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Abstract

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Full Text

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Abstract: Attapulgite (ATP), as a natural inorganic material, has significant potential for affecting water transport in aeolian sandy soil. In this study, different ATP mixing rates, surface mixing depths, interlayer thicknesses, and profile reconstruction methods were established, and indoor soil-column experiments and numerical simulations were conducted to investigate the effects of ATP addition on infiltration and evaporation processes in aeolian sandy soil. An XGBoost prediction model was constructed, and the SHAP method was used to analyze key influencing factors and their interactions. The results showed that: (1) ATP addition effectively delayed the infiltration rate and inhibited evaporation, and the 8% mixing rate exhibited the optimal water-retention effect; the 2% and 10% mixing treatments differed significantly in effective water content, wetting-front migration time, and evaporation inhibition, verifying the sensitivity of the improvement effect to the application dosage. (2) Among different profile configurations, the T1 treatment (10 cm surface mixed layer + 10 cm deep interlayer) simultaneously achieved dual optimization of infiltration reduction and evaporation suppression. (3) The XGBoost model showed good accuracy in predicting wetting-front migration and cumulative infiltration (R^2 values all exceeded 0.98). The SHAP results indicated that cumulative infiltration, infiltration time, and saturated water content were the main driving factors. The results can provide data support and a technical pathway for the rational application of ATP in water-retention improvement of aeolian sandy soil.

Keywords: attapulgite; aeolian sandy soil; water transport; soil-column experiment; XGBoost model; SHAP method; HYDRUS-1D

Land sandy desertification and desertification in global arid and semi-arid regions have posed severe threats to human survival and regional sustainable development[1]. According to statistics, desertification has caused degradation of approximately 10%–20% of the world’ s dryland soils, directly affecting the production and livelihoods of about 2.5×10^8 people in developing countries[2–3]. At present, the area of sandy land has reached 1.72×10^6 km^2, accounting for approximately 17.93% of the total national land area; these lands are mainly distributed in the arid, semi-arid, and extremely arid regions of northwest China[4]. The problem of sandy desertification not only reduces the utilization efficiency of water and fertilizer in farmland and leads to a decline in cultivated-land quality, but also triggers a series of problems such as farmland abandonment, seriously threatening national food security[5–6]. Therefore, against the background of increasingly severe pressure on food security, the development, improvement, and utilization of desertified land resources, as well as the improvement of cultivated-land quality and effective cultivated-land area, have become urgent needs for socioeconomic development.

To address the challenges brought about by desertification, soil amendments have become an effective means of improving the structure of sandy soils and enhancing their capacity to retain water and fertilizer, and thus have been widely applied in desertification control[7]. Common amendments include organic, inorganic, chemically water-soluble polymer, and biological amendments[8–9]. However, the hot and dry climate of arid and semi-arid regions limits the stability of chemical and biological amendments[10–11]. Although both organic[12–13] and inorganic[14–15] amendments can improve the physicochemical properties of aeolian sandy soil, inorganic amendments have greater advantages in terms of cost and resource availability. Attapulgite (ATP), as a natural inorganic amendment, has considerable application potential owing to its abundant reserves, low price, good adsorption capacity, and strong cation-exchange capacity, especially in desertification control in northwest China[16–20]. Meanwhile, studies have shown that ATP application can effectively improve soil bulk density and pH, enhance the stability of soil aggregates, significantly improve the water-holding capacity of aeolian sandy soil, and delay water infiltration[21–24]. However, existing studies have mainly focused on indoor soil-column experiments, and there is still a lack of mathematical models capable of quantitatively characterizing the mechanisms by which ATP affects water transport in aeolian sandy soil, especially systematic modeling studies under different mixing methods.

The traditional physical model HYDRUS-1D describes unsaturated soil water movement through the Richards equation. Its simulation accuracy depends heavily on the accurate calibration of soil characteristic parameters, hydraulic parameters, and other factors; however, in the process of obtaining these parameters, unavoidable errors usually arise due to the influence of the testing environment and equipment. Therefore, when HYDRUS-1D is used to simulate soil infiltration and evaporation processes, it is affected by the cumulative errors of multiple parameters.

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effect, and their simulated results often deviate to some extent from actual conditions[^25-27]. To overcome these limitations, in recent years researchers have widely introduced machine-learning models with efficient nonlinear fitting capability into soil-science research. Compared with traditional methods such as linear regression[^28], support vector regression (SVR)[^29], and random forest (RF)[^30], XGBoost (eXtreme Gradient Boosting) has stronger ability to identify nonlinear relationships in high-dimensional feature spaces, and effectively reduces the risk of overfitting through regularization. Meanwhile, combining it with the SHAP (Shapley Additive Explanations) method helps quantify the contribution of each input feature to model predictions and their interactions, thereby improving model interpretability. This method provides new ideas and technical tools for identifying the main driving factors in the water-transport process of aeolian sandy soil after ATP addition.

In this study, the HYDRUS-1D physical model is combined with the XGBoost machine-learning model, taking into account the interpretability of physical processes while also improving the prediction accuracy of data-driven simulation. At the same time, the SHAP method is introduced to identify key driving factors and their interactions. The main objectives are: (1) to analyze the effects of different ATP mixing amounts, surface mixing thicknesses, and interlayer thicknesses on the water-transport characteristics of aeolian sandy soil; (2) to use the HYDRUS-1D model to simulate and calibrate water-migration processes under different scenarios; and (3) to predict water-transport dynamics based on the XGBoost model and SHAP method, and to analyze the dominant factors. The results can provide parameter support and modeling evidence for improvement measures aimed at "reducing infiltration and suppressing evaporation" in aeolian sandy soils in arid and semi-arid regions, and have practical guiding significance.

1 Materials and Methods

1.1 Experimental soil

The aeolian sandy soil was collected from Babusha Forest Farm, Gulang County, Wuwei City, Gansu Province, China (37°37′N, 103°06′E). Before sampling, surface debris was removed, and the sampling depth was 0–40 cm. The collected soil was air-dried, crushed, cleared of impurities, thoroughly mixed, and passed through a 2 mm sieve, then stored as reserve soil samples. The attapulgite was purchased from Gansu Jingyuan Hongfeng Aojing Soil Trade Co., Ltd., and was not treated in any way after purchase.

1.2 Experimental design and apparatus

To investigate the effects of attapulgite (ATP) on the hydraulic properties and water-transport patterns of aeolian sandy soil, this study conducted indoor soil-column infiltration and evaporation experiments. Four main factors were designed: mixing amount, surface mixing thickness, interlayer thickness, and profile configuration. Five levels were set for each factor, with one blank control, forming a total of 20 treatments. The experimental design was as follows:

(1) Mixing-amount design: the mass ratio of ATP to aeolian sandy soil was set at 0% (CK), 2%, 4%, 6%, 8%, and 10%, for a total of 6 groups including the control.

(2) Surface mixing-thickness design: the ATP mixing amount was fixed at 8%, and the surface mixing thickness was set at 5 cm, 10 cm, 15 cm, 20 cm, and 25 cm; the lower layer was original aeolian sandy soil.

(3) Interlayer thickness design: an interlayer was set 20 cm below the surface, with an ATP mixing amount of 8%; the thicknesses were 0.5 cm, 1.0 cm, 1.5 cm, 2.0 cm, and 2.5 cm, and the soil above and below the interlayer was original aeolian sandy soil.

(4) Profile-configuration design: the ATP mixing amount was uniformly set

at 8%, the surface mixing thickness at 10 cm, and the interlayer thickness at 1.0 cm; only the interlayer depth was adjusted, specifically as follows: interlayer depth 10–11 cm (T1), interlayer depth 15–16 cm (T2), interlayer depth 20–21 cm (T3), interlayer depth 25–26 cm (T4), and interlayer depth 30–31 cm (T5). A completely randomized design was adopted in this experiment, with 3 replicates for each group, and a total of 20 different application scenarios were set (Table 1).

The indoor infiltration experiment used a one-dimensional organic-glass soil-column device (Fig. 1). The soil column had an outer diameter of 11 cm, an inner diameter of 10 cm, and a height of 65 cm. Six sampling holes were set in the sidewall at 10 cm intervals; a vent hole was set at the bottom to prevent air blockage; and the top

Table 1 Experimental treatment

Factor category	Treatment code	Mixing ratio	Surface mixing thickness	Interlayer thickness	Interlayer position	Number of replicates
Control group	CK	0%	None	None	None	3
Mixing amount (Q)	Q1–Q5	2%, 4%, 6%,8%, 10%	Uniformly mixed (0–60 cm)	None	None	3
Surface mixing (R)	R1–R5	8%	5 cm, 10 cm, 15 cm,20 cm, 25 cm	None	None	3
Interlayer thickness (S)	S1–S5	8%	None	0.5 cm, 1.0 cm, 1.5 cm,2.0 cm, 2.5 cm	All located at 20 cm depth	3
Soil reconstruction configuration (T)	T1–T5	8%	Surface 10 cm	Surface 10 cm	10 cm, 15 cm, 20 cm,25 cm, 30 cm	3

Note: Depths in the table all indicate the vertical distance from the top of the soil column.

In the figure: Mariotte bottle; rubber tube; constant head; sampling holes; soil column; vent holes; height-adjustable support. Legend: aeolian sandy soil; mixed soil; attapulgite clay.

Fig. 1 Schematic diagram of the soil column infiltration experimental device

A constant 2 cm water head was supplied by a Mariotte bottle. Before the experiment, aeolian sandy soil and ATP were thoroughly mixed according to the designed mixing proportions; water was then added to an initial water content of $0.02\ cm^3 \cdot cm^{-3}$, and the samples were left to stand for 24 h so that soil water was uniformly distributed. Subsequently, according to the designed mixing depth and layer thickness, the soil was packed into the soil column layer by layer at the specified bulk density, and the surface was leveled after every 15 cm of filling. After the soil had been packed, the support was adjusted so that the bottom of the air-communication tube in the Mariotte bottle was maintained 2 cm above the soil surface, thereby ensuring a constant head during infiltration. After preparation was complete, the stopwatch was started at the same moment that the stop clamp was opened, and the infiltration experiment began. During the experiment, different time points were set, the readings of the Mariotte bottle were recorded, and the position of the wetting front was marked on the soil-column surface with a marker pen. After the experiment, a ruler was used to measure the migration distance of the wetting front at different times.

1.3 Research methods

1.3.1 HYDRUS-1D software simulation

(1) Basic equations. Soil is a continuous, homogeneous, and isotropic porous medium in which water is continuously distributed and incompressible. Constant-head infiltration can be regarded as a one-dimensional axisymmetric water-movement problem. HYDRUS-1D software was used for the simulation, and the Richards equation was used to describe the movement of water in unsaturated soil, namely:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z} - 1\right)\right] \tag{1}$$

where θ is the soil volumetric water content (%), representing the ratio of the volume of water contained in a unit volume of soil to the total volume; t is time; h is the soil matric potential (cm); z is the vertical coordinate, positive downward (cm); and $K(h)$ is the soil unsaturated hydraulic conductivity ($cm \cdot min^{-1}$).

For the unsaturated soil matric potential h involved in the basic equation, and the relationship between the unsaturated hydraulic conductivity $K(h)$ and the water content $\theta(h)$, the VAN GENUCHTEN-MUALEM (VG-M) model was used for fitting, namely:

$$\theta(h) = \theta_r + (\theta_s - \theta_r)/(1 + |\alpha h|^n)^m \tag{2}$$

$$K(h) = K_s S_e^{0.5} \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \tag{3}$$

where S_e is the relative saturation of the soil, $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$; θ_s is the saturated soil water content (%), referring to the water content when the soil is fully saturated; θ_r is the residual soil water content (%), referring to water that remains adsorbed by soil particles under strong suction and is difficult to remove; α, n, and m are fitting parameters related to the physical properties of the soil; and K_s is the saturated hydraulic conductivity of the soil ($\text{cm} \cdot \text{min}^{-1}$).

The basic equations for the evaporation process are as follows:

$$-K(h)\left(\frac{\partial h(z,t)}{\partial z} + 1\right) = E_a(t),\ z = L \tag{4}$$

$$-h_A \leq h(L,t) \leq 0 \tag{5}$$

where $E_a(t)$ is the actual evaporation rate at the soil-column surface. According to the actual evaporation in the study area, it was set to $0.08\ \text{cm} \cdot \text{min}^{-1}$; L is the height of the soil column, taken as 60 cm; and h_A is the minimum water potential of the upper surface layer of the soil column, set to 1 cm. The soil residual water content θ_r was obtained by fitting the soil suction–water content curve, rather than being directly measured by the traditional evaporation method. Its physical meaning is that, when the matric potential approaches negative infinity, a portion of water is still firmly adsorbed by soil particles, and this water cannot participate in effective infiltration and evaporation processes.

(2) Simulation boundary conditions and scheme design. To ensure consistency between the numerical simulation and the indoor experimental conditions, the infiltration simulation was set with the same initial water content as the experimental value. The upper boundary was a constant head (2 cm water depth, with a water-supply layer thickness of 5 cm), the lower boundary was free drainage, and the left and right boundaries were zero flux. For the evaporation simulation, the water-content distribution after the wetting front had advanced to the bottom was used as the initial condition; the upper boundary was set as an atmospheric boundary, and the lower boundary was likewise free drainage. According to mass fraction, five aeolian sandy soil samples with different mixing amounts were prepared (2%, 4%, 6%, 8%, and 10%). A CR-21N centrifuge was used to determine the water characteristic curves of the original aeolian sandy soil, mixed-soil samples with different mixing proportions, and pure attapulgite clay. The RETC software was then used to fit the measured data

and obtain the VG-M model parameters. The saturated hydraulic conductivities of aeolian sandy soil and its mixed samples were measured by the constant-head method, whereas attapulgite clay (ATP) was measured by the falling-head method. The relevant parameters are shown in Table 2.

1.3.2 XGBoost model

XGBoost is an efficient machine-learning algorithm based on gradient-boosting trees. It iteratively constructs decision trees and gradually optimizes prediction performance. In predicting the target variable, in order to obtain the best prediction performance, the model parameters were tuned, and its performance was comparatively evaluated.

Table 2 Moisture characteristics of aeolian sandy soil under different ATP blending amounts

Tab. 2 Influence of different ATP blending amounts on moisture characteristics of wind-sand soil

Treatment	$\theta_r/(\mathrm{cm}^3 \cdot \mathrm{cm}^{-3})$	$\theta_s/(\mathrm{cm}^3 \cdot \mathrm{cm}^{-3})$	α/cm^{-1}	n	$K_s/(\mathrm{cm} \cdot \mathrm{min}^{-1})$
CK	0.03036	0.34255	0.04019	2.09555	0.253
2%	0.03842	0.36964	0.04364	2.07585	0.174
4%	0.04761	0.36573	0.04404	1.93534	0.101
6%	0.05102	0.36655	0.04577	1.90478	0.0681
8%	0.05704	0.35351	0.04419	1.78609	0.0303
10%	0.06043	0.36384	0.04654	1.68973	0.024
ATP	0.012	0.41	0.008	1.25	5.2×10^{-6}

performance. The dataset was divided into 70% training set and 30% test set. The main hyperparameters were set as follows: maximum tree depth of the decision tree was 5, learning rate 0.164, L1 regularization parameter 0.09, and subsampling rate 0.75. The dataset was divided at a ratio of 80% as the training set and 20% as the test set, and model performance was evaluated using indices including mean squared error (MSE), root mean squared error (RMSE), mean absolute error (MAE), and coefficient of determination (R^2).

Its core objective function is the sum of the training error and the regularization term:

$$L(\phi) = \sum_{i=1}^{n} l(y_i, \hat{y}_i) + \sum_{k=1}^{K} \Omega(f_k) \tag{6}$$

where l denotes the loss function; Ω is used to control model complexity and prevent overfitting.

1.3.3 SHAP method

SHAP is based on game theory and quantifies the contribution of each feature to the model output. Its core formula is:

$$\phi_i(x) = \sum_{S \subseteq N \setminus \{i\}} \frac{|S|(|N| - |S| - 1)!}{|N|!} \left[f_{S \cup \{i\}}(x) - f_S(x) \right] \tag{7}$$

where $\phi_i(x)$ is the SHAP value of the i-th feature for the model output; N is the complete set of features; i is the feature currently to be explained; S is a subset of features that does not contain feature i; $f_S(x)$ is the model output using only the feature subset S; and $f_{S \cup \{i\}}(x) - f_S(x)$ is the marginal contribution of feature i under the background of subset S.

SHAP values also satisfy additivity, expressed as:

$$f(x) = \phi_0 + \sum_{i=1}^{N} \phi_i \tag{8}$$

where $f(x)$ is the model output for sample x; ϕ_0 is the baseline value (the expected model output when there are no features); and ϕ_i is the SHAP contribution of the i-th feature to the prediction for that sample. SHAP values reflect the contribution of each feature to the prediction for an individual sample, supporting model interpretation and feature-importance analysis.

2 Results and Analysis

2.1 Effects of different ATP application methods on the water-transport process in aeolian sandy soil

Under treatments with different ATP blending amounts of 0%, 2%, 4%, 6%, 8%, and 10%, the water retention and transport capacity of aeolian sandy soil changed significantly (Table 3). Blended ATP generally raised the soil-water characteristic curve, significantly increasing field capacity (FC), wilting water content (WP), and available water content (TAW), among which TAW increased by as much as 135.91%. Meanwhile, saturated hydraulic conductivity decreased nonlinearly with increasing blending amount, with a maximum reduction of 90.51%, indicating that the addition of ATP significantly weakened the hydraulic conductivity of aeolian sandy soil. According to the infiltration experiment, cumulative infiltration and wetting-front advance rate decreased significantly with increasing blending amount; the time required for 1 L of water to infiltrate increased from 32 min to 382 min, indicating a significant infiltration-reducing effect. In the evaporation experiment, cumulative evaporation also decreased as the blending ratio increased.

Table 3 Indicators of water-transport characteristics in aeolian sandy soil under different ATP blending amounts

Tab. 3 Indicators of water transport characteristics in wind-sandy soil under different ATP blending ratios

Blending amount	FC/($cm^3 \cdot cm^{-3}$)	WP/($cm^3 \cdot cm^{-3}$)	TAW/($cm^3 \cdot cm^{-3}$)	K_s/($cm \cdot min^{-1}$)	Infiltration duration/min	Evaporation/mm
0%	0.0487	0.0306	0.0181	0.253	32	40.32
2%	0.0572	0.0387	0.0185 (+2.2%)	0.174	47	39.48
4%	0.0736	0.0483	0.0253 (+39.8%)	0.101	84	39.49
6%	0.0780	0.0519	0.0261 (+44.2%)	0.0681	126	36.83
8%	0.0930	0.0588	0.0342 (+89.0%)	0.0303	294	33.96
10%	0.1064	0.0637	0.0427 (+135.9%)	0.024	382	32.97

Note: FC is field capacity; WP is wilting water content; TAW is available water content; K_s is saturated hydraulic conductivity; infiltration duration refers to the time required for 1 L of water to infiltrate completely; evaporation is the cumulative value over 12 consecutive days.

lower; among them, cumulative evaporation decreased by as much as 18.3%.

However, when the mixing amount was 10%, the "infiltration-reducing and evaporation-suppressing" effect of the wind-sandy soil was the best. Yet, because the soil structure was overly compact, water may have been retained excessively in the surface layer, which was unfavorable for replenishing water in the deeper layer. The 6% and 8% treatments were more balanced in improving TAW, reducing K_s, and suppressing evaporation. In particular, the 8% mixing amount achieved a stable optimal combination among the three key indicators of water conservation, infiltration reduction, and evaporation suppression: TAW increased significantly, K_s decreased markedly, and the evaporation-suppression effect was also closest to the maximum value, indicating that soil-structure improvement was optimal under this mixing condition.

To reveal the effects of different application methods of attapulgite on the infiltration process and evaporation of wind-sandy soil, three types of scenarios were established: surface-layer mixing thicknesses (5 cm, 10 cm, 15 cm, 20 cm, and 25 cm), interlayer thicknesses (0.5 cm, 1.0 cm, 1.5 cm, 2.0 cm, and 2.5 cm, with burial depth all 20 cm), and reconstructed profiles with surface layer + interlayer (T1-T5) (Table 4).

Table 4 Comparison of water transport characteristics in wind-sandy soil under different application methods

Tab. 4 Comparison of water transport characteristics in wind-sandy soil under different application methods

Treatment type	Infiltration characteristics	Evaporation characteristics	Optimal scheme
Surface-layer mixing thickness (R1–R5, 5–25 cm)	As thickness increased → infiltration rate slowed significantly; R5 took 290 min	Evaporation first decreased and then increased; R2 (10 cm) was the lowest (20.19 mm)	R2 (10 cm) had the best evaporation-suppression effect
Interlayer thickness (S1–S5, 0.5–2.5 cm)	As thickness increased → infiltration resistance strengthened; S5 took 12,516 min	Evaporation was greater than CK (40.32 mm) in all cases, reaching a maximum of 61.58 mm	No obvious optimum; there was a trade-off between infiltration reduction and increased evaporation
Profile configuration (T1–T5)	The closer the interlayer was to the top → the slower the infiltration; T1 had the smallest infiltration amount	Evaporation was smallest in T1 (29.31 mm) and largest in T5 (75.30 mm)	T1 was optimal for reducing infiltration and suppressing evaporation

The results showed that: (1) increasing the surface-layer mixing thickness significantly delayed the infiltration rate and the advance of the wetting peak. The time required for cumulative infiltration of 1 L increased from 166 min for R1 to 290 min for R5, while evaporation showed a pattern of "decreasing first and then increasing" ; among these, the 10 cm thickness (R2) had the best evaporation-suppression effect. (2) Increasing the interlayer thickness significantly enhanced infiltration resistance. The time required for the wetting peak to reach 60 cm increased from 3,424 min for S1 to 12,516 min for S5; however, evaporation also increased at the same time (all greater than 40.32 mm for CK), showing the characteristic of "reducing infiltration but increasing evaporation." (3) In the coupled profile configurations, T1 (10 cm mixed surface layer + interlayer buried at 10 cm) showed the best effect in reducing infiltration and suppressing evaporation. The cumulative evaporation over 12 d was only 29.31 mm, far lower than CK (40.32 mm) and T5 (75.30 mm). Thus, rational configuration of the ATP surface layer and interlayer distribution can realize synergistic regulation of infiltration and evaporation processes in wind-sandy soil, with the T1 configuration being optimal.

2.2 Correlation analysis between different soil parameters and infiltration indicators

To further reveal the relationships among indicators in the improvement of the hydraulic properties and water-movement patterns of wind-sandy soil by ATP, the Pearson correlation analysis method was used to calculate the correlation coefficients among parameters including residual water content, saturated water content, shape coefficient, reciprocal of air-entry value, saturated hydraulic conductivity, mixing amount, cumulative infiltration, and wetting-front migration distance, and significance tests were performed (significance level $\alpha = 0.05$). The heat-map analysis in Fig. 2 showed that the shape coefficient was correlated with residual water content ($r = 0.87,\ P < 0.01$) and saturated water content respectively

Figure labels: residual water content; saturated water content; shape coefficient; reciprocal of air-entry value; saturated hydraulic conductivity; mixing amount; cumulative infiltration; wetting-front migration distance. Color bar: correlation coefficient.

Fig. 2 Heat map showing the correlation between the physical and chemical properties of wind-sandy soil and water dynamics parameters

water content ($r = 0.73, P < 0.01$). This indicates that the incorporation of attapulgite significantly optimized the soil structure, thereby improving the soil' s water-holding and water-retention capacities. The reciprocal of the air-entry value was significantly negatively correlated with residual water content ($r = -0.97, P < 0.01$) and saturated water content ($r = -0.80, P < 0.01$), respectively. As the soil water-holding capacity increased, the soil air-entry value decreased significantly, which was closely related to the reduction in porosity caused by the improvement of soil structure. In addition, the mixing ratio was highly positively correlated with the shape coefficient ($r = 0.89, P < 0.01$) and cumulative infiltration ($r = 0.90, P < 0.01$), respectively. This indicates that, as the ATP mixing ratio increased, the proportion of clayey particles in the soil structure increased, effectively improving soil water-holding capacity and thereby increasing soil water infiltration. Cumulative infiltration was significantly and moderately positively correlated with wetting-front migration distance ($r = 0.70, P < 0.01$), indicating that enhanced infiltration capacity effectively promoted wetting-front advancement. In addition, the reciprocal of the air-entry value showed a significant negative correlation with the mixing ratio ($r = -0.91, P < 0.01$), prolonging the residence time of water in the soil (weak: $|r| < 0.3$; moderate: $0.3 \leq |r| < 0.7$; strong: $|r| \geq 0.7$).

2.3 HYDRUS-1D Simulation Validation and Model Accuracy Evaluation

In this study, HYDRUS-1D showed good simulation performance for cumulative infiltration and wetting-front migration distance in the three types of soil bodies

–aeolian sandy soil, 6% ATP mixed soil, and interlayer-structured soil–and was generally consistent with the measured data. The coefficients of determination R^2 were all greater than 0.98, and the root mean square errors (RMSE) were controlled within 0.4 $\sim$ 0.7 cm (Fig. 3). Among them, the 6% ATP mixed soil had the best simulation performance: the fitted R^2 for wetting-front migration distance reached 0.998, and the RMSE for cumulative infiltration was 0.458 cm. However, during the initial stage of rapid infiltration (0 $\sim$ 500 s), the simulated results were slightly higher than the measured values, with a deviation range of 5%-8%, indicating that HYDRUS-1D had a certain overestimation in this stage. Part of this deviation was caused by the idealized assumptions of the model itself. HYDRUS-1D treats soil as a homogeneous porous medium, making it difficult to fully reflect the heterogeneity of the internal micropore structure of the soil after ATP incorporation [31]. In addition, boundary effects may have occurred during the experiment, including friction against the inner wall of the apparatus, uneven compaction of the filled soil, and fluctuations in boundary water head, all of which could introduce certain errors. The boundary conditions set in HYDRUS-1D are relatively idealized and therefore cannot fully reflect the actual experimental conditions [32]. Meanwhile, there is a certain uncertainty in the calibration of hydraulic parameters. Parameters such as θ_s, θ_r, α, n, and K_s were all obtained by fitting experimental data, but the addition of ATP may alter the soil pore-size distribution, reducing the fitting accuracy of the traditional VG model [33-34]. Overall, HYDRUS-1D can capture the overall infiltration behavior and wetting-front advancement trend of aeolian sandy soil relatively well; however, in the initial stage when a heterogeneous structure is present, its dynamic prediction still shows certain deviations. Subsequent studies should obtain higher-resolution soil-water characteristic curves and optimize the parameter inversion process to further improve simulation accuracy.

2.4 XGBoost Model Performance Validation and Comparative Analysis

Compared with the physical model HYDRUS-1D, XGBoost exhibited higher accuracy in predicting cumulative infiltration and wetting-front migration distance. In the test set, the prediction accuracy for cumulative infiltration was: RMSE = 0.5839, R^2 = 0.9811; the prediction accuracy for wetting-front migration distance was: RMSE = 1.3687, R^2 = 0.9885 (Fig. 4). The residual distribution was mainly concentrated near 0, with no obvious systematic bias, indicating that the model had good fitting ability and strong generalization performance. The advantage of XGBoost lies in its ability to efficiently capture nonlinear relationships among variables; through gradient-boosted trees, the model automatically learns the complex interactions among features such as infiltration time, saturated water content, and ATP content [35-36]. In combination with the SHAP method, the contribution of each input variable to the model prediction results can be further quantified [37]. The analysis results showed that the wetting-front advancement process was mainly driven by infiltration time and cumulative infiltration, with contribution rates of 28.4% and

37.5%, respectively. In the prediction of infiltration characteristics, the explanatory contribution rate of saturated water content reached 28.7%, making it one of the key influencing factors. Compared with the HYDRUS model, which requires the calibration of a large number of physical parameters, XGBoost relies only on high-quality data training to achieve relatively stable prediction performance [38]. However, it should be noted that in the initial infiltration stage, the model prediction still exhibited certain deviations, the main reason

Legend in Fig. 3: measured cumulative infiltration; simulated cumulative infiltration; measured wetting-front migration distance; simulated wetting-front migration distance.

Panel labels and annotations in Fig. 3:

- (a) Aeolian sandy soil. Axes: cumulative infiltration/cm; wetting-front migration distance/cm; infiltration time/min. Annotations: $R^2 = 0.991$, RMSE = 0.674 cm; $R^2 = 0.982$, RMSE = 0.728 cm.
- (b) Mixed soil (6%). Axes: cumulative infiltration/cm; wetting-front migration distance/cm; infiltration time/min. Annotations: $R^2 = 0.998$, RMSE = 0.935 cm; $R^2 = 0.997$, RMSE = 0.458 cm.
- (c) Interlayer. Axes: cumulative infiltration/cm; wetting-front migration distance/cm; infiltration time/min. Annotations: $R^2 = 0.998$, RMSE = 0.399 cm; $R^2 = 0.989$, RMSE = 0.382 cm.

Fig. 3 HYDRUS simulation effect

Fig. 3 HYDRUS simulation effect diagram

(a) Residuals of the training set and test set
Legend: training-set residuals; test-set residuals
Vertical axis: residual
Horizontal axis: predicted cumulative infiltration value/cm

(b) Residuals of the training set and test set
Legend: training-set residuals; test-set residuals
Vertical axis: residual
Horizontal axis: predicted wetting-front migration distance value/cm

(c) Comparison between actual cumulative infiltration and predicted cumulative infiltration
Vertical axis: predicted cumulative infiltration/cm
Horizontal axis: actual cumulative infiltration/cm
Color scale: R^2

(d) Comparison between actual wetting-front migration distance and predicted wetting-front migration distance
Vertical axis: predicted wetting-front migration distance/cm
Horizontal axis: actual wetting-front migration distance/cm
Color scale: R^2

Fig. 4 Comparison and analysis chart of the prediction effect of the XGBoost model

This may be due to insufficient data under extreme conditions and the instability of the rapid infiltration stage process[^39].

To further evaluate the predictive performance of the model, this paper also constructed random forest (RF) and support vector regression (SVR) models for comparative analysis. The results show (Table 5) that the RMSE values of the RF and SVR models on the test set were 0.78 and 0.85, respectively, and the coefficients of determination R^2 were 0.972 and 0.965, respectively, both lower than the performance of the XGBoost model (RMSE = 0.58, $R^2 = 0.981$). This indicates that although the RF model has relatively high stability, it is still inferior to XGBoost in fitting high-dimensional feature interactions. The SVR model has certain advantages under small-sample conditions, but its kernel function is relatively sensitive to parameters, and its predictive performance decreases after the data scale expands. In contrast, although the HYDRUS-1D model has a clear physical basis, it depends on the calibration of complex hydraulic parameters, making it difficult to effectively simulate the nonlinear water-migration characteristics caused by infiltration after attapulgite addition.

Table 5 Performance comparison of different models on the test set

Model	Dataset	R^2	RMSE	MAE
HYDRUS-1D	Test set	0.982	0.728	0.53
XGBoost	Test set	0.981	0.584	0.41
RF	Test set	0.972	0.78	0.56
SVR	Test set	0.965	0.85	0.61

2.5 SHAP Value Interpretability Analysis

2.5.1 Key driving factors

This study used the SHAP method to quantify the contribution of each variable to the wetting-front migration distance and cumulative infiltration (Fig. 5). After all Shapley values were normalized, their sum was 100%, intuitively reflecting the importance and direction of each variable. The SHAP scatter plot further reveals the positive or negative influence direction of variables on the prediction results: when both the feature value and the corresponding SHAP value are positive, it indicates that an increase in the variable helps promote wetting-front expansion or cumulative infiltration; otherwise, it may exert an inhibitory effect.

Figure 5a shows that cumulative infiltration and infiltration time t are the key driving factors for wetting-front advancement, with contribution rates of 37.5% and 28.4%, respectively. Other variables, such as saturated water content, shape coefficient, residual water content, reciprocal of air-entry value, and saturated hydraulic conductivity, have smaller effects, while the contribution of mixing amount is the lowest. Infiltration is strongly positively correlated with wetting-front advancement. When the infiltration amount is low, the SHAP value is negative and infiltration is restricted; when infiltration is high, the SHAP value is positive, and the wetting front advances faster. Time t exhibits a clear cumulative effect: the longer the time, the farther the advancement. In Fig. 5b, cumulative infiltration is most strongly influenced by infiltration time and saturated water content, with contribution rates of 40.2% and 28.7%, respectively. The contributions of the remaining factors, such as residual water content, shape coefficient, reciprocal of air-entry value, and mixing amount, decrease in sequence. The higher the saturated water content, the greater the infiltration; whereas when residual water content increases, downward water percolation is restricted. A larger shape coefficient is closely related to structural compactness and inhibits water migration. Enhancements in air-entry capacity and increases in the mixing ratio can both promote infiltration. Overall, time, saturated water content, and soil-structure parameters have significant effects on water dynamics.

(a) SHAP-value distribution for wetting-front migration distance
Features: cumulative infiltration; time t; saturated water content; residual water content; shape factor; reciprocal of air-entry value; admixture amount; saturated hydraulic conductivity.
Horizontal axis: SHAP value (effect on the model). Color scale: feature value, high to low.

(b) SHAP-value distribution for cumulative infiltration
Features: wetting-front migration distance; time t; saturated water content; shape factor; residual water content; reciprocal of air-entry value; saturated hydraulic conductivity; admixture amount.
Horizontal axis: SHAP value (effect on the model). Color scale: feature value, high to low.

Fig. 5 Comparison of SHAP-value distributions for factors influencing soil-water transport characteristics

significant influence.

2.5.2 Interaction effects with cumulative infiltration as a predictor

Based on the results of SHAP feature-interaction analysis, the interactions between cumulative infiltration as a predictor and other variables are mainly reflected in the following aspects. Fig. 6a shows the interaction relationship between infiltration time and wetting-front migration distance. In the initial stage (500–1000 min), the wetting front advances relatively rapidly and the SHAP value is positive. When the time extends to 3000–3500 min, the SHAP value gradually decreases and even becomes negative, indicating that the wetting front tends to stabilize and that the positive effect of infiltration time on its advance weakens. Fig. 6c shows that within 1000 min, saturated water content has a strong promoting effect on wetting-front expansion, but this influence gradually weakens over time. Fig. 6g shows that under conditions of short duration and low residual water content, the wetting front advances rapidly; however, as time increases and residual water content rises, the advance rate slows and the SHAP value shows a downward trend. Fig. 6h shows that when the duration is short and the shape factor is small, wetting-front expansion is significant; whereas when the time exceeds 3000 min and the shape factor increases, wetting-front advance is restricted.

Fig. 6b indicates that when saturated water content is relatively low (0.345–0.355), the wetting-front migration distance is small and the SHAP value is low; at 0.365–0.370, the SHAP value rises markedly and wetting-front expansion is clearly enhanced. Fig. 6e shows that under low residual water content (0.030–0.040), the wetting-front migration distance is large; when residual water content increases to above 0.050, the SHAP value gradually becomes negative, indicating that excessive retained water limits wetting-front expansion. Fig. 6f shows that the combination of low residual water content and high saturated water content is favorable for wetting-front advance, whereas the opposite combination significantly weakens it.

Fig. 6d shows that when the shape factor is relatively small (0.040–0.043), the wetting-front migration distance is large and the SHAP values are mostly positive; when the shape factor exceeds 0.045, the SHAP value gradually decreases and even becomes negative, indicating that densification of the soil structure significantly inhibits downward water infiltration. Overall, the interaction effects dominated by cumulative infiltration exhibit a temporal pattern of "rapid in the early stage—slower in the later stage," and are highly sensitive to water content parameters (saturated/residual) and soil structure. High saturated water content, low residual water content, and a loose soil structure jointly promote wetting-front expansion, whereas prolonged time and soil densification weaken this positive effect.

2.5.3 Interaction effects with wetting-front migration distance as a predictor

SHAP feature-interaction analysis shows that the interaction between wetting-front migration distance and infiltration time has obvious stage-dependent characteristics. As shown in Fig. 7a, with increasing time, the SHAP value gradually decreases, especially when $t > 2000$ min, where the decline is pronounced. This indicates that the positive driving effect of time on cumulative infiltration is mainly concentrated in the initial stage. Fig. 7c shows that over a short period, saturated water content has a significant positive effect on cumulative infiltration, but this effect gradually weakens as time increases and even turns into a negative effect. Similarly, the interaction between time and residual water content in Fig. 7d also presents a trend of "strong at first and weak later" : in the initial stage, the influence of residual water content is significant, and then gradually weakens.

The influence of water-content parameters on soil-water transport characteristics exhibits nonlinear complexity. Fig. 7b shows that as saturated water content increases, the SHAP value fluctuates between positive and negative, but the overall trend indicates that higher saturated water content helps increase cumulative infiltration. Fig. 7e indicates that when residual water content increases, the SHAP value fluctuates around 0, suggesting that its contribution to water accumulation is constrained within a certain range. Fig. 7h further reveals that when residual water content is low and saturated water content is high, the increase in cumulative infiltration is most significant; the synergistic effect of the two enhances water percolation.

Soil pore structure also plays an important role in the process of water transport. Fig. 7f shows that as the shape factor increases, the SHAP value changes from negative to positive, indicating that a larger shape factor may enhance water-retention capacity. Fig. 7g shows that when the reciprocal of the air-entry value is small, the SHAP value is positive, whereas when it increases

(a) Interaction between time t and wetting-front migration distance
Axes: SHAP value (feature contribution); time t/min; wetting-front migration distance/cm

(b) Interaction between saturated water content and wetting-front migration distance
Axes: SHAP value (feature contribution); saturated water content/($cm^3 \cdot cm^{-3}$); wetting-front migration distance/cm

(c) Interaction between time t and saturated water content
Axes: SHAP value (feature contribution); time t/min; saturated water content/($cm^3 \cdot cm^{-3}$)

(d) Interaction between shape coefficient and wetting-front migration distance
Axes: SHAP value (feature contribution); shape coefficient; wetting-front migration distance/cm

(e) Interaction between residual water content and wetting-front migration distance
Axes: SHAP value (feature contribution); residual water content/($cm^3 \cdot cm^{-3}$); wetting-front migration distance/cm

(f) Interaction between residual water content and saturated water content
Axes: SHAP value (feature contribution); residual water content/($cm^3 \cdot cm^{-3}$); saturated water content/($cm^3 \cdot cm^{-3}$)

(g) Interaction between time t and residual water content
Axes: SHAP value (feature contribution); time t/min; residual water content/($cm^3 \cdot cm^{-3}$)

(h) Interaction between time t and shape coefficient

Axes: SHAP value (feature contribution); time t/min; shape coefficient

Fig. 6 Driving factors of cumulative infiltration volume and their pairwise interaction diagrams

It then became negative, indicating that enhanced air resistance would inhibit downward water infiltration. Overall, although changes in wetting-front migration distance also exhibited a "time-decay" effect, compared with cumulative infiltration volume, wetting-front migration distance was more sensitive to soil structure and resistance to air entry.

3 Discussion

ATP (attapulgite) showed a clear effect in improving water movement in aeolian sandy soil, mainly in three aspects: optimizing pore structure, delaying infiltration, and suppressing evaporation. The chain-layer structure and high specific surface area of ATP can partially fill macropores and promote the formation of aggregate structure, thereby increasing capillary water content and total porosity, reducing bulk density, and improving field water-holding capacity and water storage capacity. This is consistent with the conclusions of Niu et al.

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regarding the enhancement of water retention in sandy soil by ATP. Second, the measured data showed that, as the ATP incorporation rate increased, both soil infiltration time and wetting-front advance time were significantly prolonged (Table 6), and the saturated hydraulic conductivity decreased by more than 86%, confirming its role in reducing infiltration. Previous studies have pointed out that the cation-exchange properties and surface activity of ATP can enhance water adsorption and retention, thereby slowing the downward infiltration of gravitational water

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. This is consistent with the phenomenon observed in this study that "the wetting-front advance velocity was significantly reduced." Third, ATP incorporation was found to reduce cumulative evaporation, with a maximum decrease of 16.5%, indicating that it has a certain inhibitory effect on surface evaporation. Related studies have also shown that evaporation loss can be reduced by more than 20% at a 3% incorporation rate

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, which is consistent with the conclusions of this paper. In summary, ATP has significant advantages in improving the water-holding capacity of aeolian sandy soil and delaying wetting-front migration, providing a feasible pathway for improving aeolian sandy soils in arid and semi-arid regions.

To clarify the appropriate application range, this study further compared the key water-movement parameters under low-rate treatment (Q1, 2%) and high-rate treatment (Q5, 10%) (Table 6). The results showed that the improvements under the high-rate treatment in water retention, infiltration reduction, and evaporation suppression were all significantly greater than those under the low-rate⋯

(a) Interaction of time t with cumulative infiltration amount
Y-axis: SHAP value (feature contribution); X-axis: time t/min; color scale: cumulative infiltration amount/cm.

(b) Interaction of saturated water content with cumulative infiltration amount
Y-axis: SHAP value (feature contribution); X-axis: saturated water content/($cm^3 \cdot cm^{-3}$); color scale: cumulative infiltration amount/cm.

(c) Interaction of time t with saturated water content
Y-axis: SHAP value (feature contribution); X-axis: time t/min; color scale: saturated water content/($cm^3 \cdot cm^{-3}$).

(d) Interaction of time t with residual water content
Y-axis: SHAP value (feature contribution); X-axis: time t/min; color scale: residual water content/($cm^3 \cdot cm^{-3}$).

(e) Interaction of residual water content with cumulative infiltration amount
Y-axis: SHAP value (feature contribution); X-axis: residual water content/($cm^3 \cdot cm^{-3}$); color scale: cumulative infiltration amount/cm.

(f) Interaction of shape coefficient with cumulative infiltration amount
Y-axis: SHAP value (feature contribution); X-axis: shape coefficient; color scale: cumulative infiltration amount/cm.

(g) Interaction of the reciprocal of the air-entry value with cumulative infiltration amount
Y-axis: SHAP value (feature contribution); X-axis: reciprocal of the air-entry value; color scale: cumulative infiltration amount/cm.

(h) Interaction of residual water content with saturated water content
Y-axis: SHAP value (feature contribution); X-axis: residual water content/($cm^3 \cdot cm^{-3}$); color scale: saturated water content/($cm^3 \cdot cm^{-3}$).

Fig. 7 Driving factors of the migration distance of wetting fronts and their pairwise interaction diagrams

Tab. 6 Comparison of key water transport parameters in wind-sandy soil under different ATP blending ratios

Indicator	Q1(2% blending)	Q5(10% blending)	Relative change(Q5/Q1)
Available water content (TAW)/($cm^3 \cdot cm^{-3}$)	0.0185	0.0427	↑ 131%

Indicator	Q1(2% blending)	Q5(10% blending)	Relative change(Q5/Q1)
Infiltration duration (1 L water)/min	47	382	↑ 712.8%
Wetting-front advance time/min	47	382	↑ 712.8%
Saturated hydraulic conductivity (K_s)/($cm \cdot min^{-1}$)	0.174	0.024	↓ 86.2%
Initial infiltration parameter k	1.061	0.234	↓ 77.9%
Wetting-front fitting parameter a	3.258	0.769	↓ 76.4%
Cumulative evaporation (12 d)/mm	39.49	32.97	↓ 16.5%

amount: the time required for infiltration of 1 L of water and the wetting-front advance time were each extended by more than sevenfold, the available water content increased by 131%, and the saturated hydraulic conductivity decreased substantially by 86.2%. This indicates that ATP has a significant effect in reducing deep percolation and improving surface-layer water retention.

However, treatment with a high blending ratio can also make the soil structure excessively compact, which may cause excessive retention of water in the surface layer, to the detriment of water uptake by the plant root zone and the replenishment of water in deeper soil layers. Therefore, by comparison, the 8% blending treatment showed a more coordinated and stable effect in both increasing available water content and "reducing infiltration and suppressing evaporation" : it not only significantly enhanced water-retention capacity, but also avoided water stagnation and uneven water distribution caused by excessive compaction.

Accordingly, on the basis of comprehensively considering improvement efficiency, the coordination of soil-water distribution, and application cost, a blending range of 6%-10% is recommended for practical application, among which 8% has the most···

the optimal recommended blending level. Therefore, in ordinary arid regions, a mixing rate of 6%-8% may be selected according to soil texture and improvement needs, whereas in extremely arid regions it may be appropriately increased to 10% according to water-retention requirements.

4 Conclusions

Through a systematic study of the influence of ATP addition on the water-transport process in aeolian sandy soil and of its simulation and prediction methods, the following main conclusions were obtained:

(1) The addition of ATP significantly improved the water-transport characteristics of aeolian sandy soil. As the mixing ratio increased, field water-holding capacity and available water content gradually increased, while saturated hydraulic conductivity and total evaporation decreased significantly. A comparison between the 2% and 10% mixing treatments showed that a higher mixing amount was more favorable for enhancing soil water retention and reducing infiltration and evaporation. In particular, under the 10% mixing treatment, available water content increased by 131%, and the infiltration time was extended by more than 7 times, demonstrating significant application potential.

(2) Different application methods exhibited different patterns of influence on water transport in aeolian sandy soil. The surface-layer 10 cm mixing treatment (R2) performed best in suppressing evaporation; increasing the thickness of the interlayer significantly slowed the advance rate of the wetting front, but evaporation increased to some extent. Among the profile configurations, T1 (surface-layer 10 cm mixing + interlayer 10 cm) combined excellent effects of "infiltration reduction and evaporation suppression" and had the best overall performance; it is recommended as the preferred configuration in practice.

(3) In terms of soil-moisture prediction accuracy, the XGBoost-SHAP model was clearly superior to the HYDRUS-1D model. This advantage was especially pronounced in predicting cumulative infiltration and wetting-front migration distance. Specifically, on the test set, the XGBoost model had an RMSE of 0.584 and an R^2 of 0.981, both superior to the RMSE (0.728) and R^2 (0.982) of the HYDRUS-1D model. This difference in accuracy indicates that XGBoost can better capture complex nonlinear water-transport processes and provide more accurate prediction results.

(4) From the perspective of model interpretability, the XGBoost-SHAP model has clear advantages in analyzing variable contributions and interaction effects. Unlike the HYDRUS-1D model, the XGBoost-SHAP model, through the SHAP method, can clearly identify major driving factors such as cumulative infiltration, time, and saturated water content, and quantify their effects on the prediction results for wetting-front migration and infiltration. This makes the model prediction process more transparent and facilitates the identification and interpretation of complex interactions among influencing factors.

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Regulatory effects of attapulgite on water transport in wind-sandy soil: Soil column tests and numerical simulations

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Abstract: Attapulgite (ATP), a natural inorganic material, has significant potential for use in the regulation of water transport in aeolian sandy soils. In this study, indoor soil column tests and numerical simulation studies were performed with different parameters (including the percentage of ATP blended, the surface blending thickness, the interlayer thickness, and the profile reconstruction method). The regulatory effects of ATP addition on the infiltration and evaporation processes occurring in aeolian sandy soil were explored, and an XGBoost prediction model was constructed. The key influencing factors and their interactions were analyzed using the SHAP method. The addition of ATP could effectively delay the infiltration rate and inhibit the evaporation process, with 8% blending achieving the optimal water-holding effect. There were significant differences in effective water content, wet front advancement time, and evaporation inhibition between the 2% and 10% blending treatments, confirming that the regulatory effects were dependent on the applied dosage. Under different profile configurations, T1 treatment (10 cm surface blending + 10 cm deep interlayer) simultaneously optimized both seepage reduction and evaporation suppression. The XGBoost model demonstrated excellent accuracy for the prediction of the moist front migration and cumulative infiltration ($R^2 > 0.98$). The SHAP results indicated that the cumulative volume of infiltration, the time, and the saturated water content were the main driving factors. The findings of this research provide supporting data and technical methodology for the rational application of ATP to improve water retention in wind-sandy soil.

Keywords: attapulgite; wind-sandy soil; water transport; soil column test; XGBoost model; SHAP method; HYDRUS-1D

Note: Figure translations are in progress. See original paper for figures.