{5}$$

in which N_j is the number of pores in the i-th pore fraction, exposed at the cross-sectional area, R_j is the pore radius for a given i-th fraction of particles on the PSD curve (m), τ_i is the number of spherical particles that could be formed using the fraction solid mass and A_b is the cross-sectional area (m^2) of the sample given by $A_b = (1/\rho_b)^{2/3}$ and c and x are empirical parameters described in Silva et al. (2020b).

In this approach, the sum of the flow rates of each saturated pore of a given soil sample is computed assuming the Hagen-Poiseuille's law for capillary flow (Prevedello and Armindo, 2015). Therefore, $K(\theta)$ is expressed as

$$K(\theta_i) = \frac{1}{A_b}\sum_{j=1}^{j=i}\left(q_j\right)N_j \qquad i = 1, 2, \ ...., n \tag{6}$$

in which N_j is the number of pores in the i-th pore fraction exposed at the cross-sectional area, A_b is the cross-sectional area of the sample (m^2), given by $A_b = (1/\rho_b)^{2/3}$, and q_j is the volumetric flow rate for a single pore (m^3 s^{-1}), calculated by $q_j = c\,R_j^x$. A more complete description of the $K(\theta)$ estimation is provided in Arya et al. (1999a).

5. Flowchart of the Splintex 2.0 algorithm

The interface of the Splintex 2.0 program was developed with an input structure, optional information and output data (Fig. 1).

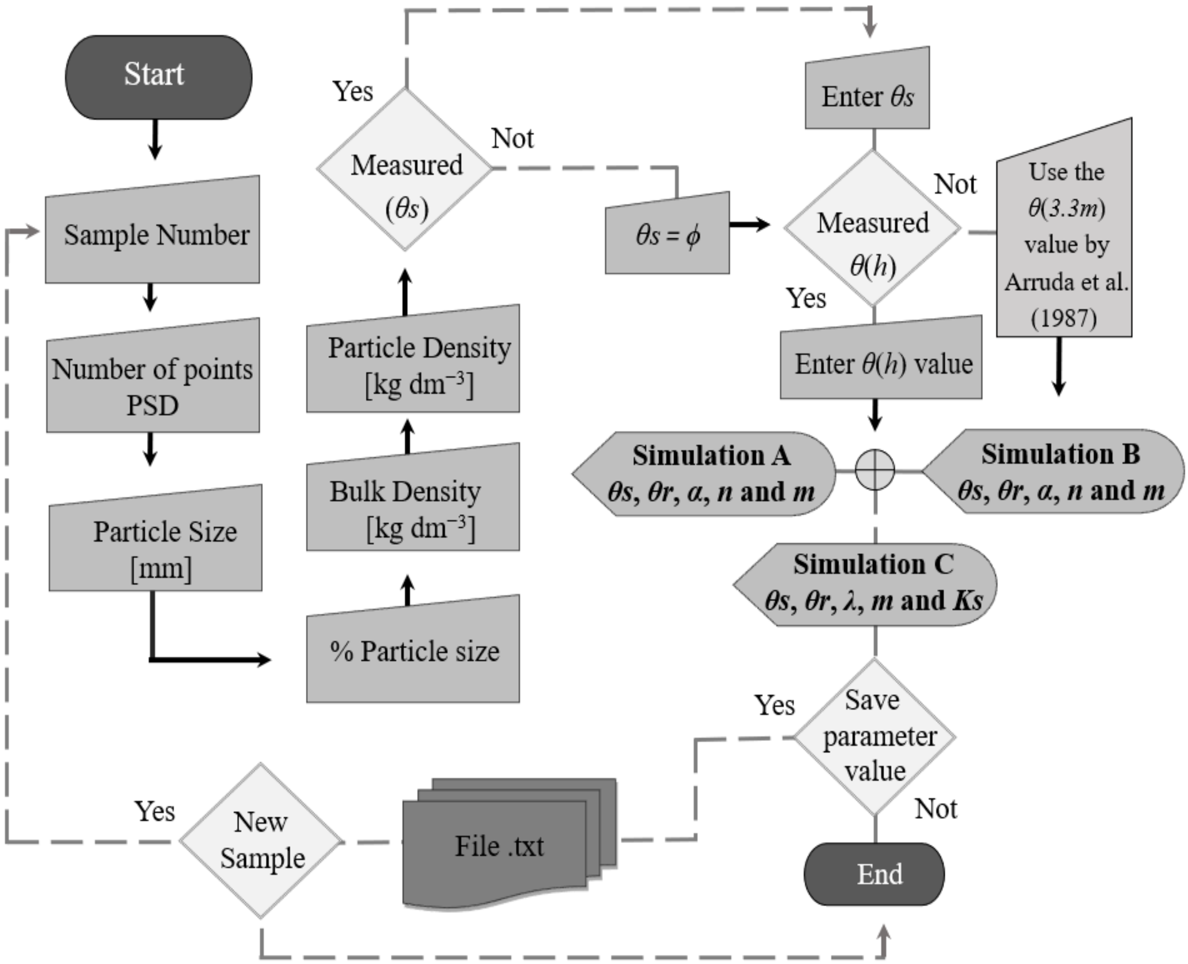


Fig. 1. Flowchart of the Splintex 2.0 algorithm. The output of the vGM parameters are presented in three ways; simulation A: θ_s was set as its measured value and θ_r, α, n and m estimated; simulation B: all parameters θ_s, θ_r, α, n and m estimated; simulation C: all parameters θ_s, θ_r, λ, m and K_s estimated; PSD: particle size distribution.

- **Required inputs**

The program requires the sample identification and the number of texture data points (N) to create a dimension vector continuously stored in its memory. Each particle diameter and its percentage values are then inserted. After that, a cubic spline function is fitted to these data for describing the cumulative PSD function. We standardized PSD for 16 classes of particle diameters: 2, 4, 6, 8, 10, 20, 40, 50, 60, 80, 100, 200, 400, 600, 800 and 1000 μm. To finish the procedure, the values of ρ_b and ρ_p are required.

- **Optional inputs**

The measured θ_s is required, but if its value is unknown the total porosity (ϕ) is used to replace it by $\phi = 1 - \rho_b/\rho_p$. Subsequently, the algorithm proceeds to equations (3), (4) and (5). Some deviations in these estimation procedure may occur due to the transformation of PSD into pore size distribution data to estimate the parameters of equations (1) and (2). The deviations in the estimation of $\theta(h)$ parameters can be minimized if any measured $\theta(h)$ point is provided, otherwise it is accomplished to find the best value of β. A more complete description to obtain the value of β is given in Arya and Paris (1981) and Silva et al. (2020a). According to these, the estimated $\theta(h)$ values are fitted to equation (1) and the estimated $K(\theta)$ data fitted to equation (2) applying the non-linear regression optimization.

- **Output window division**

Two outputs of the parameters of equation (1) are presented. In the second column (*SWRC parameters*) is the *simulation A*, where four parameters (θ_r, α, n *and* m) are estimated and θ_s is set to the measured θ_s or ϕ. In the third column, *Simulation B* results in five estimated parameters (θ_s, θ_r, α, n and m). Parameter m is calculated by $m = 1–1/n$ for both simulations.

The fourth column (SHCC parameters) provides estimates of the parameters θ_s, θ_r, λ, m and K_s, described in equations (2) (*Simulation C*).

6. Developed environment and graphical interface of the Splintex 2.0 program

The newly developed version of the Splintex model is shown in Fig. 2. On the left side of the window, a box with the description of the input data is presented. The output results of the parameters of equation (1) and (2) are revealed in another box at the right side of the window. In the upper left corner, the information about the system menu is organized with options to "Import" and "Export" data, quit and a file with the previous published studies with Splintex 2.0.

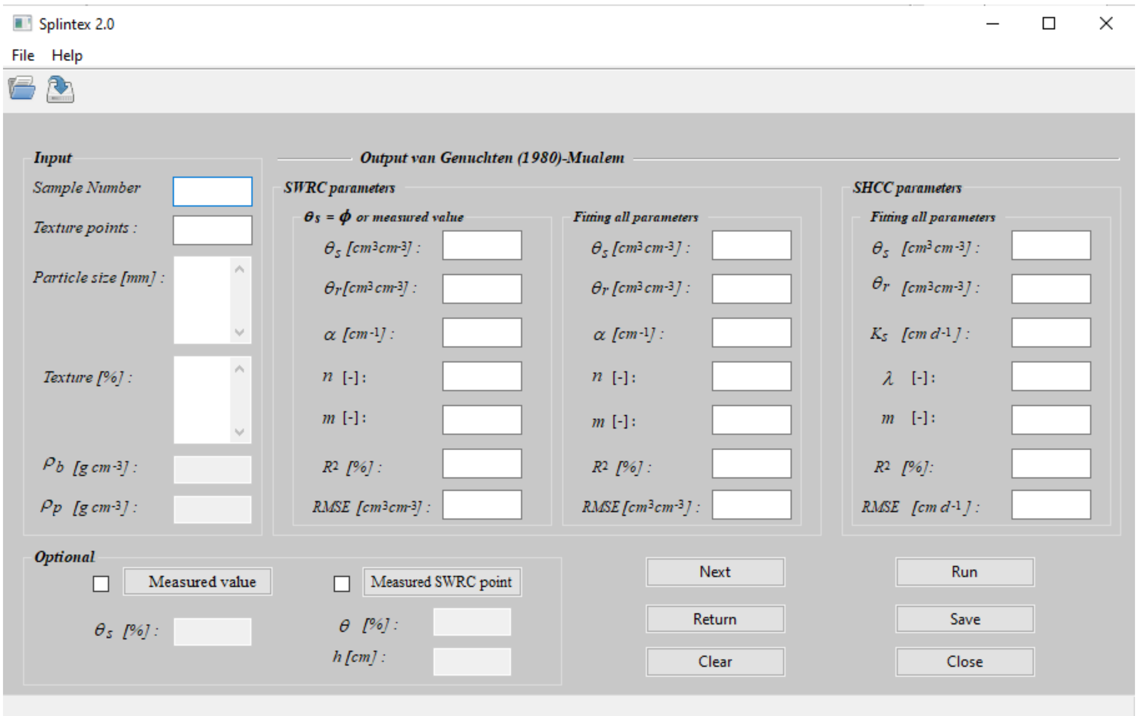


Fig. 2. Initial window of the pedotransfer model Splintex 2.0.

- **Manual use:** Users can manually enter the values of the requested variables in a sequential way. The sample number and values of the diameters (mm) of the particles that compose the PSD increasing values, textural contents (%), ρ_b and ρ_p (g cm^{-3}) and the optional values of measured θ_s and any other *θ(h)* point should be filled in here. To run the Splintex 2.0 program, click the "Run" button, and click the "Export" button to save each simulation in a .txt file or click on the "Save" button to save each simulation. If the user clicks the "Save" button, the file named "RESULT SPLINTEX 2.0 .txt" will be automatically stored in the program's installation folder.

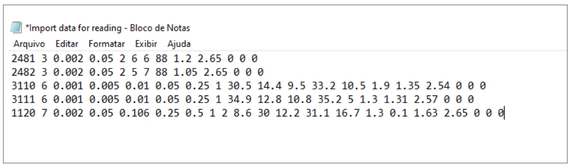
  Note: The buttons "optional Measured" and "Measured SWRC point" should not be activated if values of measured θ_s and any other *θ(h)* point are not available. The information should not be filled in this file, leaving the information window blank.

- **Importing a data file:** This item is used to import a *.txt* file and read input variables for simulation with input data in sequence. To do so, the button "Import File" should be used to choose the *.txt* file containing the sample number and the diameters (mm) of the particles that compose the PSD increasing values, textural contents (%), ρ_b and ρ_p (g cm^{-3}) and the optional values of measured θs and any other *θ(h)* point should be filled in this file. Then, to run the Splintex 2.0 model, click the "Run" button and "Next" for a new iteration. The estimated vGM parameters will be saved for each iteration by clicking on the “Save” button, in the same folder as the initial file named "RESULT SPLINTEX 2.0 .txt".

Example of input files:

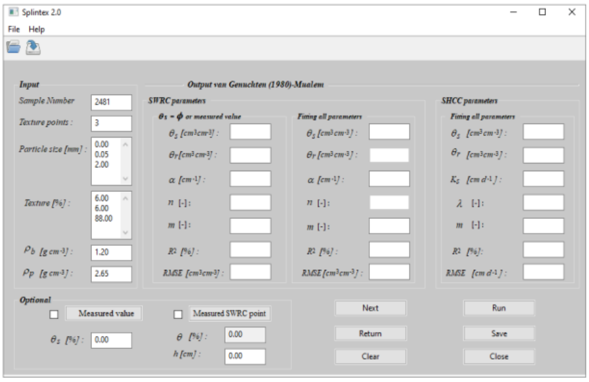
The inputs used in the first PTF (Splintex-PTF1) were PSD, *ρb*, *ρp*.

The sequence of input variables:
Sample Number >> Points >> Particle Size >> ρ_b >> ρ_p.



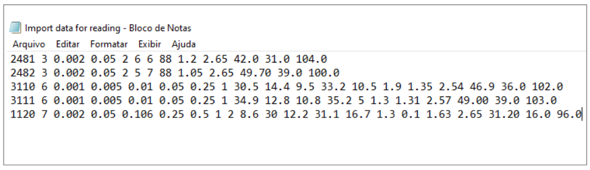
*Import data for reading - Bloco de Notas
Arquivo Editar Formatar Exibir Ajuda

```
2481 3 0.002 0.05 2 6 6 88 1.2 2.65 0 0 0
2482 3 0.002 0.05 2 5 7 88 1.05 2.65 0 0 0
3110 6 0.001 0.005 0.01 0.05 0.25 1 30.5 14.4 9.5 33.2 10.5 1.9 1.35 2.54 0 0 0
3111 6 0.001 0.005 0.01 0.05 0.25 1 34.9 12.8 10.8 35.2 5 1.3 1.31 2.57 0 0 0
1120 7 0.002 0.05 0.106 0.25 0.5 1 2 8.6 30 12.2 31.1 16.7 1.3 0.1 1.63 2.65 0 0 0
```



The inputs used in the second PTF (Splintex-PTF2) PSD, *ρb*, *ρp*, *θs* and measured *θ(h)* point were inserted.

The sequence of input variables:
Sample Number >> Points>> Particle Size >> *ρb* >> *ρp* >> θ_s >> θ_i >> *h*.



Import data for reading - Bloco de Notas
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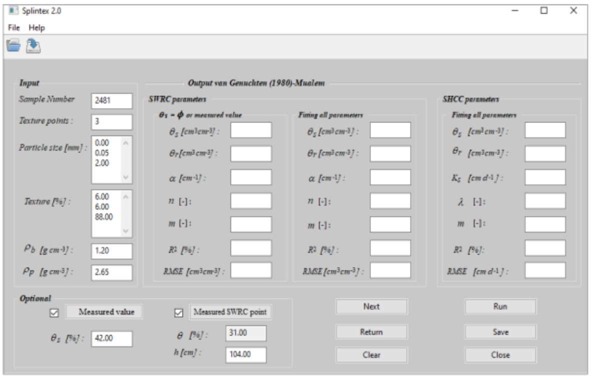
```
2481 3 0.002 0.05 2 6 6 88 1.2 2.65 42.0 31.0 104.0
2482 3 0.002 0.05 2 5 7 88 1.05 2.65 49.70 39.0 100.0
3110 6 0.001 0.005 0.01 0.05 0.25 1 30.5 14.4 9.5 33.2 10.5 1.9 1.35 2.54 46.9 36.0 102.0
3111 6 0.001 0.005 0.01 0.05 0.25 1 34.9 12.8 10.8 35.2 5 1.3 1.31 2.57 49.00 39.0 103.0
1120 7 0.002 0.05 0.106 0.25 0.5 1 2 8.6 30 12.2 31.1 16.7 1.3 0.1 1.63 2.65 31.20 16.0 96.0
```



Note: If no measured θ_s and any other *θ(h)* are available, one point should be filled in the *.txt* file with zero values. The optional buttons “Measured value” and “Measured SWRC point” should not be activated due to the internal process of the algorithm, if the measured parameters θ_s and θ*(h)* are not obtained.

- **Saving results:** For each iteration, the estimated vGM parameters can be saved in two ways. Either the “Export file” button can be used to create a *.txt* file with the results in a folder, or the “Save” button can be used to save the results in the same folder as the initial file named "RESULT SPLINTEX 2.0 .txt".

Example of output parameters:

The output of the vGM parameters are presented in three ways; simulation A, B and C. Note the sequence of output parameters:

i. Soil water retention curve [SWRC_1st, $\theta(h)$] =

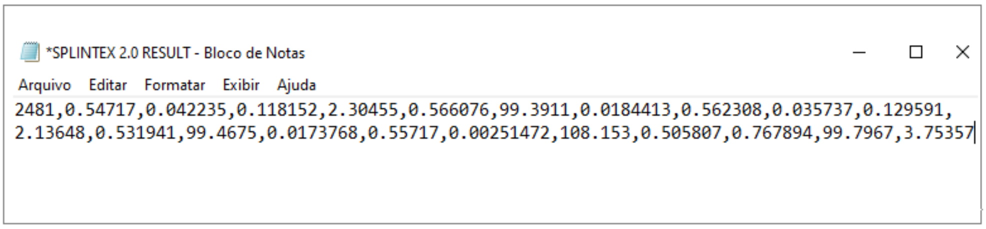
Sample Number >> θs >> θr >> α >> n >> m >> R^2 >> RMSE.

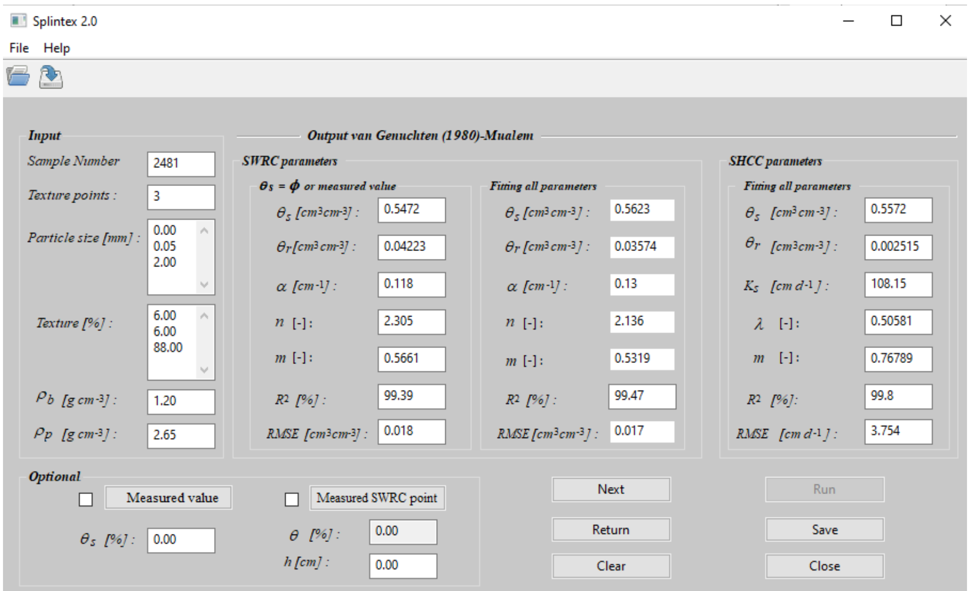
ii. Soil water retention curve [SWRC_2nd, $\theta(h)$] =

Sample Number >> θs >> θr >> α >> n >> m >> R^2 >> RMSE.

iii. Soil hydraulic conductivity curve [SHCC, $K(\theta)$] =

Sample Number >> θs >> θr >> K_{sat} >> λ >> m >> R^2 >> RMSE.





7. *Help system and tutorials*

Splintex 2.0 contains extensive help files that explain how to use the various menu options and screens. The help system also contains two tutorials that illustrate most of the functions of Splintex 2.0. In addition, the help system contains *.txt* files illustrating the basic soil physical properties as input variables and output parameters of the vGM equation.

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