

Local sensitivity analysis of fitting parameters for the water retention curve in unsaturated flow models in filtered tailings

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Abstract

Accurate modelling of unsaturated flow in filtered tailings is critical for understanding their hydrological behaviour and improving resource management in mining operations. This study investigates the sensitivity of fitting parameters in the van Genuchten model, which characterises the water retention curve (WRC), through a comprehensive local sensitivity analysis. Laboratory challenges in determining WRCs, due to time and resource constraints, have led to reliance on estimates derived from material index properties which often fail to accurately represent moisture retention behaviour.

3,000 1D simulations were performed, using HYDRUS-1D, to assess the influence of six key parameters: residual moisture content (θ_r), saturated moisture content (θ_s), initial moisture content (θ_i), fitting parameters (α and n) and saturated hydraulic conductivity (K_s). The study focused on filtered tailings from a mining site in northern Chile, with simulations reflecting the region's typical environmental conditions. The results show that n , θ_s and θ_i are the most sensitive parameters, significantly affecting water flow predictions. The presence of a foundation soil alters hydrological responses, in contrast to scenarios with free drainage.

This research provides critical insights into the effects of WRC fitting parameters on unsaturated flow behaviour, enabling the definition of parameter variation ranges and improving the accuracy of flow models. The findings are invaluable for improving the reliability of tailings management and risk assessment strategies in Chile and similar environments worldwide, contributing to sustainable mining practices.

Keywords: water retention curve, sensitivity analysis, filtered tailings, unsaturated flow modelling.

1 Introduction

The water retention curve (WRC) is a fundamental component in unsaturated flow modelling, particularly in the context of filtered tailings. Accurately describing the relationship between moisture content and suction is critical for predicting the hydrological behaviour 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 limited points are typically measured (Luo et al. 2017). This has led to the use of estimations based on the index properties of materials for obtaining soil–water characteristic curves (SWCC). Nevertheless, deriving the WRCs from estimates based on index properties, such as the Fredlund & Wilson (2002) or Vereecken (1989) methods, often proves to be unrepresentative for anthropogenic materials originated from mining processes. These estimates can significantly differ from those determined in laboratory settings (Riquelme & Godoy 2017) and may lead to issues in resource estimation for a project (Torres & Riquelme 2021).

The van Genuchten model (1980) is widely used to characterise the moisture retention behaviour in porous materials. However, the fitting parameters required for this model can vary considerably, affecting the accuracy of unsaturated flow simulations. Previous studies suggest that the most sensitive parameters are residual moisture (θ_r), followed by the fitting parameters alpha (α) and n (Chen et al. 2016).

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This study aims to assess the impact of each fitting parameter on the WRC in unsaturated flow problems. Through a comprehensive local sensitivity analysis, varying the parameters of the van Genuchten model and two key parameters of the unsaturated flow model, 3,000 simulations were conducted on 1D flow models considering filtered tailings from a mining site in northern Chile. The hydrological conditions employed in the simulations reflect the typical environmental conditions of this region. To achieve this objective, a local sensitivity analysis was performed following the guidelines provided in Lenhart et al. (2002). Based on the partial derivation principle and assuming that the flow problem is represented by a fixed set of parameters (baseline), the local sensitivity index I (see Section 2.4) allows estimation of the degree of influence of a parameter by calculating the relative difference between the output of the baseline results and the output obtained when a single parameter moves from its baseline value. Then the relative output difference is normalised by the relative change in the tested parameter, obtaining a magnitude of the relative influence of the parameter. Based on the obtained I values, the influence of the parameters is classified into four levels, as shown in the work of Li et al. (2023). Further descriptions are given in the next section.

2 Methodology

2.1 van Genuchten model

The van Genuchten model (1980) was used to assess the behaviour of filtered tailings under unsaturated flow conditions. This model allows the characterisation 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 by the following equation:

$$\theta(\psi) = \theta_r + \left[\frac{\theta_s - \theta_r}{[1 + (\alpha\psi)^n]^{(1-1/n)}} \right] \quad (1)$$

where:

- ψ = suction
- $\theta(\psi)$ = moisture content at suction ψ
- θ_s = saturation moisture content
- θ_r = residual moisture content
- α, n = model fitting parameters.

2.2 Materials

The materials studied are filtered tailings sourced from a mining site in northern Chile. The tailings are classified as silt (ML) in the unified soil classification system (USCS), with a fines content (under 0.075 mm) of approximately 80%, and the fines exhibit no plasticity. The specific gravity of the solids (G_s) is 2.74. Relevant properties include a dry density of 15.6 kN/m³ and a porosity of 0.431. The suction curves were determined experimentally and fitted using the van Genuchten parameters: residual moisture content (θ_r), saturated moisture content (θ_s), the shape parameter (α) and the slope parameter (n). To represent the foundation soil, a typical material from northern Chile was selected, classified as silty sand (SM) in USCS, with an approximate fines content of 30% (under 0.075 mm), non-plastic, and a G_s equal to 2.65. The particle size distribution of the materials used in the modelling is shown in Figure 1, and the relevant properties are detailed in Table 1. In addition, Figure 2a shows the SWCCs, while Figure 2b shows the unsaturated hydraulic conductivity curves. In terms of saturated hydraulic conductivity, the filtered tailings have a value of 0.023 m/d (2.7 E-07 m/s), while the foundation soil has a value of 0.1 m/d (1.1 E-06 m/s).

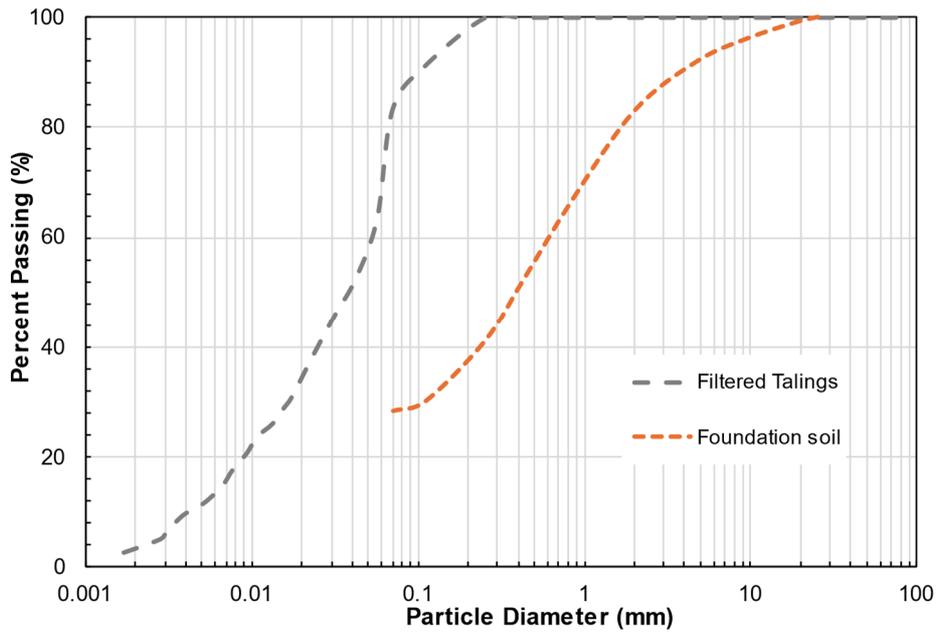


Figure 1 Materials studied: particle size distribution

Table 1 Material properties and van Genuchten parameters

Parameter		Filtered tailings	Foundation soil
Dry unit weight	γ_d (kN/m ³)	15.6	17.0
Porosity	n	0.431	0.36
Specific gravity of solids	G_s	2.74	2.65
Fitting parameters of van Genuchten model	α (1/kPa)	0.032	0.816
	n	1.76	1.35
Volumetric moisture content at saturation	θ_s	43.1%	36.0%
Residual volumetric moisture content	θ_r	1.5%	0.5%
In situ volumetric moisture content	θ_0	12.9%	6.0%

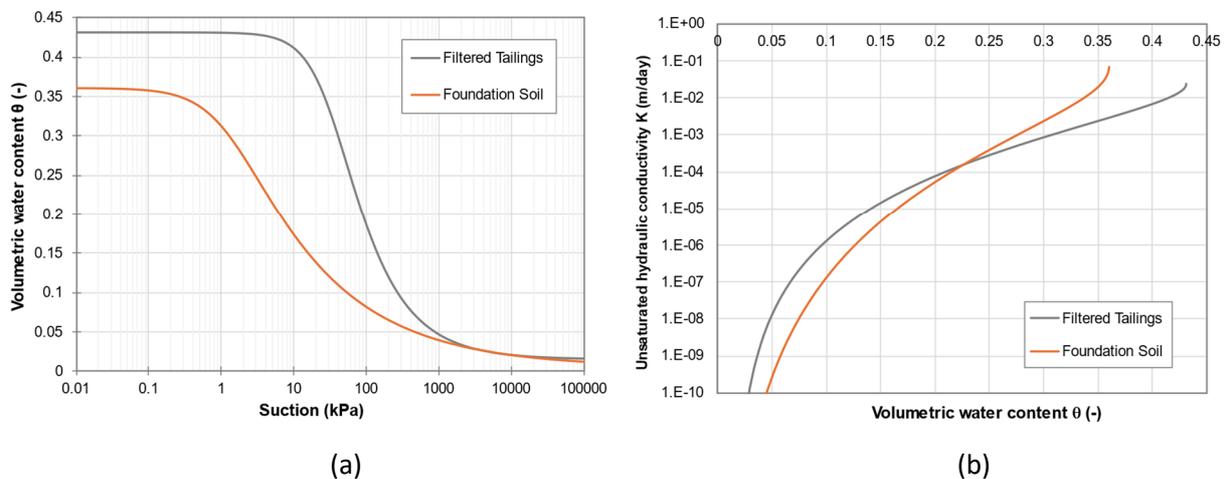


Figure 2 Materials studied. (a) Soil–water characteristic curves; (b) Unsaturated hydraulic conductivity

2.3 Unsaturated flow model

The modelling was conducted using HYDRUS-1D software (Šimůnek et al. 2018), which specialises in simulating unsaturated flow systems through the finite element method. Its intuitive user interface, combined with its capacity to integrate Python scripts, provides substantial flexibility for customising models to suit specific site conditions. This functionality enables comprehensive simulations and analyses across a diverse range of scenarios, including water infiltration and contaminant migration.

One-dimensional models were developed to represent a 30-metre-thick profile of tailings overlying a 30-metre-depth layer of foundation soil. This configuration allows for the assessment of vertical water flow from the tailings into the ground material.

The models were simulated over a period of 50 years to capture the long-term behaviour of the system. A climate boundary condition was applied to the surface of the column. Climatic conditions are representative of those found in northern Chile. At the bottom of the column a unit gradient is assigned to permit free drainage in vertical direction. As an initial condition, the in situ volumetric water content was used for each material (see Table 1). Figure 3 shows a conceptualisation of the model geometry.

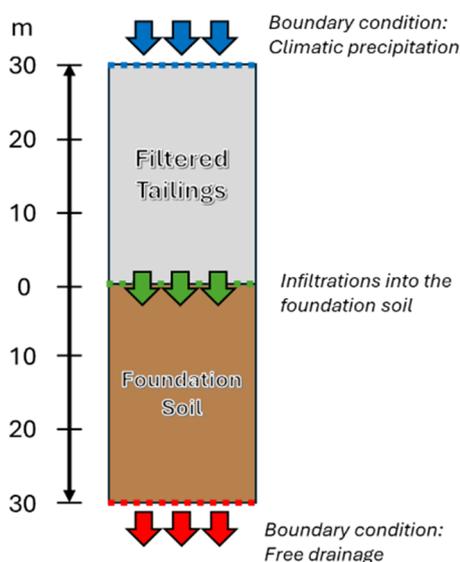


Figure 3 Model geometry

2.4 Local sensitivity analysis

Local sensitivity analysis is a method used to evaluate the impact of minor changes in model parameters on the output of a model. This approach involves altering one parameter at a time while keeping others constant to observe the effect on the model’s results. It provides insights into which parameters have the greatest influence on model behaviour, allowing for the identification of key parameters that need accurate estimation. The quantitative evaluation is carried out using the sensitivity index (defined in equation 2).

The sensitivity analysis performed in this study corresponds to a classical approach focused on the calculation of the partial derivative of the parameter with respect to the outcomes of the model results. This allows estimation of the degree of influence of each parameter with respect to a baseline parameter set. In summary, six parameters were considered, and 500 simulations were performed for each (i.e. 3,000 simulations in total) to explore the variability in unsaturated flow behaviour due to different combinations of fitting parameters for the WRC. The van Genuchten parameters θ_r , θ_s , α and n were varied within predefined ranges based on experimental data and relevant literature. In addition, two key parameters of the flow model were modified: the saturated hydraulic conductivity (K_s) and the initial moisture content (θ_i).

Each simulation assessed the water flow from the tailings to the foundation soil, providing insights into the influence of each parameter on the hydrological behaviour of the system. The hydrological conditions of the

simulations were adapted to those typical of northern Chile. The local sensitivity analysis procedure used in this study is described below.

Local differentiation method—explanation of the sensitivity analysis steps:

1. A set of parameters of interest is defined. A range of values for each parameter (p_i) is established using field/literature references. The parameters of interest P_i are assumed to lie within a specific range, that is, $p_{in} \in [P_{i_{min}}, p_{i_{max}}]$ (see Table 3)
2. A set of uniform distributed parameters is generated for the parameter p_i using the Latin hypercube sampling method (Dutta & Gandomi 2020). A number of 500 is used as the size sample and the specified ranges of values defined for each parameter are used as lower/upper boundary values.
3. For each parameter (i), 500 flow simulations are executed, obtaining 500 outputs, i.e.
4. $\{\{O_1, \dots, O_n\}_K, \{O_1, \dots, O_n\}_\alpha, \{O_1, \dots, O_n\}_n, \{O_1, \dots, O_n\}_{\theta_r}, \{O_1, \dots, O_n\}_{\theta_{sat}}, \{O_1, \dots, O_n\}_{\theta_i}\}$
5. For each parameter i in the set $\{O_1, \dots, O_n\}_{p_i}$, an evaluation of the partial derivative is performed (rate of change of the output results with respect to the change of the input parameter). This calculation gives us a sensitivity index value (I).

$$I = \left| \frac{\partial O_i}{\partial p_i} \frac{p_i}{O_i} \right| \sim \left| \frac{(O_i - O_0) p_i}{(p_i - p_0) O_i} \right| \tag{2}$$

obtaining

$$I_{p_i} = \{I_1, \dots, I_n\}_{p_i} \tag{3}$$

6. Perform a statistical analysis on the resulting sensitive index sets.
7. Compare and analyse the results.

The sensitivity index can be classified according to the parameters established in Table 2, as defined in the work of Liu et al. (2019).

Table 2 Parameter sensitivity classification

Classification	Index	Susceptibility
I	$0 \leq I \leq 0.05$	Insensitive
II	$0.05 \leq I \leq 0.2$	Commonly sensitive
III	$0.2 \leq I \leq 1$	Highly sensitive
IV	$I \geq 1$	Overwhelmingly sensitive

3 Results

3.1 Moisture content profiles

Figure 4 shows the simulated moisture content profile representative of a 50-year drainage period for the different scenarios tested. The base case is shown in white, and the results obtained for the full range of variation considered for each parameter during local sensitivity analysis are shown in blue. The results show the wide range of configurations that can be achieved in the tailings profile, depending on the different values adopted for each soil parameter. In all the tested scenarios the results showed a limited advance of the water from the tailings through the soil foundation. In this case, given the typical conditions in northern Chile, the foundation material is considered to be initially in an almost dry condition with an extremely low effective hydraulic conductivity, lower than that of the tailings and thus providing powerful hydraulic restraint for the water transmission among materials.

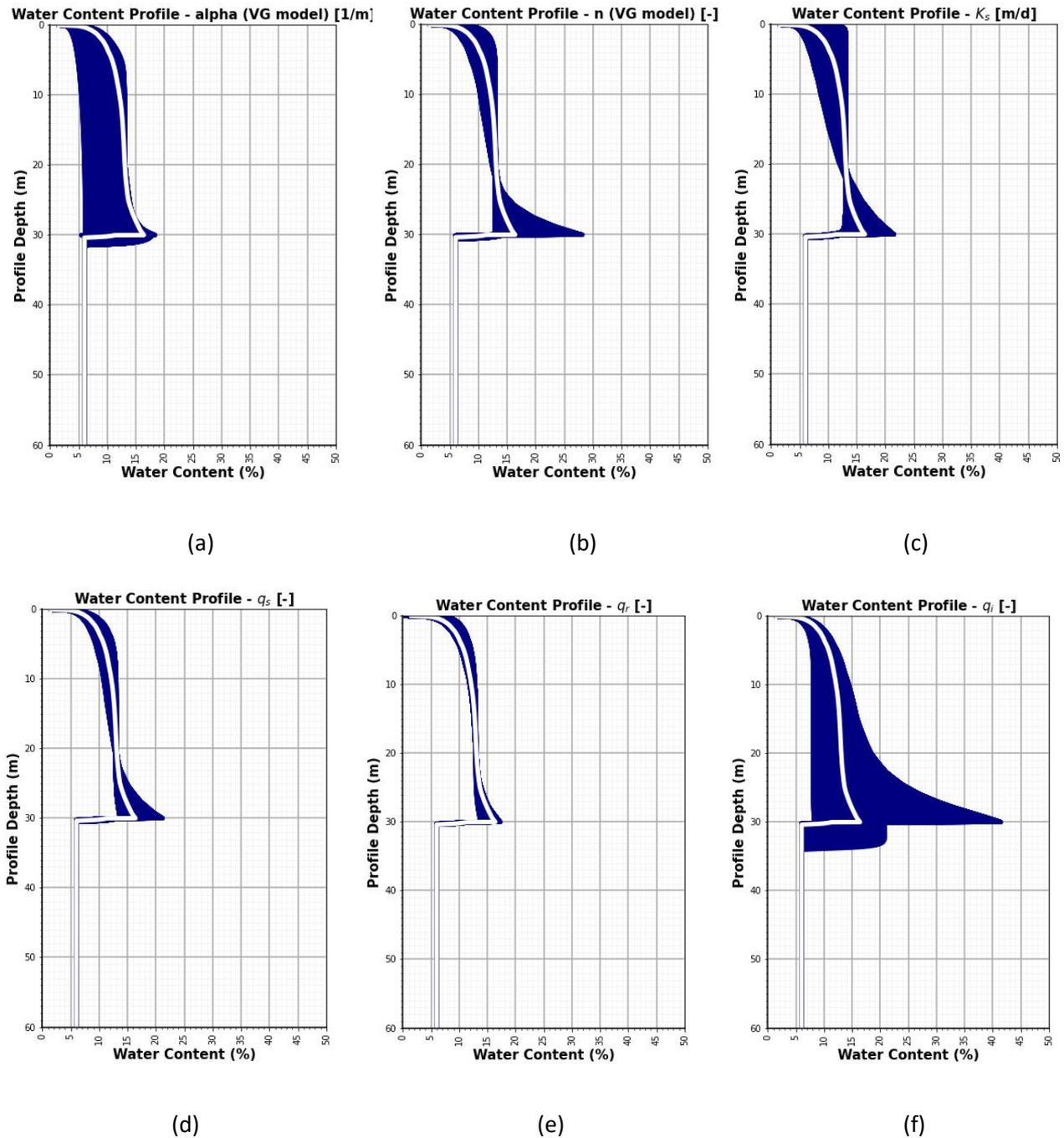


Figure 4 Water content profiles

3.2 Variation ranges of parameters

Figure 5 shows the sensitivity index (I) determined for all parameters over the entire range of variation studied. Results are presented for a 50-year simulation period, but this index could vary depending on the time selected (as shown in Figure 5). In most cases the simulated trend for the sensitivity index I along of the range of different parameter values tested could lead to the setting of a range of variation where the sensitivity analysis for each parameter could be constrained in order avoid evaluation of a range of values so wide that considered values are associated with a completely different material. In the figures, base case (filtered tailings, Table 1) is plotted as a 0 index value. With the aim of defining a rank of variation for each parameter where the sensitivity analysis could be performed, the next criteria used were as follows: firstly, a mean index I for the full evaluated rank, tested for specific time and standard deviation of this index, was

calculated. Next, a second constrained mean index I and its standard deviation were performed by filtering the values of I by the rank of the parameter values, i.e. the mean I value was computed by considering just a subset of values but not the whole rank. Regarding the standard deviation of the mean index, in general this increased as the parameter rank did, so constraining the boundaries of the rank used in the calculation also reduced the variance. To obtain the I constrained value for each sensitivity parameter tested, the constrained rank for the sensitivity analysis was obtained by defining a neighbourhood centred on the mean value where the calculated standard deviation of index I was the minimum. These results are shown in Table 3. For each parameter, a rank of variation for realisation of sensitivity analysis is presented. For values where its ranks of tested values vary within several orders of magnitude of difference, the rank is expressed in terms of order of magnitude. In the cases of characteristic moisture content values, rank of variation is evaluated with respect to the total porosity, i.e. the maximum volume of water possible to be managed. As stated before, the rank limits are centred with respect to the mean value of the parameter.

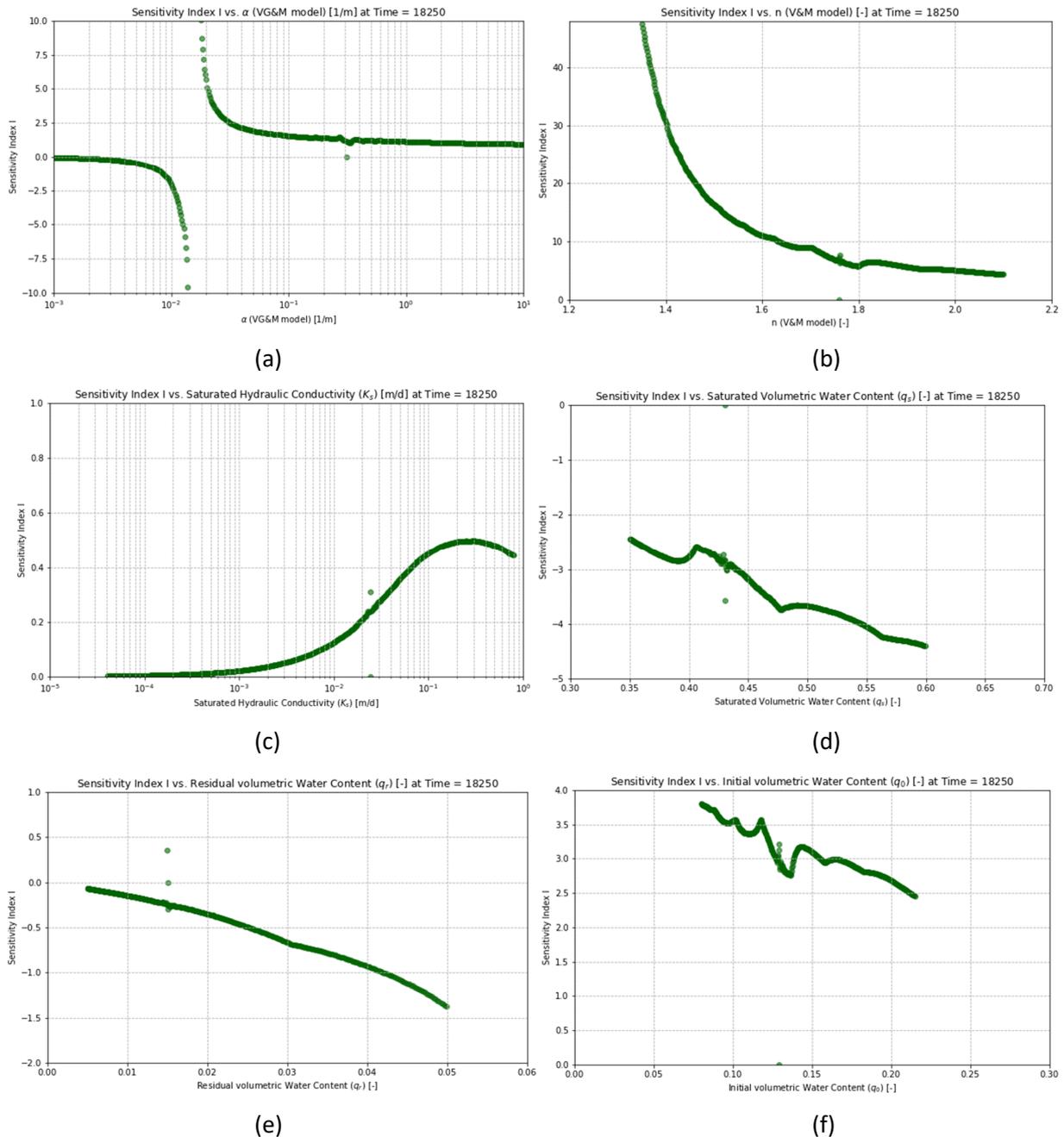


Figure 5 Sensitivity index across the entire range of variation of each parameter

Table 3 Rank variation for each parameter

Parameter	Mean value	Lower limit (full)	Upper limit (full)	Lower limit (filtered)	Upper limit (filtered)	Rank variation with respect to mean value
K_s (m/d)	0.023	0.0	0.8	0.003	0.1	+/- 1 magnitude order
α (1/kPa)	0.032	0.001	10	0.05	1.1	+/- 1 magnitude order
n	1.76	1.35	2.1	1.71	1.8	+/- 3–5% of mean value
θ_s	43.1%	35%	60%	39%	47%	+/- 10% of saturated moisture content
θ_r	1.50%	0.05%	5%	0%	3%	+/- 5% of saturated moisture content
θ_i	12.30%	8%	21.5%	10%	15%	+/- 5% of saturated moisture content

3.3 Local sensitivity index

Sensitivity indices were calculated for the different parameters α , n , θ_r , θ_s , θ_i and K_s . The output result that was used as a control parameter to calculate the I index was the cumulative infiltration flow from tailings to the soil foundation. Figure 6 shows the evolution of the average sensitivity index of the filtered data, in absolute terms, according to the recommended variation ranges presented in Table 3, over the evaluated period. After 50 years the sensitivity index associated with the residual moisture (θ_r) and saturated hydraulic conductivity K_s is slightly above 0.2, classifying them as ‘highly sensitive’. The parameter α is above 1. The parameters for saturation moisture (θ_s) and initial moisture (θ_i) show values close to 3, while the parameter n shows sensitivity index values around 7, classifying it as ‘overwhelmingly sensitive’.

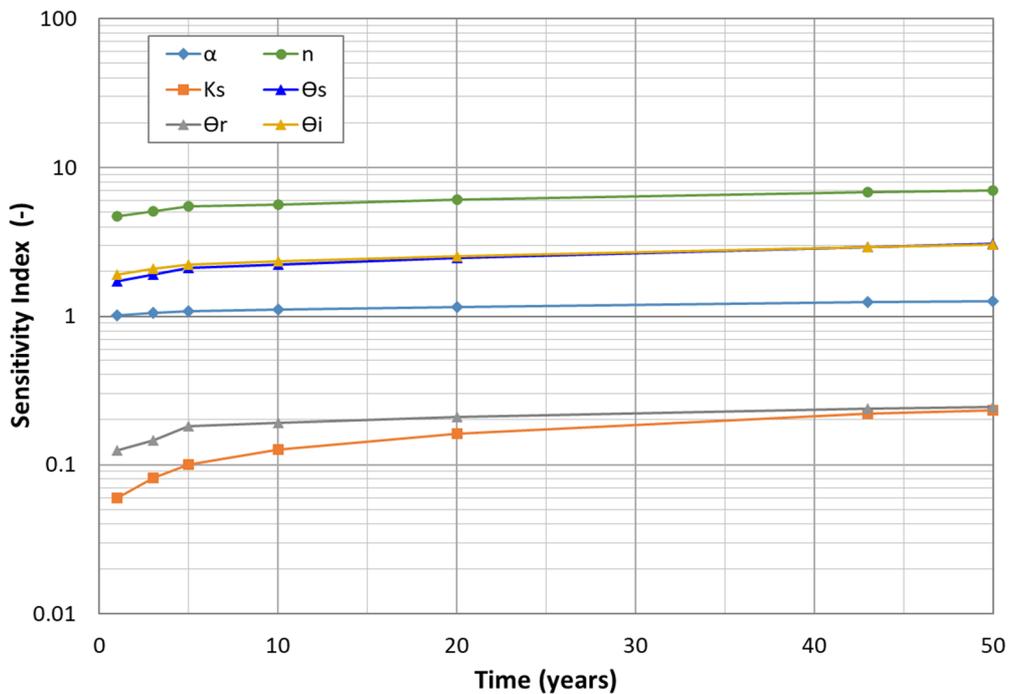


Figure 6 Sensitivity index, in absolute value

3.4 Evaluation under free drainage without foundation soil

In addition to the model with foundation soil, an alternative scenario with free drainage at the base of the filtered tailings was evaluated. This approach allows for the analysis of the unsaturated flow behaviour without the influence of the underlying soil, providing an additional perspective on the system’s dynamics. Figure 7 shows the evolution of the average sensitivity index of the filtered data, in absolute terms, in accordance with the recommended variation ranges for the alternative scenario without foundation soil.

In this scenario, the influence coefficients showed a change in trend for the parameters K (hydraulic conductivity) and α , which now exhibit greater sensitivity compared to the models with foundation soil. However, the parameter n , saturated moisture (θ_s) and the initial moisture (θ_i) continue to be the most significant factors in determining flow behaviour.

The increased sensitivity of K_s and α in the free drainage case suggests that these parameters play a more critical role in the material’s ability to manage water flow when there is no restriction at the base. This highlights the need to consider different drainage scenarios when designing management strategies for filtered tailings deposits.

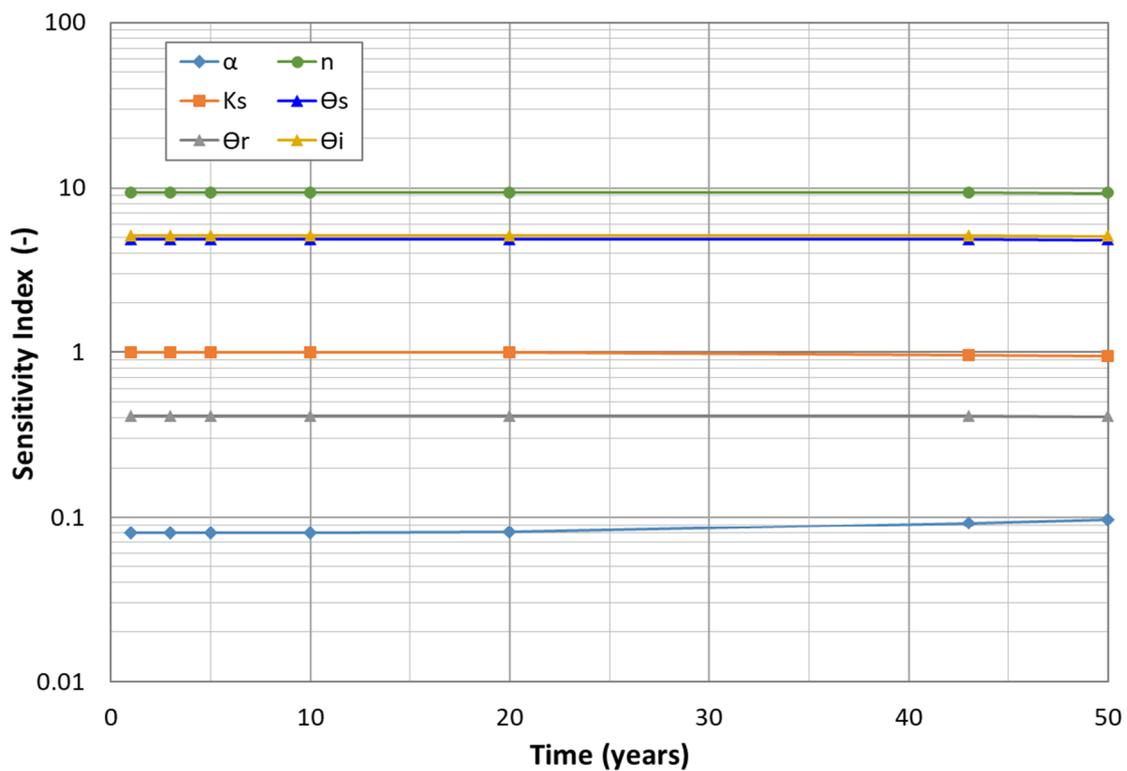


Figure 7 Sensitivity index, absolute value: case without foundation soil

4 Discussion

The results of this study highlight the critical importance of the WRC fitting parameters in modelling unsaturated flows in filtered tailings. The moisture profiles with depth show significant variation, and the flow at the material interface, namely from the filtered tailings to the foundation soil, also show considerable dispersion. It is noteworthy that filtering the results based on the identified ranges yields a more constrained behaviour, allowing for a more realistic representation of the phenomenon. The pronounced sensitivity of the parameters n , θ_s , and θ_i suggests that these are key determinants of the material’s capacity to manage water infiltration in the tailings deposit, while the parameters K_s and θ_r are the least sensitive. However, this is only applicable to the model constructed for this study. When executing the same procedure solely with

filtered tailings and a free drainage boundary condition at the base, i.e. without foundation soil, the most relevant sensitive parameters remain n , θ_s , and θ_i , but the least sensitive parameters shift to α and θ_r .

This finding is consistent, although not identical, with previous studies (Chen et al. 2016) that have identified the parameters α and n as significant influences on the hydraulic behaviour of soils and porous materials. When comparing results with the existing literature, there are similarities in the relative importance of the van Genuchten parameters. However, the focus on a specific context of filtered tailings in northern Chile provides a unique perspective that highlights the need to consider local site characteristics when applying generic SWCC models.

The knowledge gained about the sensitivity of the fitting parameters has direct implications for tailings storage facilities management. The ability to more accurately predict water flow towards the foundation soil can improve risk mitigation strategies, particularly in high precipitation scenarios. In addition, identifying the most influential parameters allows engineers and designers to concentrate their efforts on measuring and adjusting these values to optimise deposit stability at design stages.

5 Conclusion

This study provides a detailed insight into the influence of the fitting parameters of the WRC on the unsaturated flow behaviour in filtered tailings from northern Chile, and specifically for a particular case in a 1D unsaturated flow model with extensive local sensitivity analysis.

The parameters n and θ_s of the van Genuchten model, in addition to the initial moisture (θ_i), are the most influential in determining the water flow towards the foundation soil. These parameters must be carefully selected to improve the accuracy of the flow predictions. It is important to note that the sensitivity of the parameters depends on the case studied, with a significant change observed in the sensitivity of the parameters α and K_s for cases with and without foundation soil.

Significant variability was observed in the accumulated flow towards the foundation soil, depending on the combinations of fitting parameters and initial moisture conditions. It is important to mention that the results are strongly controlled by the presence of the foundation soil, which, due to its almost negligible initial moisture, presents an unsaturated hydraulic conductivity lower than that of the filtered tailings. When filtered tailings only are analysed the behaviour is different.

The results of this study will enable designers and practitioners to understand which parameters of the van Genuchten model are most relevant when performing a sensitivity analysis. This will allow parameters to be varied within recommended ranges and will save modelling time in more complex 2D or 3D unsaturated flow models.

The methodology used in this study is easily reproducible for other types of problems and/or materials. It is recommended that this type of sensitivity analysis be performed to determine which parameters are most sensitive in the phenomenon to be reproduced and then that the variation ranges be determined before performing sensitivity analyses in complex unsaturated flow models.

Despite the progress made, this study has limitations due to the variability of field conditions and the simplification of the 1D model. It is always advisable to carry out laboratory tests to obtain the most realistic WRC. Performing sensitivity analyses based on measured data is preferable to using indirect estimation methods.

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