MATEC Web of Conferences **337**, 02001 (2021)
PanAm-UNSAT 2021

https://doi.org/10.1051/matecconf/202133702001

Modelling of soil-water retention curve considering the effects of existing salt solution in the pore fluid

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Abstract. Soil-water retention curve (SWRC) has a wide application in geoenvironmental engineering from the predication of unsaturated shear strength to transient two-phase flow and stability analyses. Although various SWRC models have been proposed to take into account some influencing factors, less attention has been given to consider the effects of pore fluid osmotic potential. Therefore, the key objective of this study is to extend van Genchten's model so that osmotic potential is considered as an independent factor governing the SWRC behavior. The new model comprises only six variables, which can be calibrated through minimal experimental measurements. More importantly, most of the model parameters have physical meaning by correlating macroscopic volumetric behavior and general trends of SWRC to osmotic potential. The results of validation tests revealed that the new osmotic-dependent SWRC model can predict the retention data in terms of both total and matric suction for two different soils and various molar concentrations very good. The proposed modeling approach does not require any advanced mercury intrusion porosimetry (MIP) tests, yet it can deliver excellent predictions by calibrating only six parameters which are far less than those incorporated into similar models for saline water permeating through the pore structure.

1 Introduction

The soil-water retention curve (SWRC) expresses the relationship between soil moisture content and suction [1, 2]. Despite various technical terminologies commonly used, and wide applications in different disciplines including geoenvironmental engineering, hydro-geological processes, and petroleum engineering, the physical implication of SWRC is the ability of porous media to retain fluid at specified aqueous potential under steady-state or transient conditions [3, 4]. In other words, the SWRC is one of the key elements in conjunction with the hydraulic conductivity for reliable analysis of subsurface two-phase flow under transient wetting or drying scenarios [5, 6, 7]. As a result, the rigorous characterization and modeling of this hydro-mechanical feature is inevitable for investigation of slope stability, two-immiscible phase flow, volumetric and shear strength behavior [8, 9, 10, 11, 12].

Current approaches for modeling of the SWRC can be categorized into four groups [5]. The first group includes parametric functions that are suitable for fitting existing data, such as the Brooks and Corey [13] or van Genuchten [14] model. The second group consists of models based on soil particle size distribution such as those introduced by Aria and Paris [15] or Hovercamp and Perlang [16], generally making use of statistical concepts. The third group employs the pore size distribution as a fundamental soil feature determined usually from the mercury intrusion porosimetry (MIP) test. Accordingly, soil porosity is usually divided into two groups of micro- and macro-pores, and water retention behavior is hence interpreted and modeled in the capillary and adsorption domain separately [17]. For example, the recent models introduced by Qiao [18] and Dieudonne [19] belong to this category. The last group belongs to pedotransfer functions (PTF), correlating the SWRC functions to some basic and easily-determined soil properties such as porosity, organic carbon content, and soil texture [5].

However, most of these modeling approaches have the shortcoming of ignoring the impurity of permeating aqueous fluid through pore structure by simplifying it with distilled water. In other words, the SWRC models capable of considering pore water salinity into the water retention trends are rather limited and recent [20]. On the other hand, the inclusion of water salinity into a reliable model cannot be denied as recent experimental measurements proved the significant role of fluid salinity on SWRC, swelling and collapse potential, hydraulic conductivity, and compressibility [21, 22, 23, 24, 25]. Further details on these phenomena are provided accordingly.

He et al. [22] investigated the effects of salt on both volumetric and retention behavior of GMZ bentonite. The measured laboratory data were simulated based on the retention model proposed by Gallipoli et al. [26]. He et al. [23] also employed the Fredland and Xing [27] modeling approach to mathematically mimic the results of water retention experiments. However, it is worth mentioning that the proposed models [22, 23] are mainly restricted to

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the specific soil type and salt used, i.e. bentonite and sodium chloride, and hence it may not be generally used for various soil types and salt species. Ma et al. [9] explored the effects of salinity on the SWRC of sandy soil for soil remediation and agricultural development along the coast. The van Genuchten model [14] was used to simulate the hysteresis of soil-saline water retention behavior. An analytical closed-form solution was proposed recently by Scelsi et al. [20] to model the SWRC of compacted bentonite at different salt concentrations. The satisfactory performance of the model, however, relies on incorporating a relatively large number of parameters, i.e. 11, into the analytical modeling. To calibrate this model, it is necessary to conduct a MIP test which is relatively advanced and expensive to some extent [28].

As a result of this brief literature survey, there has been still a lack of a simple model that can simulate the SWRC of soils subjected to pore fluid containing different concentrations of various salt solution species. Therefore, this study aims to provide a simplistic, yet precise modeling approach to consider the influence of salt solution concentrations in simulating the SWRC behavior based on minimal experimental data excluding the requirement of advanced testing. Details on the development, calibration procedure, and validation of the new model which is an extension of the original van Genuchten model [14] with three additional parameters are presented in this paper. Before introducing the new modelling framework, a complete section is presented to review the detailed influence of salt solution on some aspects of the soil behavior relevant to this study.

2 The influence of salt solution on soil behavior

Total suction in soil consists of two components: matric suction and osmotic suction. The former is mainly governed by the pore structure and air-water interface properties, while the presence of dissolved salt into the pore fluid gives rise to the latter. Indeed, the existence of the osmotic suction can greatly affect the mechanical behavior of clayey soils because of the clay-salt interactions [23, 29, 30]. Moreover, several other previously well-studied factors such as the soil microstructure, type of soil, mineralogy, density, initial water content, stress history, sample preparation technique, and confining stress can also affect the behavior of unsaturated soils [31, 32].

There have been several studies revealing the significant role of pore fluid concentration on different hydro-mechanical aspects of compacted bentonite. The reason lays behind some unique properties of bentonite such as low permeability and good adsorption characteristics, resulted in the global usage of this buffer/backfill engineered material as a choice of the first priority in high-level radioactive waste repository across many countries [22, 23]. Previous studies indicated that a rise in molar concentration of salt species including NaCl [22, 23, 33, 34], $CaCl_2$ [33, 34], and KCl [33] reduces the swelling potential of bentonite but at different rates. The observed mechanical feature is attributed to the two mechanisms of osmotically induced consolidation and osmotic consolidation. Indeed, the presence of salt in pore fluid leads to a decrease in the level of chemical potential compared to distilled water, so to achieve the chemical balance, water flowing outward the clay surface in response to osmotic gradients. This flow process induces negative pore fluid pressure that increases the effective stress and some consolidation occurs accordingly. Osmotic consolidation, on the other hand, occurs due to a reduction in interparticle repulsive stresses upon changes in pore fluid concentration. As a result, the increase in salt concentration reduces both the swelling rate and porosity of the soil samples [35].

Microstructural evidence has shown that compacted bentonite comprises a dual-porosity structure, consisting of two groups of macro- and micro-pores [19]. Looking into the effects of salt concentrations on pore characteristics has revealed a decline in the total pore volume with increasing salt concentration. Indeed, salt diffusion into clay results in a reduction in the thickness of the diffuse double layer (DDL), and hence the repulsive interparticle forces be reduced [36]. These pore-scale salt-clay interactions eventually lead to a rise and drop in the volume of macro- and micro-pores, respectively. As a result, less water retention capability, and the steeper curve is delivered by increasing pore water salinity when the retention data be depicted in terms of matric suction [37]. However, if the retention data is expressed in terms of total suction, the opposite behavior is expected as the inclusion of osmotic suction can significantly enhance the water retention capabilities [22, 23]. Therefore, it is very important that a modeling approach can be effectively used to predict the retention data not only in terms of matric suction but also in terms of total suction without any preference of each component over the other.

3 The newly proposed retention model for different salt solution concentration

van Genuchten [14] proposed a smooth three-parameter model based on an analytical solution for the soil-water retention curve [38] according to equation (1):

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = [1 + (\alpha\,\psi)^n]^{-m} \tag{1}$$

where θ is volumetric water content, θ_r is residual volumetric water content, and θ_s is saturated volumetric water content which is equal to the porosity, ψ represents the soil suction (matric or total), α is the model parameter related to air entry value, n is related to the pore size distribution, and m can reflect the overall symmetry of the retention curve [38], which also can be expressed as a function of parameter n [38, 39]. van Genuchten [14] model has been used in the development of many subsequent SWRC models. For example, Gallipoli [26] modified the van Genuchten [14] model by taking into account the effects of void ratio. Zhou et al. [28] also developed the model proposed by Gallipoli with inclusion of microstructural evolution determined from the MIP test results as a consequence of hydro-mechanical loading. Following the contribution of Zhou et al. [28] in correlating the α parameter to the net stress level, one can infer that similar phenomenological consequence be expected for the influence of water salinity on retention behavior. The reason is the previous experimental observations revealing an enhancement of water retention capability in terms of total suction due to a rise in pore water salinity. In other words, both net stress and osmotic suction seems to affect the SWRC of clayey soil in similar way [35]. Therefore, the original van Genuchten model can be further modified according to Equation (2) to consider the influence of osmotic suction, assuming the above postulation is valid at least from a qualitative point of view at the moment.

$$\theta = \theta_{\mathrm{r}} + (\theta_{\mathrm{s}} - \theta_{\mathrm{r}}) \left\{ 1 + \left[\alpha \left(1 + \frac{\pi}{\psi_{\mathrm{ref}}} \right)^{\beta} \psi \right]^{n} \right\}^{-m} \qquad (2)$$

where β is a new parameter that depends on the salt concentration or the osmotic potential. This parameter, in addition to the three main parameters of the van Genuchten model, namely n, m, and α, forms the four main parameters of the present model. There is no need to mention that the three van Genuchten model parameters have been calibrated and available for many soils in the literature or they can be easily determined based on conventional distilled water retention data. Besides, to calibrate the new parameter, β, only one retention dataset corresponding to a given salt specie having a certain pore fluid concentration is also needed.

The osmotic suction, π, in Equation (2) can be calculated using the van't Hoff formulation expressed according to Equation (3):

$$\pi = iRTM \qquad (3)$$

where i is the number of ions for the salt dissolved in solution (e.g. 2 for NaCl), R is the universal gas constant equals to 8.32 J/(mol.K), T is the absolute temperature in Kelvin and M is the molar concentration [29]. The last parameter in Equation (2) is ψ_{ref}, denoting a reference suction of 1 MPa to normalize the osmotic suction with the same unit and hence to make it dimensionless. In addition, the surplus unity inside the parentheses of Equation (2) contributes to the stability of the relationship. Therefore, it makes the smooth transform from the new model to the original van Genuchten model for distilled water possible, which can be of primary importance in numerical modeling.

It should be noted that there is no general consensus on the interpretation and definition of the residual volumetric water content (θ_{r}) in the literature. Some researchers consider this parameter simply as a fitting parameter with no specific physical meaning, but others consider it corresponding to a physical state where the water phase starts to be discontinuous [5]. A simplistic approach, however, considers it equivalent to the amount of water corresponding to the matric suction of 1500 kPa [40]. According to the experimental observations, salinity mainly affects the water retention behavior at suction (matric or tatal) range limited to the residual state, while all the retention curves are assumed to converge to that of distilled water at high matric or total suction range independent of salt concentrations [8]. Given that this assumption is correct at a premature state of measurements and knowledge for higher range of matric or total suction beyond the residual state, the value of θ_{r} is assumed a constant independent of salinity conditions. In other words, the retention data of distilled water is used to infer the residual water content for a soil under consideration. The procedure is explained in the following section.

The saturated volumetric water content, θ_{s}, is the same as soil porosity according to the mass-volume relationships. Experimental results indicated that porosity at saturated conditions varies with changes in the salt concentration. He et al. [23] used a hyperbolic function to correlate the porosity with salt concentration. In this study, it is assumed that a power relationship similar to Equation (4) can also be reliably used to correlate the abovementioned variables. This postulation will be supported by validation test results presented in the next section.

$$\theta_{\mathrm{s}} = b \left(1 + \frac{\pi}{\psi_0} \right)^{r} \qquad (4)$$

where b and r are the additional two model parameters which can be determined by fitting the Equation (4) to the measured data for saturated volumetric water content against salt concentrations. As a result, the present model contains three additional parameters to the original van Genuchten model or six parameters in total. It should also be noted that the influence of salt solution on SWRC could be different and even opposite if the data are represented in terms of matric, or total components of suction. However, the modelling framework is flexible in adapting to both matric and total suction components if the basic calibration measurements are available. The performance of this modelling approach in prediction of the SWRC in the presence of different salt solution concentrations is explained and validated for two different types of soils.

4 Model predictions and validation against experimental results

4.1. GMZ bentonite

The experimental results reported by He et al. [23] was used as the first dataset for calibration and validation the new model. The GMZ bentonite used in that study was Na-type bentonite with a high cation exchange capacity (77.6 mmol/100g) and high adsorption. Some of the most important characteristics of this type of bentonite are the specific gravity of 2.66, the liquid limit of 276%, and the plastic limit of 37%. Bentonite from Gaomiaozi (GMZ), located 300 km northwest of Beijing, has been reckoned as the preferred buffer/backfill material for constructing engineering barriers in deep geological repositories. In the study of He et al. [23], the GMZ bentonite powder with an initial water content of 11.7% was oven-dried at 105°C for 24 h. Afterwards, distilled water, 0.5 mol/L, 1.0 mol/L, and 1.5 mol/L NaCl solutions were sprayed on the dried powder to achieve a target water content of 20%. Eventually, the SWRC for different concentrations was determined using the vapor phase technique as illustrated in Figure 1 [23].

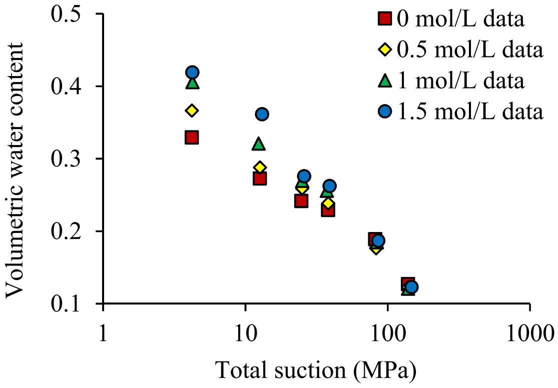

Fig. 1. SWRC data of compacted GMZ bentonite for different NaCl molar concentrations [23].

According to Figure 1, there is a rise in drying water retention capability with an increase in the pore water salinity in the total suction space. Moreover, measured data points indicates that differences vanishes with enhancement of total suction and hence the value of residual water content can be approximately assumed 0.15 where all the retention data converge to corresponding values of distilled water. In addition, the variations in the saturated volumetric water content (porosity) with molarity can be inferred from the results of Figure 1.

As explained in the previous section, a power relationship is used according to Figure 2(a) to obtain the two model parameters related to salt concentrations. According to this figure, the parameters b and r introduced in Equation (4) is determined as 0.32 and 0.12, respectively. In the rest of the calibration process, the values of the four main parameters, namely n, m, α, and β, must be determined. The first three parameters are the van Genuchten model parameters determined for the SWRC corresponding to distilled water. The determination of β parameter requires the use of a retention curve corresponding to an arbitrary salt concentration. For example, the retention data corresponding to 1 mol/L concentration was used to calibrate this parameter (Figure 2b). A summary of the calibrated model parameters for the GMZ bentonite permeated with different salt concentrations is given in Table 1. Eventually, the water retention behavior of the soil can be predicted using the calibrated model for all desired pore fluid molar concentrations. The performance of the model, for example, is checked against the measured SWRCs corresponding to 0.5 mol/L and 1.5 mol/L in Figure 2(c). The results confirm the capability of this model in precise capturing of the retention data.

To examine the accuracy of the proposed model in predicting retention behavior quantitatively, two statistical parameters of root mean square errors (RMSE) and the coefficient of determination (R^2) were adopted. The RMSE is an indicator of the overall error in the model and should vanish for the best model performance, while an R^2 as close as possible to unity is desirable to achieve the best model performance [41]. The following equations can be used to calculate these two quantities, respectively.

$$\mathrm{RMSE} = \sqrt{\sum_{i=1}^{n}\left(\theta_i - \theta_i'\right)^2} \tag{5}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(\theta_i - \theta_i'\right)^2}{\sum_{i=1}^{n}\left(\theta_i - \bar{\theta}\right)^2} \tag{6}$$

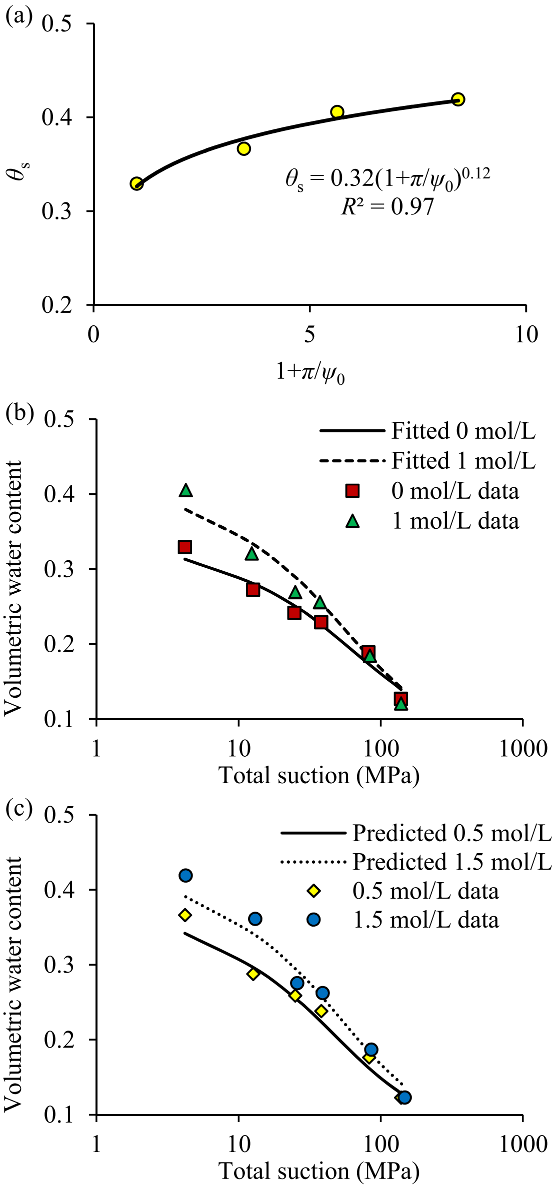

Fig. 2. Calibration and validation test results for GMZ bentonite: (a) and (b) model calibration, and (c) performance of the model

prediction of SWRC data in terms of total suction for the two levels of 0.5 and 1.5 mol/L NaCl molar concentrations.

where *n* is the number of soil-water retention data points for each test, θ_i and $\theta_i^{'}$ are the measured and predicted volumetric water content of the i^{th} data points, respectively, and $\bar{\theta}$ is the mean value of the measured volumetric water content for each test. According to the last two columns of Table 1, the R^2 value is about 0.98 and the values of RMSE varies from 0.01 to 0.02 for all salt concentration levels. As a result, the present model can give excellent predictions of the SWRC as a function of pore fluid saline concentration.

Table 1. Model parameters and its prediction capability for GMZ bentonite [23].

α	β	n	m
0.0002	0.09	0.8	36.4
Pore fluid concentration (mol/L)	**Osmotic suction (kPa)**	**RMSE**	R^2
0	0.0	0.012	0.97
0.5	2476.4	0.013	0.98
1.0	4636.0	0.017	0.98
1.5	7429.0	0.017	0.98

4.2. Karnataka clay

The second validation dataset was selected based on the experimental work of Thyagaraj and Rao [35] in which the effect of osmotic suction on retention characteristics of compacted Karnataka clay was investigated. The maximum dry density and the optimum water content corresponding to the standard proctor effort for this soil were 1.42 Mg/m^3 and 28%, respectively. In addition, the soil had a specific gravity of 2.71, and a cation exchange capacity of 56.6 meq/100 g. This soil was classified as CH according to the unified soil classification system [35].

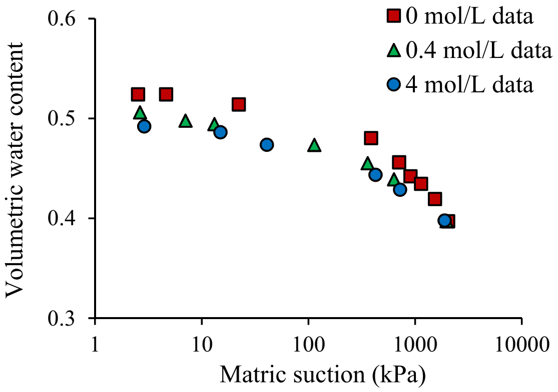

Fig. 3. SWRC data of of Karnataka compacted clay for different NaCl solutions [35].

Thyagaraj and Rao [35] explored the influence of induced osmotic suction gradient on the wetting retention curve of compacted clay specimens inundated with sodium chloride solutions/distilled water at vertical stress of 6.25 kPa in oedometer cells. In the experiments, soil samples were first prepared with distilled water and then subjected to concentrations of 0.4 mol/L and 4 mol/L. The results of wetting SWRC obtained from the experiment are depicted in Figure 3.

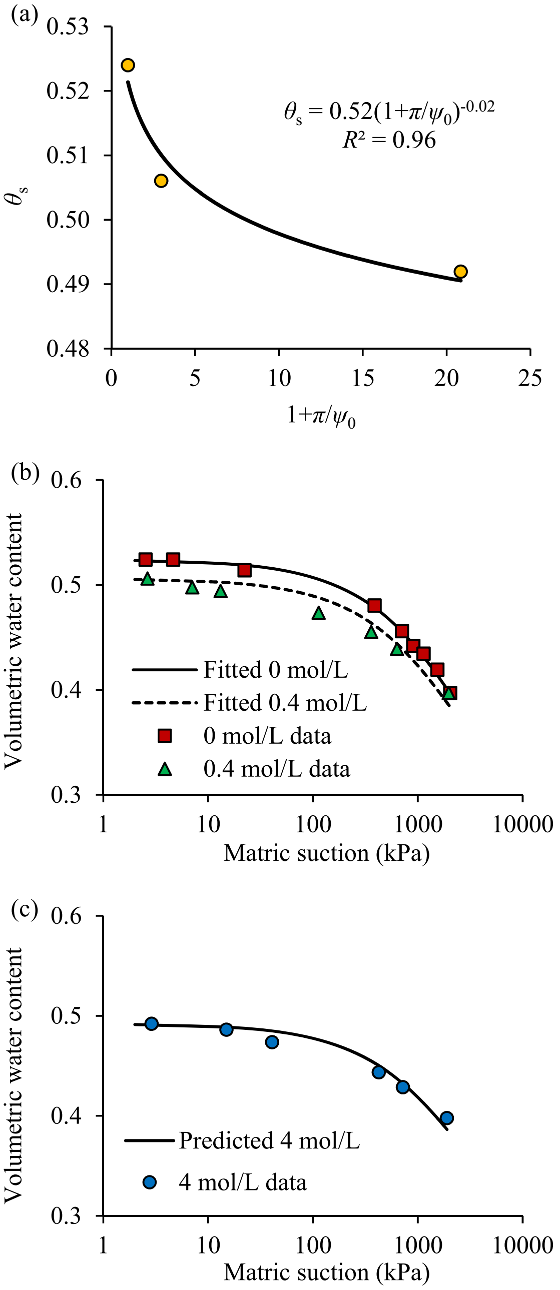

Fig. 4. Calibration and validation test results for Karnataka compacted clay: (a) and (b) model calibration, and (c) performance of the model prediction of SWRC data in terms of matric suction for the 4 mol/L NaCl molar concentrations.

It is worth noting that the original results [35] were reported in terms of gravimetric water content. Therefore, the corresponding volumetric water contents in Figure 3 were inferred on the basis of information provided for void ratios and specific gravity.

According to the results of Figure 3, it can be assumed that the amount of residual water is approximately equal to 0.4 and for all different concentrations of salt, this amount is assumed to be constant. In addition, the parameters b and r introduced in Equation (4) are obtained equal to 0.52 and -0.02, respectively. In the rest of the validation process of the proposed model, the values of the four main parameters of the model, namely n, m, α, and β, must be determined. The first three parameters will be obtained from distilled water data. The β parameter is calibrated based on the retention data corresponding to 0.4 mol/L (Figure 4b). Consequently, the SWRC of arbitrary concentrations can be predicted very straightforward based on the calibration results summarized in Table 2. For example, the predictions of SWRC corresponding to 4.0 mol/L concentration are compared with the experimental measurements in Figure 4(c). The results confirm that the present model can well predict the wetting SWRC in terms of matric suction for different salt concentrations.

The statistical results presented in Table 2 reveal that the model can deliver excellent predictions reflecting in the two statistical parameters considered. For a concentration of 4.0 mol/L, the RMSE and R^2 are equal to 0.022 and 0.98, respectively. It is worth noting that for this soil, unlike the GMZ soil, results were presented in terms of matric suction. In other words, the new model is robust enough to predict the retention behavior along both drying and wetting processes in terms of matric and total suction.

Table 2. Model parameters and its prediction capability for Karnataka compacted clay [35].

α	β	n	m
0.000002	0.08	0.8	63.6
Pore fluid concentration (mol/L)	**Osmotic suction (kPa)**	**RMSE**	R^2
0	0.0	0.005	1.00
0.4	1980.8	0.016	0.98
4.0	19840.0	0.022	0.98

5 Conclusions

In this paper, a new SWRC model was presented to consider the effects of pore water salinity. The proposed model made use of the van Genuchten's model [14] by incorporating three additional parameters into the original model. In order to calibrate the model parameters, the SWRC data corresponding to distilled water and a distinct salinity level is required. In addition, the osmotic-dependent porosity of a given soil should be determined either from a set of available data or a few oedometer measurements. According to the results, the following conclusions can be drawn:

1) The new model can predict water retention behavior of two different soils at various salt concentrations very well. The capability of model was proved through presenting two statistical criteria revealing high accuracy.

2) The proposed model relies only on data obtained from the conventional SWRC tests, implying that relatively costly experiments such as MIP tests are not required.

3) The model has the merit of predicting water retention behavior in terms of both total and matric suction.

4) In addition to the drying retention curve, the new model can predict the wetting branch as well, a capability which has been rarely reported in other modelling approaches.

5) Despite the simplicity of the new modelling framework, it can predict the retention behavior very precisely. It is therefore expected that this model can be reliably incorporated into numerical codes where the permeating aqueous fluid is not distilled water and has certain impurity, which is the case of many geoenvironmetal problems.

Acknowledgements

The financial support provided by the Research Grant Office at Sharif University of Technology for fundamental investigation of flow characteristics through deformable porous media by way of grant G970902 is gratefully acknowledged.

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