Global Sensitivity analysis of Water Retention Curve parameters for mine tailings flow models

Kevin Vidal*,1 and José Riquelme1
1*SRK Consulting, Chile*
**Corresponding author's email:* kvidal@srk.cl

Abstract: Determining the Water Retention Curve (WRC) is a key factor in properly solving unsaturated flow through a material. Commonly, its characterization is obtained by means of laboratory tests, but these methods are quite challenging due to time and resource constraints. Alternatively, estimations based on material index properties can be made; however, this approach does not always produce results that fit well with the data obtained from laboratory tests. The aim of the current study is to evaluate the impact of each adjustment parameter used to characterize the WRC of a material on unsaturated flow problems. This was carried out through a global sensitivity analysis of 1D flow models, considering representative materials from Chilean mine tailings, whose unsaturated behavior is modeled using the equation proposed by van Genuchten (1980). In summary, three different types of tailings from various mining operations in Chile were considered, and for each case, 2000 simulations were run following a Monte Carlo scheme. Each run represents a different combination of parameters that define a specific WRC for the material. Likewise, the hydrological conditions used in the numerical simulations were adapted to the typical environmental conditions of Northern Chile. The results of the sensitivity analysis conducted in this study aim to improve and strengthen the numerical work performed through 1D models, providing a deeper understanding of how the adjustment parameters of the water retention curve affect the unsaturated behavior of Chilean mine tailings and, consequently, how these changes influence the flow results obtained through unsaturated modeling performed for this kind of material.

Introduction

The water retention curve (WRC) is a fundamental component in the modeling of unsaturated flows, particularly in the context of tailings. Accurately describing the relationship between moisture content and suction is crucial for predicting the hydrological behavior of materials under unsaturated conditions. However, the experimental determination of the WRC in laboratories presents significant challenges in terms of time and resources, and in practice, only a limited number of points are typically measured [1]. This has led to the use of estimations based on the index properties of materials for obtaining the WRC. Nevertheless, deriving WRCs from estimations based on index properties, such as the Fredlund & Wilson [2] or Vereecken [3] methods, often proves to be unrepresentative for anthropogenic materials originating from mining processes. These estimates can significantly differ from those determined in laboratory settings [4] and may lead to issues in resource estimation for a project [5]. The van Genuchten model [6] is widely used to characterize the moisture retention behavior in porous materials. However, the fitting parameters required for this model can vary considerably, affecting the accuracy of unsaturated flow simulations. This study aims to assess the impact of each fitting parameter of the WRC (van Genuchten) and the key volumetric water content values for three different types of mine tailings in the context of an unsaturated flow problem. A total of 2000 numerical simulations were performed using 1-D models in Hydrus 1-D [7] for the three tailings tested. The simulations were conducted following a Monte Carlo scheme, meaning each run is characterized by a different set of material parameters, resulting in a spectrum of output results for each tailing. The rank variation value for each parameter was defined using the results of previous analyses conducted for filtered tailings [8], where recommendations to vary these values in the context of a local sensitivity analysis are provided. Using the spectrum of results, a global sensitivity analysis was conducted. Different correlations between outputs and parameter variations were evaluated to measure the degree of the parameter's effect on the output. The results provide insights into the impact of each parameter individually as well as the synergistic effects of varying different parameters simultaneously. Material property values used are characteristic of mine tailings from operation sites located in northern Chile, namely filtered tailings, thickened tailings, and conventional tailings. The hydrological conditions employed in the simulations reflect the typical environmental conditions of this region.

In this study, simulations assessed the exposure of tailings to atmospheric conditions and the vertical drainage from tailings to the soil foundation over a 50-year period. Additional correlation analysis was performed by examining two typical outputs of 1-D models: the degree of saturation at the bottom of the tailings (contact zone between materials) and the soil penetration height, which represents the advance of a humidity front. These results highlight critical aspects of geotechnical and hydrogeological evaluations.

Methodology

van Genuchten Model

To assess the behavior of filtered tailings under unsaturated flow conditions, the van Genuchten model (1980) was employed. This model enables the characterization of the WRC through fitting parameters that describe the relationship between moisture content and suction in porous materials. The model proposed by van Genuchten is described using the following equation:

$$\theta(\psi) = \theta r + \left[\frac{\theta s - \theta r}{\left[1+(\alpha\psi)^{n}\right]^{(1-1/n)}}\right] \tag{1}$$

Where ψ is the soil suction, $\theta(\psi)$ is the instant moisture content, θs is the saturated moisture content, θr is the residual moisture content, and α and n are the model fitting parameters of the van Genuchten model.

Materials

The materials studied were filtered tailings, thickened tailings, and conventional tailings sourced from various mining operations in northern Chile. The tailings are classified as silts (ML), according to the Unified Soil Classification System (USCS), with fines content (less than 0.075 mm) ranging from 66% to 83%. The specific gravity of the solids (Gs) varies between 2.74 and 2.8. WRCs were experimentally determined and fitted using the van Genuchten parameters. To represent the foundation soil, a typical material from northern Chile was selected, classified as silty sand (SM) in the USCS, with an approximate fines content of 30% (less than 0.075 mm), non-plastic, and a Gs of 2.65. The particle size distribution of the materials used in the modeling is presented in Figure 1, and the relevant properties and variations of each parameter are detailed in Table 1. Additionally, Figure 2(a) illustrates the SWRC, while Figure 2(b) represents the unsaturated hydraulic conductivity curves.

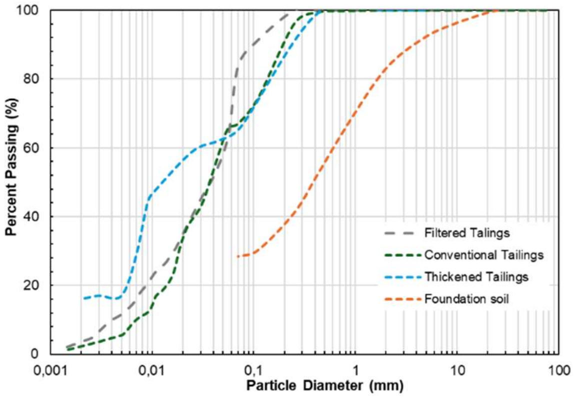
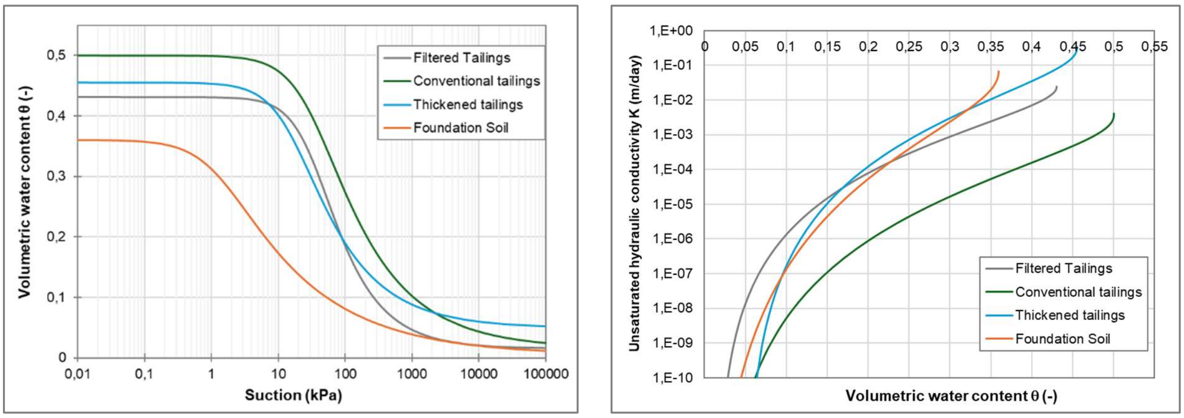


Figure 1: Materials studied - Particle size distribution.

Table 1: Materials properties and van Genuchten parameters and rank variation

Parameter		*Filtered Tailings*	*Conventional Tailings*	*Thickened Tailings*	*Foundation Soil*	*Rank variation respect to mean value*
Dry unit weight	γ_d *(kN/m3)*	*15.6*	*14.0*	*15.0*	*17.0*	-
Porosity	*n*	*0.431*	*0.5*	*0.455*	*0.36*	-
Specific gravity of solids	G_s	*2.74*	*2.8*	*2.75*	*2.65*	-

Fitting parameters of van Genuchten model	*a (1/kPa)*	*0.032*	*0,032*	*0,0633*	*0,816*	*+/- 1 magnitude order*
	n	*1.76*	*1.4974*	*1.5672*	*1.35*	*+/- 5% of mean value*
Volumetric moisture content at saturation	θ_s	*43.1%*	*50.0%*	*45,5%*	*36.0%*	*+/- 10% of saturated moisture content*
Residual volumetric moisture content	θ_r	*1.5%*	*1.6%*	*4.9%*	*0.5%*	*+/- 5% of saturated moisture content*
In-situ volumetric moisture content	θ_0	*12.9%*	*32.5%*	*29.6%*	*6.0%*	*+/- 5% of saturated moisture content*
Saturated hydraulic conductivity	*Ks (m/s)*	*2.80E-07*	*5.00E-08*	*4.06E-06*	*1.10E-06*	*+/- 1 magnitude order*
Saturated hydraulic conductivity	*Ks (m/d)*	*0.023*	*0.004*	*0.351*	*0.100*	*+/- 1 magnitude order*



(a) (b)

Figure 2: Materials studied – SWCC and Unsaturated hydraulic conductivity.

Unsaturated 1-D flow model

Simulations were executed using the HYDRUS-1-D software [7], which specializes in simulating unsaturated flow systems through the finite element method. It features an intuitive and user-friendly interface, and model construction relies on several text files. This structure provides flexibility to integrate external customized scripts, offering several advantages during model construction and the execution of simulations. One-dimensional models were developed to represent a 30-meter-thick profile of tailings overlying a 30-meter-deep layer of foundation soil.

This configuration allows for the assessment of vertical water flow from the tailings into the underlying ground material. The models were simulated over a period of 50 years to capture the system's long-term behavior. At the surface of the column, a climatic boundary condition was applied, with climatic values representative of northern Chile. Precipitation and evaporation were distributed monthly. At the bottom of the column, a unit gradient was assigned to permit free drainage in the vertical direction. As an initial condition, the in-situ volumetric water content was used for each material (see Table 1). Figure 3 presents a conceptualization of the model geometry.

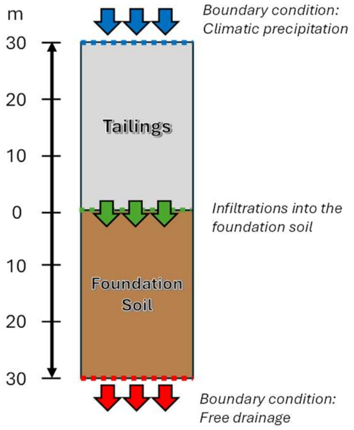


Figure 3: Materials studied – SWCC and Unsaturated hydraulic conductivity.

Global sensitivity analysis

Sensitivity analysis is a technique used to evaluate how variations in model parameters influence its outputs. It helps identify the most critical parameters of a specific problem, providing valuable insights to support decision-making and prioritizing actions based on the uncertainty or sensitivity of the system. It can be broadly categorized into local sensitivity analysis and global sensitivity analysis. Local sensitivity analysis focuses on assessing the impact of small, incremental changes in parameters around fixed points, typically using partial derivatives. This approach assumes linearity and independence of parameters, making it suitable for exploring the model's behavior in the vicinity of specific scenarios. In contrast, global sensitivity analysis examines the influence of parameters within a range of values, considering nonlinearities and interactions between parameters. By exploring the simultaneous and combined effects of multiple inputs, it provides a comprehensive understanding of the model's behavior, identifying key drivers of variability and interactions that may not be apparent in a local context.

The global sensitivity analysis conducted in this study utilized a Monte Carlo simulation approach. Variations in six parameters were considered: the van Genuchten parameters θ_r, θ_s,α, and n, the saturated hydraulic conductivity (Ks), and the initial moisture content (θ_i). For each one, a uniform distribution was assumed, generated using Latin Hypercube Sampling (LHS) within a predefined range of values. The parameter ranges were established based on a prior local sensitivity analysis [8] performed on a 1D model for filtered tailings. This earlier study provided recommendations for parameter variation around their mean values based on the evaluation of a sensitivity index (I) calculated through a classical partial derivation method (see Table 1). Monte Carlo scenarios were constructed by randomly sampling parameter values within the subspace defined by the LHS-generated ranges. For the three types of tailings studied, variations in the six parameters under consideration were performed, resulting in a total of 2,000 Monte Carlo simulations per tailings. The sensitivity analysis was conducted by evaluating the degree of correlation between the outputs and the range of variation of the parameters. In this study, analysis results are limited to the evaluation of the degree of saturation at the bottom of the tailings (contact zone between materials) and the soil penetration depth, which is a representative value of the advance of a humidity front. These results are indicative of key aspects of geotechnical and hydrogeological evaluations. The degree of correlation was measured by the computation of three coefficients, namely: Pearson, Spearman, and Kendall. These values allow us to evaluate the relative significance of parameter variation on the model outputs. Additionally, two non-linear analyses are included: Mutual Information and Feature Importance techniques—advanced correlation methods that permit capturing complex interactions between parameters and model outputs.

Monte Carlo Simulations Results

Figure 4 presents the results of Monte Carlo simulations for the three tested tailings materials. In Figure 4 (a-b), simulated volumetric water content profiles over a 50-year period are shown for tailings and foundation soil materials. The full set of Monte Carlo simulations is displayed in blue, while the mean values for each tailings material (see Table 1) are plotted in white.

Sensitivity analysis focuses on two key aspects of the water content profile: the degree of saturation at the interface between materials (at 30 m depth) and the soil penetration depth, which is an indicator of water migration from tailings to the soil foundation. The sensitivity of these results is evaluated by measuring the correlation between variations in six parameters and the final outputs. Results for the six parameters are shown in Figure 4 (d-f) for the degree of saturation and in Figure 4 (g-i) for the soil penetration depth. In the next section, correlation results for each parameter are evaluated.

Discussion

In Figures 4 (d-i), a visual inspection reveals significant dispersion across all parameters. However, marked trends are particularly distinguishable for the parameters α, Ks, and θ_i, with the most evident trends observed in α and Ks. For α, a non-monotonic behavior is noted across the entire evaluated range, while for the remaining parameters, slight trends are perceived but are accompanied by extremely high dispersion. To evaluate the degree of correlation between variables, three typical coefficients will be used: Pearson (P), Spearman (S), and Kendall (K). A ranking will then be calculated by summing the absolute values of these three coefficients (P +

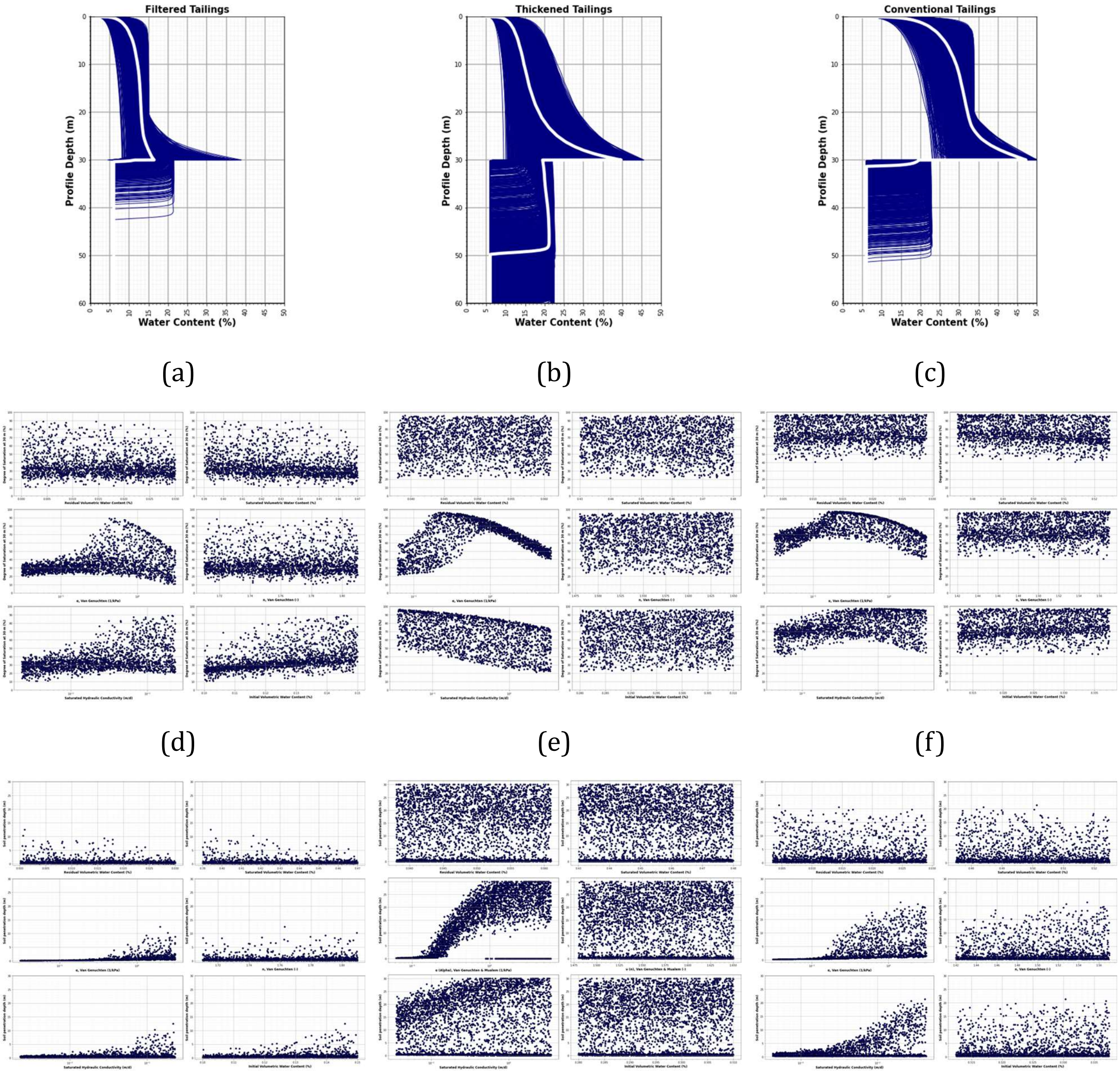
S + K). The parameter with the highest combined coefficient will be identified as the most influential. These correlation results and the weighted ranking value are shown in Table 2.

For soil penetration depth, the most influential parameter across all tailing types is consistently α, while the least influential is θ_r. Conversely, for the degree of saturation, the most influential parameters are θ_i for filtered tailings and Ks for thickened and conventional tailings. The least influential parameter is n for filtered tailings and θ_r for the other two types. If these results are compared against the simulated trends in Figure 4 (d-e), where the parameter α demonstrates a high influence on the degree of saturation, classical correlation methods may fail to appropriately capture the influence of α due to its non-linear and non-monotonic behavior. To verify this sensitivity result, alternative methods better suited to identifying non-linear and non-monotonic trends will be employed, specifically Mutual Information (MI) and Feature Importance (FI) correlation methods. As the soil penetration depth appears consistent between the classical correlation results and the visual inspection, the calculation of these two non-linear methods will be focused exclusively on the degree of saturation. The results of the MI and FI analyses for the three tailings tested are presented in Table 3.

Results in Table 3 indicate that, across all tailing types, α is consistently the most influential parameter for the degree of saturation, as it has the highest Mutual Information (MI) and Feature Importance (FI) values in all cases. Ks emerges as the second most important parameter, particularly for thickened and conventional tailings, while parameters such as n, θ_r, and θ_s have minimal influence across all tailing types. Unlike classical correlation methods (P + S + K, see Table 2), which struggle to capture non-linear and non-monotonic behaviors, these approaches reflect the significant influence of α, demonstrating their ability to provide a more robust understanding of parameter importance in the sensitivity analysis.

Finally, with the results presented, a ranking has been established to determine the importance of each tested parameter in the sensitivity analysis. For each analysis performed (Table 2 and Table 3), a ranking system was applied where the parameter with the highest sensitivity index received 6 points, and the parameter with the lowest index received 1 point. A final score index is obtained when the scores of the three correlation analyses are summed. The ranking from each analysis, as well as the final score combining the three analyses, is presented in the form of a histogram in Figure 5. The black curve represents the sum of absolute values for the classical correlation coefficients (Kendall, Pearson, and Spearman), while the blue curve corresponds to the ranking based on Mutual Information (MI), and the purple curve corresponds to the ranking based on Feature Importance (FI). The red curve represents the final score, calculated as the sum of the rankings from the three individual methods (K + P + S, MI, FI), where the parameter with the highest total ranking is considered the most influential.

From the sensitivity analysis, it is evident that the most important parameters are α and Ks across all tailing types. These parameters consistently rank highest in all methods and contribute most significantly to the variability of the degree of saturation response. Conversely, θ_r and n consistently emerge as the least influential parameters within the range of values tested. This ranking provides clear guidelines on which parameters should be prioritized in further modeling and experimental efforts.



(a) (b) (c)

(d) (e) (f)

(g) (h) (i)

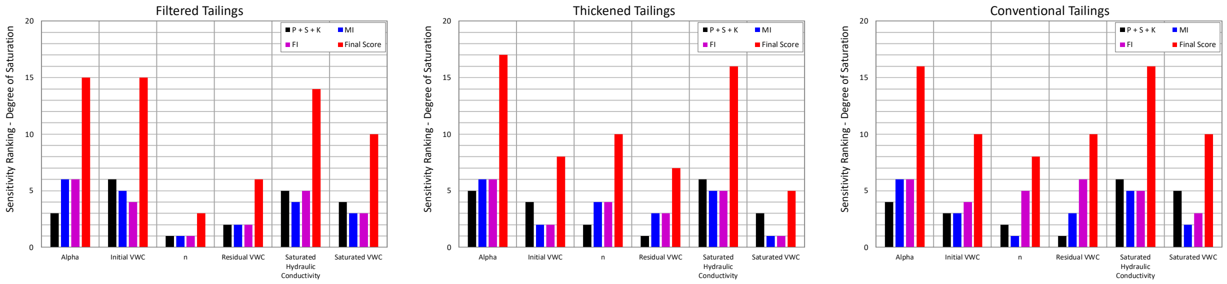
Figure 4: Sensitivity analysis results after 50 years of simulation: (a-c) Volumetric water content profile; (d-f) Degree of saturation at 30 m depth vs Parameters variation; and (g-i) Soil penetration depth vs Parameters variation.

Table 2: Sensitivity analysis correlation results between Degree of Saturation/Soil penetration depths and parameter

Parmeter	*Filtered*				*Thickened*				*Conventional*			
	Correlations index for degree of Saturation											
	Pearson	*Spearman*	*Kendall*	***ranking***	*Pearson*	*Spearman*	*Kendall*	***ranking***	*Pearson*	*Spearman*	*Kendall*	***ranking***
a, Van Genuchten (1/kPa)	0.12	0.24	0.18	**0.54**	-0.17	0.12	-0.03	**0.32**	-0.26	0.12	0.08	**0.46**
Initial Volumetric Water Content (%)	0.48	0.58	0.41	**1.46**	0.03	0.03	0.02	**0.08**	0.14	0.16	0.11	**0.41**
n, Van Genuchten (-)	0.05	0.04	0.03	**0.13**	-0.02	-0.02	-0.01	**0.06**	0.07	0.08	0.05	**0.20**
Residual Volumetric Water Content (%)	-0.13	-0.10	-0.07	**0.30**	0.00	0.00	0.00	**0.01**	0.01	0.01	0.01	**0.03**
Saturated Hydraulic Conductivity (m/d)	0.38	0.38	0.27	**1.03**	-0.40	-0.45	-0.31	**1.17**	0.19	0.36	0.26	**0.81**
Saturated Volumetric Water Content (%)	-0.21	-0.24	-0.16	**0.62**	-0.03	-0.02	-0.02	**0.06**	-0.18	-0.19	-0.13	**0.51**
Parameter	*Correlations index for soil penetration depth*											
a, Van Genuchten (1/kPa)	0.55	0.94	0.80	**2.29**	0.37	0.52	0.49	**1.38**	0.51	0.86	0.70	**2.07**
Initial Volumetric Water Content (%)	0.23	0.20	0.14	**0.57**	0.03	0.01	0.01	**0.05**	0.11	0.09	0.06	**0.25**
n, Van Genuchten (-)	0.06	0.09	0.06	**0.21**	0.02	0.01	0.01	**0.05**	0.14	0.10	0.07	**0.31**
Residual Volumetric Water Content (%)	-0.12	-0.07	-0.05	**0.24**	-0.01	-0.01	-0.01	**0.03**	-0.03	-0.02	-0.02	**0.07**
Saturated Hydraulic Conductivity (m/d)	0.30	0.16	0.11	**0.58**	-0.12	-0.09	-0.05	**0.25**	0.53	0.33	0.25	**1.11**
Saturated Volumetric Water Content (%)	-0.12	-0.05	-0.04	**0.21**	-0.04	-0.04	-0.03	**0.11**	-0.13	-0.12	-0.08	**0.33**

Table 3: Sensitivity analysis (Mutual Information and Features Importance) for degree of Saturation.

Parameter	*Filtered*		*Thickened*		*Conventional*	
	Correlations index for degree of Saturation					
	MI	*FI*	*MI*	*FI*	*MI*	*FI*
a, Van Genuchten (1/kPa)	0.30	0.34	1.05	0.72	0.78	0.56
Initial Volumetric Water Content (%)	0.26	0.26	0.00	0.00	0.02	0.02
n, Van Genuchten (-)	0.01	0.01	0.03	0.01	0.00	0.02
Residual Volumetric Water Content (%)	0.01	0.04	0.02	0.00	0.04	0.00
Saturated Hydraulic Conductivity (m/d)	0.16	0.28	0.37	0.27	0.24	0.36
Saturated Volumetric Water Content (%)	0.03	0.06	0.00	0.00	0.01	0.04



(a) (b) (c)

Figure 5: Sensitivity analysis rankings stablished for the three tested tailings.

Conclusion

A global sensitivity analysis was conducted for three types of tailings to evaluate the influence of six key hydraulic parameters on their unsaturated behavior. Both classical correlation methods and advanced metrics designed to capture non-linear and non-monotonic trends were employed. The results indicate that while classical correlations provide useful insights, they are not always appropriate for capturing the full complexity of parameter behavior, especially in cases where non-linear or non-monotonic relationships are expected. This highlights the importance of exploring alternative approaches, such as Mutual Information and Feature Importance, to better understand parameter sensitivities under such conditions.

Finally, while this study provides a robust framework for identifying the most influential parameters in unsaturated flow problems, it also opens the door for the development of an uncertainty analysis to further refine the understanding of how parameter variability affects the output results of these types of models. However, such an analysis is beyond the scope of the current work.

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