Simulation of the soil water content under different water deficits for apple trees via improved WOFOST-HYDRUS coupled model

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Abstract: As a crucial fruit tree crop, the health and yield of apple trees are intricately linked to soil moisture conditions. This study aimed to integrate the enhanced WOFOST model with the HYDRUS model to simulate the growth and development of apple trees, as well as the dynamics of soil moisture under varying degrees of water deficit. The outputs of evapotranspiration (ET_0) and leaf area index (LAI) from the WOFOST model during the apple growth phase were specifically integrated with HYDRUS-1D. These parameters served as intermediaries to assess the impact of different water deficit scenarios on apple tree growth and soil moisture content. The experimental design included three levels of water deficit treatments in addition to control, with irrigation volumes for the deficit treatments set at 85%, 70%, and 55% of the control's volume, respectively. The model-predicted LAI across all irrigation treatments exhibited an R^2 range of 0.89-0.95, a normalized root mean square error (NRMSE) between 8.02% and 14.57%, and yield prediction errors ranging from 6.27% to 9.61%, closely aligned with empirical data. The accuracy of simulated soil moisture content was enhanced in the 0-30 cm layer, with a slight decrease in accuracy observed in the 30-60 cm layer. For each irrigation treatment, the R^2 values for simulated soil moisture content ranged from 0.77 to 0.89 in the 0-30 cm layer and from 0.75 to 0.81 in the 30-60 cm layer. This study validated the capability of the WOFOST-HYDRUS model to accurately simulate the effects of varied water deficit treatments on soil moisture, LAI, and apple tree yield, providing valuable insights for developing optimal irrigation strategies.

Keywords: growth model, WOFOST-HYDRUS, apple trees, water simulation, water deficit treatment
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1 Introduction

The WOFOST model, renowned for its high accuracy, simulates the entire crop life cycle, from sowing to maturity. It accounts for environmental factors such as daily solar radiation, temperature, and precipitation, while also integrating the unique attributes of the crops, thereby ensuring a comprehensive and precise simulation outcome. In their research, Bai et al.[1,2] successfully modeled the growth of date palms using WOFOST, demonstrating its potential for simulating apple tree growth as well. However, despite the WOFOST model's strengths in reproducing crop growth and development under varying conditions, its reliance on a simplified "bucket model"[3] for soil water movement fails to account for lateral flow and the effects of moisture and nutrient distribution across soil layers on crop growth. This simplification limits the model's ability to accurately simulate critical hydrological processes - including soil moisture fluctuations, evaporation, and transpiration - which are pivotal to crop growth and development. The accurate simulation of hydrological cycle variables is essential for assessing the impact of environmental changes on crop growth and development, particularly in arid regions. Enhancing the model's hydrological cycle calculation is essential for accurately simulating crop transpiration under water stress, thereby improving the model's predictive accuracy regarding the effects of water stress on growth, development, and yield. Hydrological models, such as HYDRUS, serve as instrumental tools for simulating water cycle processes within water resource systems[4]. In agricultural production, these models can evaluate the impact of various irrigation and drainage strategies on crop growth and yield[5], thus supporting sustainable agricultural management. Consequently, integrating the strengths of both models can enhance crop growth simulation. The WOFOST and HYDRUS models have been extensively integrated with others[6]; Shelia et al.[7] combined HYDRUS-1D with DSSAT to simulate soil moisture dynamics, facilitating the coupling of crop growth with hydrological models. Kodeš et al.[8] utilized HYDRUS-1D to simulate 16 scenarios, featuring free drainage or a fixed water table at a depth of 250 cm, thereby showcasing the influence of groundwater on soil moisture balance. Zhou et al.[9] coupled HYDRUS-1D with WOFOST for wheat planting and irrigation simulation, optimizing irrigation strategies and simulating wheat production under fluctuating water

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conditions. Li[10] established a bidirectionally coupled crop growth-hydrological model by integrating WOFOST with HYDRUS-1D. Given the limited research on fruit tree simulation using WOFOST and its constraints in accurately capturing detailed soil moisture stratification, this study employs the WOFOST-HYDRUS coupling to simulate and analyze the LAI, yield, and soil moisture content of apple trees. This approach enhances the accuracy of growth simulations through WOFOST's sensitivity analysis and parameter calibration. The specific procedure involves inputting the ET_0 and LAI, as simulated by the WOFOST model, throughout the entire growth period as intermediate variables into the HYDRUS model.

2 Materials and methods

2.1 Experimental field site overview

The experimental work was conducted from March to September 2022 at the Fuguo Feng Agricultural Co., Ltd. apple planting demonstration park, where a rain-shelter system was implemented at the experimental site. Located in Fufeng County, Baoji City, Shaanxi Province, China (coordinates: 107°53′20″E, 34°28′49″N), the park is situated at an elevation of 735 m and experiences a warm temperate continental monsoon climate. The region receives an average annual precipitation of 569.9 mm, primarily occurring from July to September 2022. The park's soil is classified as loamy, with a pH value of 8.42 and a bulk density of 1.55 g/cm^3.

2.2 Experimental treatments

The experimental subjects consisted of "Gala" apple trees grafted onto M9-T337 rootstocks. These 7-year-old dwarf trees were densely planted with dimensions of 3 m × 1 m for plant height and row spacing. The growth period was delineated into four distinct stages: bud break and flowering, vegetative growth, fruit enlargement (subdivided into Phase I and Phase II), and fruit maturation.

An experiment assessing continuous water deficit was established, featuring three water deficit treatments and one control treatment (CK) for each growth stage. The control treatment irrigation volumes were determined based on field capacity, specified as 0.0635 m^3/plant for Phase I, 0.6345 m^3/plant for Phase II, 0.5979 m^3/plant for Phase III, and 0.4493 m^3/plant for Phase IV. The water deficit treatments were configured to 85%, 70%, and 55% of the CK treatment volumes, designated as low deficit (LD), moderate deficit 1(MD1), and moderate deficit 2 (MD2), respectively. To mitigate the impact of lateral soil moisture migration, a barrier film was installed 1.0 m beneath the soil surface in each plot, supplemented by protective rows at the plot boundaries. Uniform agronomic practices, including weed management, pruning, and pesticide application, were applied across all treatments.

2.3 Measurement and collection of experimental data

In this study, the data utilized encompass verification data for apple trees from the WOFOST model as well as parameter data for growth simulation.

2.3.1 Soil moisture content verification data measurement

Within each cohort of apple trees, a random sample of three trees was selected, resulting in a total of nine trees per treatment group. Soil moisture probes were strategically inserted at a depth of 15-20 cm radiating from the base of each tree trunk. Measurements of soil moisture content were conducted on the orchard soil profile, extending from 0 cm to 60 cm in depth at 10 cm increments, utilizing the TRIME-TDR soil moisture sensing system. The mean of these measurements was calculated, with assessments performed both pre- and post-irrigation at each developmental phase.

2.3.2 Leaf area index verification data measurement

In each group of apple trees, one leaf was randomly selected from the upper, middle, and lower canopy layers, resulting in a total of nine leaves per treatment. Photographs were taken with a fisheye camera on specific dates: April 14th, May 2nd, May 24th, June 13th, June 24th, and July 8th. LAI was subsequently measured using the Plant Canopy Analysis System software, and the average value of the measurement results was calculated for each date.

2.3.3 Yield verification data measurement

Following the maturation of the apples, three apple trees were randomly selected from each treatment group. The apples were harvested, weighed, and counted individually. The average weight of a single apple was multiplied by the total number of apples on each tree to calculate the yield per tree.

2.3.4 WOFOST simulation data collection

The operation of the WOFOST model requires both meteorological and soil data. The necessary meteorological data were obtained from the China Meteorological Data Sharing Service Platform, specifically from the Fufeng County station, covering the period from March to August 2022. Key meteorological parameters include saturation vapor pressure, average wind speed, daily minimum temperature, daily maximum temperature, daily radiation, and cumulative precipitation. The utilization of these precise and comprehensive datasets serves as the foundation for the simulation operations of the WOFOST model and its coupling with HYDRUS, thereby ensuring the accuracy and credibility of the simulation outcomes.

The construction of the soil parameter database in this study integrates field surveys with literature research. The core attributes of the soil have been established, including soil bulk density, particle size distribution, field capacity, and wilting coefficient. The accuracy of the measured soil data is crucial for soil management, crop growth, and irrigation strategies. The bulk density is measured at 1.55 g/cm^3, the volumetric water content at wilting point is 0.12 m^3/m^3, the field capacity is 0.32 m^3/m^3, the gravel content is 10.00%, the silt content is 72.20%, the calcium carbonate content is 7.20%, the cation exchange capacity is 10.40 cmol/kg, and the pH is 8.42.

2.4 Introduction and coupling analysis of the WOFOST and HYDRUS models

2.4.1 Overview of the WOFOST model

The WOFOST model, developed collaboratively by Wageningen University in the Netherlands and the World Food Studies Center, is a crop growth simulation tool that enables the assessment of yield under three distinct growth conditions: potential, water-limited, and nutrient-limited scenarios[11]. This model is primarily utilized for quantitative land evaluation, regional yield forecasting, risk analysis, and the assessment of interannual yield variability and the impacts of climate change. The WOFOST model is grounded in the principles of crop physiology and ecology, incorporating processes such as photosynthesis, respiration, transpiration, and dry matter distribution. To effectively apply the WOFOST model, it is essential to compile meteorological data, which includes parameters such as temperature, precipitation, humidity, wind speed, and other relevant meteorological variables, formatted to conform with the model's specifications. The outputs generated by the model include phenological development, leaf area index, and yield, among other results.

In the WOFOST model, the growth and developmental rate of crops can be accurately simulated, as represented by Equation (1).

$$D_{r,t} = \frac{T_{\mathrm{ei}}}{\mathrm{TSUM}_j} \tag{1}$$

where, the growth rate $D_{r,t}$ (in d^{-1}) of the crop at time t is closely related to the effective accumulated temperature required for its growth. For different growth stages j (where j=1 represents germination and flowering, and j=2 represents the period from flowering to maturity), the crop requires a cumulative effective accumulated temperature TSUM$_j$ (in °C·d) to facilitate its growth, which is essential for completing a specific developmental stage. T_{ei} is the effective accumulated temperature threshold for crop growth, °C.

$$T_{\mathrm{ei}} = \begin{cases} 0, & T_i < T_b \\ T_i - T_b, & T_b < T_i < T_{\max.e} \\ T_{\max} - T_b, & T_i \geq T_{\max.e} \end{cases} \tag{2}$$

where, T_i denotes the average daily temperature, °C; T_b represents the lower temperature threshold for crop growth and development, °C; $T_{\max.e}$ signifies the upper temperature threshold for crop growth and development, °C.

$$\mathrm{DVS} = f_{\mathrm{red}} \times \frac{\sum T_{\mathrm{ei}}}{\mathrm{TSUM}_j} \tag{3}$$

where, the crop development stage (DVS) is numerically represented, with DVS=0 indicating the germination stage, DVS=1 representing the flowering stage, and DVS=2 signifying the maturity stage. The DVS is calculated as the ratio of the actual accumulated effective temperature for the current growth stage to the theoretical effective temperature required for that stage, multiplied by the photoperiodic influence factor f_{red}, This calculation yields a quantitative indicator of the crop's current developmental phase.

$$f_{\mathrm{red}} = \frac{D - D_C}{D_O - D_C} (0 \leq f_{\mathrm{red}} \leq 1) \tag{4}$$

where, D represents the daily effective duration of radiation, h; D_o denotes the effective duration of solar radiation, h; D_C signifies the critical effective duration of solar radiation, h.

The daily total assimilation in the WOFOST model refers to the total energy absorbed and utilized by the crop through photosynthesis within a single day. This value is obtained by accumulating and integrating the instantaneous CO_2 assimilation rates throughout the day. This value is one of the key input parameters for the WOFOST model to calculate critical ecological processes such as crop growth, development, and yield. The daily total assimilation is typically expressed in the form of total effective radiation for photosynthesis, with units of kJ/m^2 (or MJ/m^2). The WOFOST model simulates the temporal changes in crop growth, development, and yield by calculating the daily total assimilation and predicts and manages crops under different ecological environments.

In the WOFOST model, the response function of single-leaf CO_2 assimilation rate to light is represented in a negative exponential form as Equation (5):

$$A_L = A_{\mathrm{m}} \left(1 - \mathrm{e}^{\frac{-\varepsilon_0 \mathrm{PAR}_a}{A_{\mathrm{m}}}}\right) \tag{5}$$

where, A_L represents the instantaneous total assimilation rate of CO_2 per unit leaf area at a relative height L from the canopy top (with L=0 at the canopy top), expressed in kg CO_2/(h·hm^2 leaf); A_m is the instantaneous total assimilation rate of CO_2 at light saturation, also in kg CO_2/(h·hm^2 leaf); PAR$_a$ is the available photosynthetically active radiation, μmol/m^2·s; and ε_0 is the initial light use efficiency, kg CO_2·J.

The calculation proceeds in two stages. First, the instantaneous total assimilation rate of CO_2 was calculated, followed by the calculation of the daily total assimilation rate of CO_2. When calculating the instantaneous total assimilation rate of CO_2, the entire canopy was divided into three layers. LAI at the canopy height L was calculated using Equation (6); p is an adjustment factor, which takes values of −1, 0, and 1 for different layers.

$$\mathrm{LAI}_L = (0.5 + p\sqrt{0.15}\ \mathrm{LAI}) \quad p = -1, 0, 1 \tag{6}$$

where, LAI$_L$ represents the LAI at the relative height L from the canopy top (in hm^2/hm^2), distinguishing between shaded leaves and sunlit leaves to calculate the corresponding total instantaneous CO_2 assimilation rates A_{sh} and A_{sl}, respectively.

$$A_{\mathrm{sh}} = A_{\mathrm{m}} \left(1 - \mathrm{e}^{\frac{-\varepsilon \mathrm{PAR}_{a,\mathrm{sh}}}{A_{\mathrm{m}}}}\right) \tag{7}$$

$$A_{\mathrm{sl}} = A_{\mathrm{m}} \left(1 - (A_{\mathrm{m}} - A_{\mathrm{sh}}) \frac{1 - \mathrm{e}^{\frac{-\varepsilon \mathrm{PAR}_{a,\mathrm{dr,sl}}}{A_{\mathrm{m}}}}}{\varepsilon \mathrm{PAR}_{a,\mathrm{dr,sl}}}\right) \tag{8}$$

where, A_{sh} represents the instantaneous total photosynthetic CO_2 assimilation rate of shaded leaves, kg/(hm^2·h); A_{sl} represents the instantaneous total photosynthetic CO_2 assimilation rate of sunlit leaves, kg/(hm^2·h); A_{m} is the instantaneous total photosynthetic CO_2 assimilation rate at light saturation, kg/(hm^2·h); ε is the light use efficiency, kg·J; PAR$_{a,\mathrm{sh}}$ is the total photosynthetically active radiation absorbed by shaded leaves, J/(m^2·s); and PAR$_{a,\mathrm{dr,sl}}$ is the total photosynthetically active radiation absorbed by sunlit leaves, J/(m^2·s). The proportion of shaded and sunlit leaves in the LAI is distinguished to calculate the proportion of leaf area occupied by sunlit leaves, and f_{sl}; and K is the extinction coefficient (as shown in Equation (9)).

$$f_{\mathrm{sl}} = \mathrm{e}^{-K \cdot \mathrm{LAI}_L} \tag{9}$$

The instantaneous total photosynthetic CO_2 assimilation rate of the entire layer at a relative height L from the canopy top, $A_{T,L}$ [in kg/(hm^2·h)], was calculated as follows:

$$A_{T,L} = f_{\mathrm{sl}} A_{\mathrm{sl}} + (1 - f_{\mathrm{sl}}) A_{\mathrm{sh}} \tag{10}$$

The total instantaneous photosynthetic CO_2 assimilation rate of the canopy, A_c [in kg/(hm^2·h)], was obtained by weighting and calculating as follows:

$$A_c = \frac{\mathrm{LAI}\left(A_{T,D,-1} + 1.6A_{T,D,0} + A_{T,D,1}\right)}{3.6} \tag{11}$$

At three diurnal points, the instantaneous total photosynthetic CO_2 assimilation rates at various canopy locations are converted into a daily total CO_2 assimilation rate through weighting. In Equation (12), T_h denotes the calculation time point (in h), while Equation (13) defines A_d as the daily total CO_2 assimilation rate [in kg/(hm^2·h)], which is derived by averaging the weighted values at three heights and three intervals.

$$T_h = 12 + 0.5D\left(0.5 + p\sqrt{0.15}\right) \quad p = -1, 0, 1 \tag{12}$$

$$A_d = \frac{D\left(A_{c,-1} + 1.6A_{c,0} + A_{c,1}\right)}{3.6} \tag{13}$$

Regarding soil water balance, the WOFOST model employed a simplified framework, known as the "bucket model" to simulate crop water balance under stress conditions. This framework delineates the soil into three distinct layers: the root zone, which extends from the soil surface to the depth of the root system; the subsoil zone, located between the root system's depth and the soil's maximum depth; and the deepest soil layer, situated beneath the maximum extent of the root system. In the WOFOST model, the soil moisture available to crops, specifically the water in the root zone, is determined by multiplying the root depth by the prevailing soil water content. Upon precipitation, an initial portion is allocated to surface runoff, proportional to the volume of rainfall. If the soil's water content exceeds field capacity, the excess water percolates downward to the subsoil and deeper layers. In subsequent model simulations, crops are considered unable to access water that has percolated to the deeper soil layers. The WOFOST model calculates crop water uptake potential based on actual root depth and soil moisture levels, rather than the distribution of soil water within the root zone. The model assumes that soil water distribution within the root zone is uniform throughout the day, with the crop's water uptake capacity being independent of root distribution and the daily water uptake rate per unit length. In instances of water limitation, WOFOST utilizes the Penman-Monteith equation to estimate potential ET_0. The water stress factor is derived from the ratio of the crop's actual water uptake to its potential evapotranspiration. However, this simplified approach may not adequately simulate the hydrological cycle throughout the crop's developmental stages.

2.4.2 Overview of HYDRUS model

The HYDRUS model[12], developed by Simunek and colleagues in the early 1990s, is primarily designed to simulate the movement of water in the soil and the transport of other substances within it. Based on a set of mathematical equations and computational techniques, the HYDRUS model discretizes and numerically approximates the complex geometric soil medium into uniform or heterogeneous blocks, equating them to multiple physical quantities. Parameters and data required for the model include soil material properties, initial conditions, boundary conditions, and more.

The core equation of the HYDRUS model is the Richards equation, which describes the one-dimensional variation of water in the soil, including the movement and transformation of moisture[13]. To more accurately simulate the transport of water and substances, the HYDRUS model also incorporates additional equations such as the mass conservation equation and biological reaction equations. The HYDRUS model can simulate the anisotropic movement of fluids and various nonlinear reactions and is suitable for predicting environmental hydrological issues at both small and large scales. Its advantages lie in its high degree of precision and flexibility. The model is capable of simulating the movement of water and other substances in the soil and providing quantitative predictions of substance transport. Furthermore, the HYDRUS model takes into account the physical and chemical properties of the soil medium, more closely resembling the natural environment, and can offer useful recommendations for land use and management.

In the process of simulating soil water levels, considering that moisture primarily undergoes one-dimensional vertical migration, the model employs the Richards equation to calculate the dynamic changes in soil moisture within the vertical soil profile[14]. The Richards equation integrates soil permeability and porosity to accurately simulate the movement of water in the soil. Through this equation, the fluctuations in soil water levels can be more precisely predicted, providing scientific guidance for crop management and irrigation. The calculation method is shown in Equation (14).

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial t}\left[k(h)\left(\frac{\partial h}{\partial x}+1\right)\right]-S \tag{14}$$

In the Richards equation, key parameters include the soil's volumetric water content θ (cm³/cm³), time t (d), coordinate value x (cm) (positive upwards), pressure head h (cm), as well as the crop root water uptake rate S (cm³/(cm³·d)) (which is 0 for bare areas), and the soil water unsaturated hydraulic conductivity $K(h)$ (cm/d). These parameters together form an accurate framework for simulating soil moisture movement.

The HYDRUS model utilizes a water stress index to investigate root water uptake, employing the Feddes model to calculate the root water uptake issue as follows:

$$S(h)=a(h)S_p=a(h)b(x)T_p \tag{15}$$

where, $a(h)$ is the water stress response coefficient; S_p is the potential water uptake rate, cm/d; $b(x)$ is the root water uptake distribution density function; T_p is the potential transpiration rate, cm/d.

2.4.3 Coupling analysis of WOFOST and HYDRUS

The WOFOST model, from an ecological perspective, meticulously describes the interactions and dependencies between crops and the environment during their growth process. The model aims to simulate crop growth and development under various environmental conditions. However, in dealing with the water cycle, it employs a simplified "bucket model" to simulate the dynamics of soil moisture and does not consider lateral flow in the horizontal direction. This simplification limits the model's ability to simulate key hydrological processes such as soil moisture changes, evaporation, and transpiration, which are crucial for crop growth. The hydrological cycle is the foundation of physical and physiological processes between soil, crops, and the atmosphere; therefore, accurately simulating these hydrological variables is of great significance for understanding how environmental changes impact crop growth, especially in arid regions. To enhance the model's accuracy in simulating crop transpiration under water stress and its effects on growth and yield, it is necessary to improve the hydrological cycle calculation process of the WOFOST model.

As one of the core projects of the International Geosphere-Biosphere Programme, the study of Biospheric Aspects of the Hydrological Cycle emphasizes the importance of considering the impact of the biosphere in the hydrological cycle. The HYDRUS-1D model, on the other hand, adopts a traditional hydrological perspective, focusing primarily on hydrological processes with less attention to the biophysics and biochemistry of vegetation. In this model, growth parameters related to vegetation characteristics, such as the LAI, root depth, and crop height, are provided as static data, implying that these parameters do not dynamically adjust with changes in the water cycle and water balance. Given the complex interactions and feedback mechanisms between crop growth and the hydrological cycle, the static treatment approach of the HYDRUS-1D model may lead to significant deviations in simulation results due to the lack of dynamic feedback. Therefore, when simulating the interaction between crop growth and the hydrological cycle, it is necessary to dynamically describe the interaction between crops and hydrological processes to more realistically reflect actual conditions, thereby more accurately predicting the impact of environmental changes on crop growth.

Therefore, it is necessary to couple the two models to complement each other's strengths, allowing the crop growth model to provide dynamically changing vegetation characteristics such as the LAI, root depth, and crop height for the hydrological cycle processes; and allowing the hydrological model to provide dynamic changes in soil moisture and other hydrological cycle variables for the simulation of the crop growth process, enhancing the analytical and understanding capabilities of the crop growth-hydrological cycle dynamics.

The specific operation involves the WOFOST module for simulating the crop growth process, while the HYDRUS-1D module is used to simulate soil moisture changes and the water balance process in the crop root zone. The WOFOST module and the HYDRUS-1D module achieve data flow coupling by exchanging crop growth parameters and water stress response factors. The WOFOST module passes crop growth parameters required for simulating soil moisture changes and the water balance process to the HYDRUS-1D module (using the ET_0 and LAI simulated by the WOFOST model throughout the entire growth period as intermediate variables input into the HYDRUS model). The HYDRUS-1D module passes water stress response factors that determine the actual CO_2 assimilation rate to the WOFOST module, thereby achieving coupling between the two.

Regarding the potential evapotranspiration of crops, both models employ the Penman-Monteith method for calculation, hence using ET_0 as one of the intermediate variables to input WOFOST results into the HYDRUS model. The P-M model, established based on aerodynamics and the principles of energy balance, takes into account all influencing factors comprehensively. Compared to other calculation methods, the P-M model does not require parameter adjustments according to climatic differences across regions when calculating ET_0. It has been tested with global meteorological station data, and its calculated ET_0 accuracy is universally applicable, thereby better guiding crop irrigation and water management. The equation is as follows:

$$\mathrm{ET}_0=\frac{0.408\Delta(R_n-G)+\Upsilon\left(\dfrac{900}{T+273}\right)u_2(e_s-e_a)}{\Delta+\Upsilon(1+0.34u_2)} \tag{16}$$

where, ET_0 represents the daily reference evapotranspiration, mm/d; R_n is the net radiation at the crop surface, MJ/(m^2·d); G is the soil heat flux density, MJ/(m^2·d); T is the daily average air temperature at 2 m height, °C; u_2 is the daily average wind speed at 2 m height, m/s; e_s is the saturation vapor pressure, kPa; e_a is the actual vapor pressure, kPa; Δ is the slope of the saturation vapor pressure curve with respect to temperature, kPa/°C; γ is the psychrometric constant, kPa/°C.

The calculation formulas for potential transpiration and soil evaporation are as follows:

$$T_p=\mathrm{ET}_p\left(1-\mathrm{e}^{-k\cdot\mathrm{LAI}}\right) \tag{17}$$

$$E_p=\mathrm{ET}_p\mathrm{e}^{-k\cdot\mathrm{LAI}}=\mathrm{ET}_p-T_p \tag{18}$$

where, k represents the canopy extinction coefficient, and LAI stands for the leaf area index.

2.5 Sensitivity analysis and parameter calibration of the model

2.5.1 Redefine model parameters

Expanding on the WOFOST model framework, this study meticulously adjusted parameters to accurately simulate apple tree growth. Given that apple trees are perennial, their growth traits markedly differ from annuals, necessitating parameter adaptations to accommodate their distinct physiological attributes. To begin, an exhaustive analysis of the WOFOST model's internal structural parameters was performed, followed by calibration aligned with the growth patterns and physiological traits of apple trees[15]. Notably, for the pivotal parameter set defining phenological stages, the developmental phases of apple trees were redefined. The DVS quantifies the developmental status of apple trees, with its scale calibrated to map onto discrete growth phases. For example, the DVS is set at −0.10 for the bud break stage, −0.05 for flowering, 0 for the fruit set, incrementing to 1 as the branches renew, and peaking at 2 upon fruit maturity. With these refinements, the WOFOST model more precisely mirrors the growth patterns and physiological conditions of apple trees during simulation, bolstering the accuracy and applicability of the predictive outcomes.

2.5.2 Sensitivity analysis

The WOFOST model encompasses a vast array of parameters, necessitating a global sensitivity analysis to quantitatively evaluate the influence of individual parameters and their interactions on output variability. Typically, a subset of model parameters predominantly dictates the variability in model output, whereas the remaining parameters exert a negligible influence. To concentrate calibration efforts on a select few biologically significant sensitive parameters, ensuring simulation efficacy and concurrently minimizing computational demands, the Sobol method[16] is leveraged. This approach utilizes uniformly distributed sample points to assess the impact of input factors on output, incorporating their interactive effects. It systematically prioritizes and filters input factors, delineating the relative significance of each parameter and augmenting the model's predictive precision.

The Sobol method is a typical global sensitivity analysis technique[17,18] and has been proven to be one of the most effective methods for model parameter sensitivity analysis[19]. The Sobol method is based on the concept of variance decomposition, representing the parameterized model as:

$$y=f(X,\theta) \tag{19}$$

where, y represents the objective function, X denotes the driving data, and θ is the vector of parameters.

The model's total variance $D(y)$ is decomposed into the effects of individual parameters and the combined effects of the parameters.

$$D(y)=\sum_{i=1}^{k}D_i+\sum_{i=1}^{k-1}\sum_{j=i+1}^{k}D_{ij}+\ldots+D_{1,\ldots,k} \tag{20}$$

where, the range of values for i is from 1 to k, where k is the total number of input parameters. D_i represents the first-order partial variance of parameter θ_i on the objective function y, D_{ij} denotes the second-order partial variance due to the interaction between parameters θ_i and θ_j, and k is the dimension of the parameters.

Equation (20) is normalized, and the sensitivity indices of the parameters are calculated by the ratio of the partial variance to the total variance.

First-order sensitivity index:

$$S_i=\frac{D_i}{D} \tag{21}$$

Total sensitivity index:

$$S_{\mathrm{oi}}=\sum S_i \tag{22}$$

where, S_{oi} denotes the sensitivity including all parameters θ_i, which is the sum of the individual effect of parameter θ_i on the objective function y and the combined effect with other parameters on y[20].

2.5.3 Parameter calibration

At the commencement of the crop model, this study, leveraging actual monitored data, meticulously calibrates the germination base temperature (TBASEM) to 7°C for enhanced model fidelity. This calibration ensures alignment of the model's germination simulation with the actual environmental conditions. Subsequently, aligning with the observed trends in LAI, the leaf lifespan (SPAN) is adjusted to 50 to emulate the natural lifecycle of leaves, from emergence to senescence. In light of the stable and enduring nature of the root systems in perennial fruit trees, this study establishes the root mortality rate at 0, indicative of the minimal occurrence of root death under natural growth conditions.

Following the identification of sensitive parameters via WOFOST model's sensitivity analysis, this study employs the PEST parameter estimation software to refine and select parameters that are challenging to ascertain or susceptible to measurement inaccuracies. For the remaining parameters, this study harmonizes actual measurement data with the model's default parameter values[21], performing judicious estimations and configurations to ensure an accurate depiction of environmental factors' influence on crop growth across the entire simulation process. This initialization approach, grounded in empirical growth data and scientific estimation, not only enhances the model's capacity to accurately simulate the crop growth process but also augments its predictive precision and practical utility in agricultural production scenarios.

2.6 Performance evaluation of model simulation accuracy

This study employed the coefficient of determination R^2 and the NRMSE as evaluation metrics[2,21]. R^2 is a statistical metric that measures the consistency between the model's predicted values and the observed values. NRMSE is another statistical indicator of model prediction accuracy, which normalizes the root mean square error (RMSE) by dividing it by the mean or range of the observed values, thus making the error measure independent of the data's scale. An R^2 value typically ranging from 0.8 to 0.9 or higher is considered a good fit. For NRMSE, a value less than 0.1 indicates that the model's prediction accuracy is very high and can be considered an extremely accurate simulation, a value between 0.1 and 0.2 is usually considered high-precision simulation, between 0.2 and 0.5 is considered medium-precision simulation, and greater than 0.5 is considered low-precision simulation. The calculation formulas for each metric are shown in Equations (23)-(25).

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \tilde{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y}_i)^2} \tag{23}$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} (\tilde{y}_i - y_i)^2}{n}} \tag{24}$$

$$\text{NRMSE} = \frac{\sqrt{\frac{\sum_{i=1}^{n} (\tilde{y}_i - y_i)^2}{n}}}{\bar{y}_i} \tag{25}$$

where, $\tilde{y}_i$ represents the simulated values, y_i represents the measured values, $\bar{y}_i$ is the average of the observed values, and n is the sample size.

3 Results and analysis

3.1 Sensitivity analysis and main parameter calibration of the model

This study employed the Sobol method to conduct a comprehensive sensitivity analysis on yield parameters. The Sobol analysis was configured with a parameter sample size of 15×2000, aimed at identifying parameters with a substantial impact on yield. The study primarily utilized the water-limited mode within the WOFOST model framework and performed the sensitivity analysis using meteorological data corresponding to the 2022 growth period of apple trees. The results of this analysis are presented in Figure 1. The findings reveal that the first-order and global sensitivity patterns among various crop parameters exhibit notable similarities. Parameters demonstrating high sensitivity to yield include the TBASEM, accumulated temperature to the juvenile fruit stage (TSUMEM), SPAN (leaf area life cycle at 35°C), initial dry weight of roots and trunk (TDWI), conversion rate of assimilates to storage organs (CVO), and conversion rate of assimilates to stems (CVS). Notably, SPAN and TSUMEM exhibit higher sensitivity indices, indicating that yield is predominantly influenced by the maximum effective germination temperature and the leaf area life cycle at 35°C.

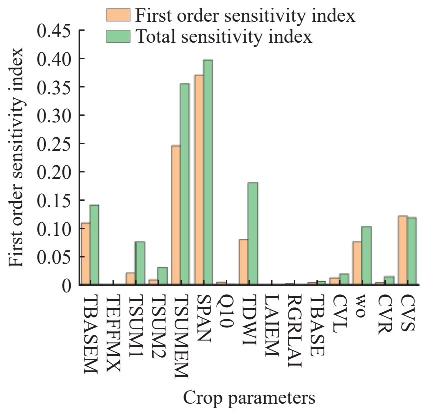


Figure 1 Sensitivity analysis for the apple tree model

Utilizing the aforementioned calibration techniques, the PEST parameter estimation software was employed to refine high-sensitivity data, leading to the selection of the calibrated outcomes. For the remaining parameters, this study aligned empirical measurement values with the model's default parameter ranges to facilitate informed estimations and configurations. The parameters specific to apple trees are listed in Table 1.

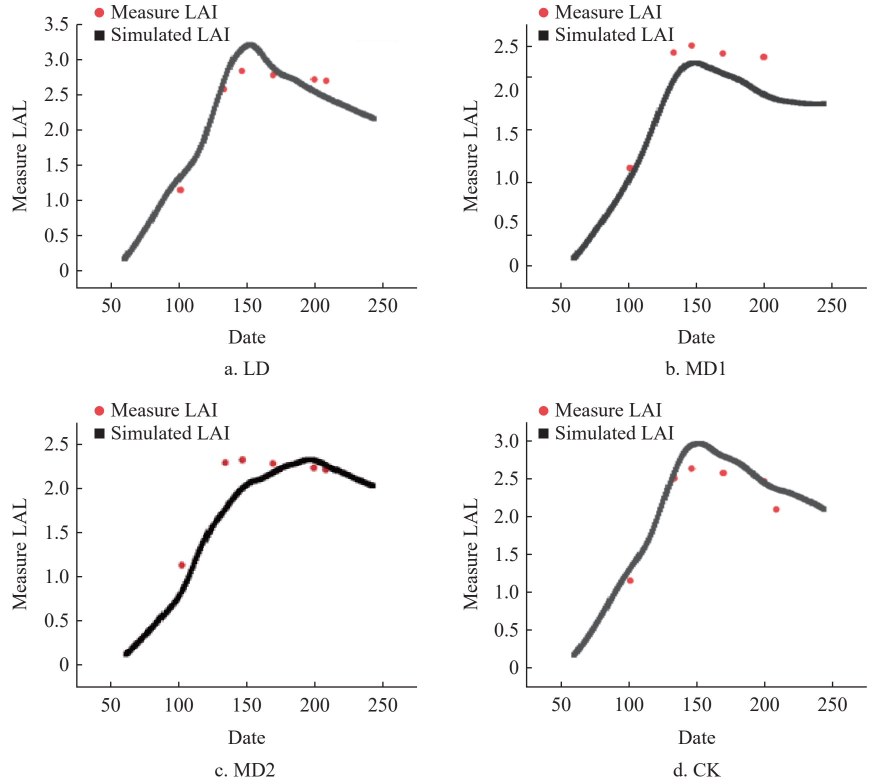
Table 1 Calibration table of main parameters for the apple tree model

Parameter	Parameter definition	Calibration value	Unit
TBASEM	Minimum germination temperature	7.0	°C
TEFFMX	Maximum effective temperature for germination	30	°C
TSUMEM	Accumulated temperature from germination to juvenile fruit stage	170	$°C \cdot d^{-1}$
TSUM1	Accumulated temperature from juvenile fruit to rapid expansion stage	456	$°C \cdot d^{-1}$
TSUM2	Accumulated temperature from rapid expansion to maturation stage	1023	$°C \cdot d^{-1}$
TDWI	Initial dry weight of roots and stems	89	$kg \cdot hm^{-2}$
RGRLAI	Daily maximum increase in leaf area index (LAI)	0.09	$hm^2 \cdot hm^{-2} \cdot d^{-1}$
LAIEM	Maximum growth rate of LAI	0.02	$hm^2 \cdot hm^{-2}$
SPAN	Life cycle of leaf area at 35°C	50	d
TBASE	Low-temperature threshold for leaf age	10	°C
CVL	Conversion rate of photosynthates to leaves	0.762	$kg \cdot kg^{-1}$
CVO	Conversion rate of photosynthates to storage organs	0.720	$kg \cdot kg^{-1}$
CVR	Conversion rate of photosynthates to roots	0.790	$kg \cdot kg^{-1}$
CVS	Conversion rate of photosynthates to stems	0.901	$kg \cdot kg^{-1}$
Q10	Relative change in respiration rate with a 10°C temperature increase	2.0	-

3.2 Model validation and evaluation

3.2.1 LAI verification

The fidelity of the LAI simulation serves as a pivotal metric for evaluating the accuracy of apple tree growth simulation. Figure 2 shows the outcomes of the LAI simulation across varying degrees of water deficit, while Figure 3 presents a comparative analysis between the LAI simulation and empirical data. The findings reveal a strong concordance between the model's projections and actual measurements, with R^2 values exceeding 0.84. Notably, the LAI simulation under the LD treatment demonstrates the highest precision, achieving an R^2 of 0.9525 and an NRMSE of 8.02%, which is below the 10% threshold. For the MD1 treatment, the corresponding values are R^2=0.9284 and NRMSE=14.57%; for the MD2 treatment, R^2=0.8412 and NRMSE=13.62%; and for the CK treatment, R^2= 0.9471 and NRMSE=9.14%. The accuracy of the LAI simulation is notably lower under the MD2 treatment, with an R^2 value falling below 0.9. These outcomes suggest a decrease in model simulation accuracy with excessive water deficit in apple trees. In conclusion, the LAI simulation maintains a relatively high level of accuracy when water deficit treatments exceed 55% of field capacity.



Note: The water deficit treatments were configured to 85%, 70%, and 55% of the CK treatment volumes, correspondingly labeled as LD, MD1, and MD2. Same below.

Figure 2 LAI simulation diagram for the apple tree model

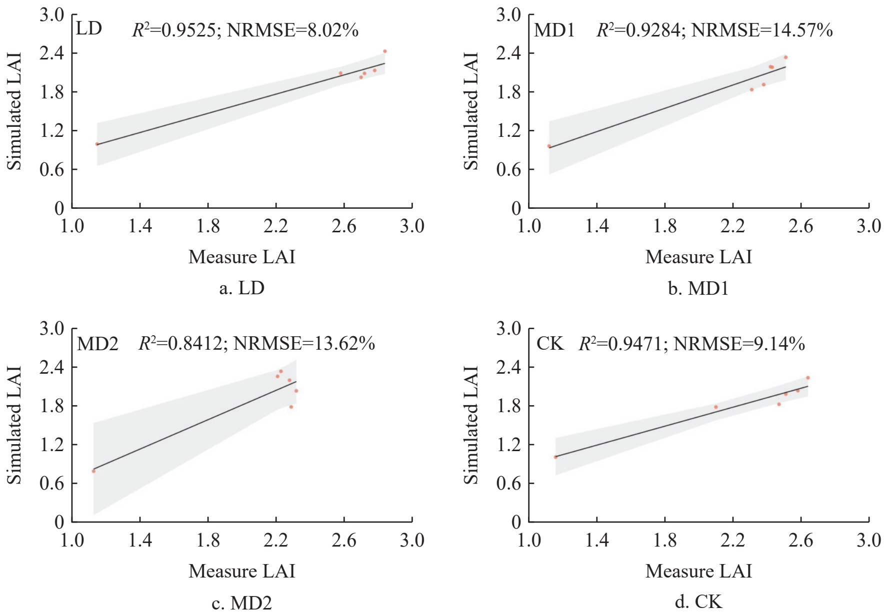
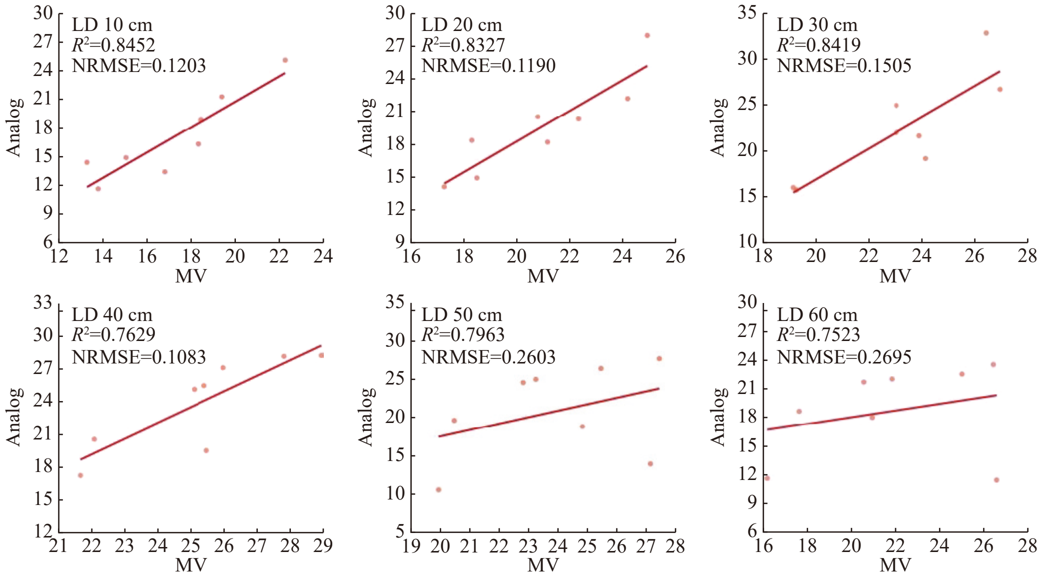


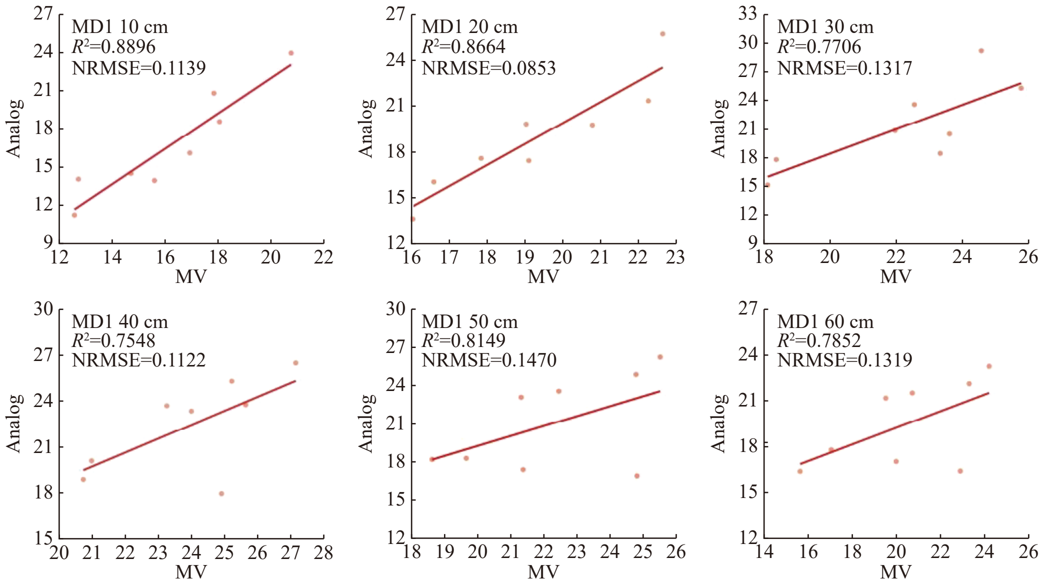
Figure 3 Scatter plot for the apple tree model

3.2.2 Soil moisture content verification

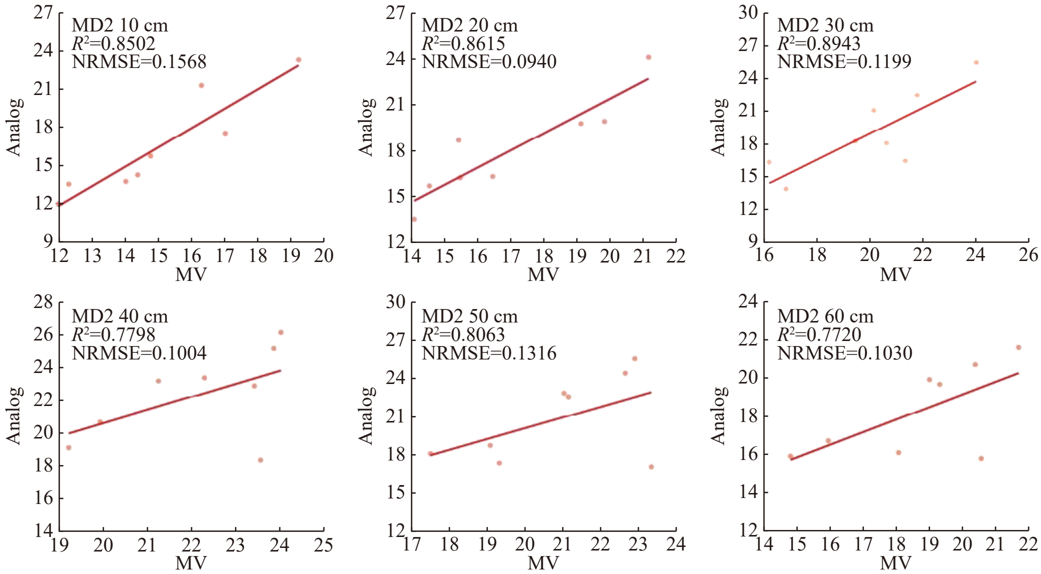
Across various water deficit treatments, a comparison of the measured versus simulated WOFOST-HYDRUS values (shown in Figure 4) and the soil moisture simulation outcomes (shown in



a. LD



b. MD1

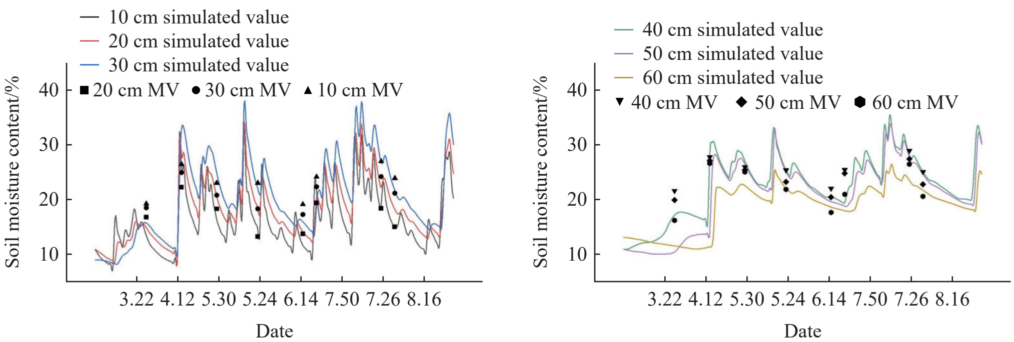


c. MD2

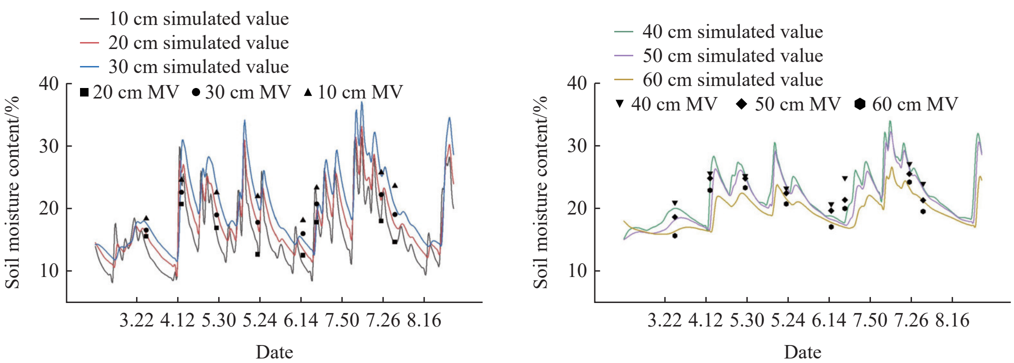
Note: Each subplot, in order from left to right and top to bottom, represents the comparison of actual and simulated soil moisture content at depths of 10 cm, 20 cm, 30 cm, 40 cm, 50 cm, and 60 cm. MV denotes the actual soil moisture content, and Analog denotes the simulated value.

Figure 4 Scatter plot comparing measured and simulated soil moisture content values

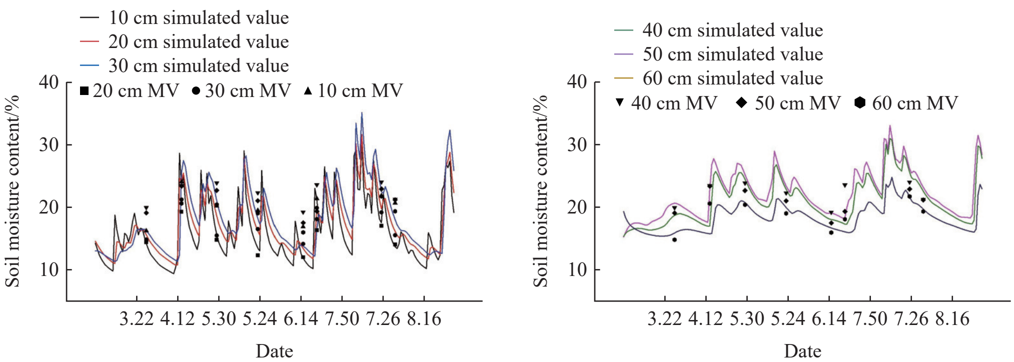
Figure 5) demonstrate that the developed WOFOST-HYDRUS model effectively simulates soil moisture at multiple depths for apple trees, achieving a model accuracy R^2 exceeding 0.75 across diverse water management scenarios. Specifically, under the LD treatment, the WOFOST-HYDRUS model exhibits marginally higher simulation accuracy for shallow soil moisture, registering R^2 values from 0.8327 to 0.8452 for the 0-30 cm layer, compared to 0.7523 to 0.7963 for the 30-60 cm layer. Under the MD1 treatment, the model maintains relatively high simulation accuracy for shallow soil moisture, with R^2 values ranging from 0.7706 to 0.8896, while the accuracy for deeper soil moisture falls within the range of 0.7548 to 0.8149. Similarly, under the MD2 treatment, the model's simulation accuracy for shallow soil moisture remains relatively high, with R^2 values from 0.8502 to 0.8943; and for deeper soil moisture, the accuracy is between 0.7720 and 0.8063. The study suggests that excessive water deficit may diminish simulation accuracy, potentially due to the model's failure to account for the physiological adaptations of apple trees to water stress conditions[22].



a. LD



b. MD1



c. MD2

Figure 5 Moisture simulation results for the apple tree model

3.2.3 Production verification

Variations in actual apple tree yields were observed across the spectrum of water deficit treatments. In the experimental analysis, the LD treatment produced the highest individual tree yield at 18.1 kg, while the MD2 treatment resulted in the lowest yield at 15.7 kg. The MD1 treatment yielded 17.2 kg, and the CK treatment generated 17.6 kg, establishing the following descending order of yields: LD, CK, MD1, MD2. Table 2 lists the discrepancies between simulated and actual yields across the various water deficit treatments, all of which fall within a 10% margin. The LD treatment exhibited a minimal yield error of 6.27%, in contrast to the maximal error observed under the MD2 treatment at 9.61%. The MD1 and CK treatments recorded respective errors of 7.36% and 6.85%. These findings suggest that apple trees exhibit enhanced growth and yield under moderate water deficit conditions; however, severe water deficits can adversely impact yield.

Table 2 Yield errors under different water deficit treatments

Deficit irrigation	Measured	Simulated	Yield error
MD2	15.7	17.4	9.61%
MD1	17.2	18.6	7.36%
LD	18.1	19.3	6.27%

4 Discussion

4.1 Analysis of model simulation accuracy

Validation against empirical data confirms that the LAI simulation achieves a high degree of precision (R^2>0.88), while the yield simulation accuracy is also commendable, exhibiting errors within a 10% margin. Furthermore, the simulation of soil moisture content yields positive outcomes. The accuracy of the simulations surpasses that of the MD2 treatment for CK, LD, and MD1 treatments. Initially, simulated accuracy increases with reduced irrigation volumes but subsequently declines. An exceedingly low irrigation volume may diminish simulation accuracy, potentially due to the enhanced water use efficiency of apple trees under specific moisture conditions. Moderate water deficiency, as observed in the LD treatment, can enhance water utilization efficiency in apple trees, thereby moderately increasing yield. In contrast, severe water scarcity, characteristic of the MD2 treatment, induces more pronounced drought stress[23]. Under the MD2 treatment, soil moisture may decrease to very low levels, potentially complicating the dynamics of soil moisture. Alternatively, the model may not have employed the most appropriate parameter set for extreme drought conditions, resulting in discrepancies between the simulation results and actual conditions. Furthermore, under extreme drought conditions, measuring soil moisture may become more difficult as the soil hardens, which can lead to increased measurement errors. These errors may propagate into the model, thereby affecting the accuracy of the simulation results. In some instances, the CK treatment may lead to excessive soil moisture, which can impair soil aeration and root respiration, ultimately detracting from crop growth. The LD treatment is likely more effective in maintaining optimal soil moisture conditions. In practical agricultural settings, its impact on apple tree growth may exceed the corrections for simulated drought stress, potentially exacerbating errors in LAI and yield estimations[24]. LAI, a critical input for HYDRUS, can propagate errors into soil moisture content simulations, if it is inaccurate, with these errors becoming more pronounced as soil depth increases. This variability may be attributed to significant differences in the physical and chemical properties of the soil, including texture, organic matter content, and porosity, across varying depths. Such heterogeneity complicates the simulation of deep soil moisture, thereby increasing the potential for error[25,26].

4.2 Uncertainty in model input parameters and considerations for model improvement

The WOFOST-HYDRUS model requires comprehensive datasets that include meteorological, soil, and crop data[27]. Meteorological data, including precipitation, temperature, humidity, and radiation, are critical input parameters for the model. Measurement errors, spatial representativeness, and temporal resolution of these data can significantly impact the simulation results. For instance, the accuracy of precipitation measurements may be influenced by the precision and location of rain gauges, while temperature and humidity readings can be affected by sensor calibration and environmental conditions. The physical and chemical properties of soil, including texture, organic matter content, and porosity, are essential for water retention and transport. Measurement errors and spatial variability in these parameters can introduce uncertainties in simulation outcomes. For example, variations in soil texture can influence water infiltration and retention, while changes in organic matter content can influence soil water-holding capacity and nutrient supply. Additionally, physiological parameters of crops, such as LAI, root distribution, and stomatal conductance, are vital for accurately simulating the crop's response to water deficits. Measurement errors and biological variability in these parameters can introduce uncertainties in simulation results. For instance, inaccuracies in LAI measurements can influence the simulation of photosynthesis and transpiration, while uncertainties in root distribution can alter water uptake simulations. The accessibility of these datasets is often limited, and updates may not be timely, which impacts the model's practical utility. Furthermore, deep soil moisture is influenced by various factors, including capillary action, gravitational drainage, and infiltration. These processes become increasingly complex with soil depth, thereby amplifying the uncertainty of simulations. The accuracy of the HYDRUS simulation relies on precise input parameters, such as soil hydraulic properties and boundary conditions[28]. Accurately obtaining these parameters for deep soil layers is challenging, further contributing to simulation uncertainty. This parameter uncertainty, combined with the model's inherent simplifications, may consequently affect the simulation outcomes[29,30].

This study validated the soil moisture component of the WOFOST-HYDRUS model using actual measurement results; however, further exploration is necessary to confirm the model's broader applicability. The model can be evaluated using long-term datasets from various climatic regions and soil types to assess its stability and suitability. Dynamically adjusting model parameters in accordance with the progression of the crop growth season can effectively reflect changes in crop growth status and environmental conditions. To enhance the accuracy of parameter acquisition, advanced sensors and measurement technologies should be employed to minimize measurement errors in meteorological, soil, and crop physiological parameters. Integrating ground observations, remote sensing data, and model simulations can significantly improve the spatial and temporal resolution of these parameters. Future research studies will incrementally verify and analyze the model's application in simulating growth parameters and yield of apples, calibrating model parameters with empirical data related to the growth and development of apple trees to enhance the model's simulation accuracy.

The current iteration of the WOFOST-HYDRUS coupled model accounts solely for water movement and does not incorporate solute transport dynamics. Future research endeavors could integrate solute transport processes within the soil into the WOFOST-HYDRUS model to elucidate the effects of fertilization on soil and crops. By incorporating solute transport, the model would more accurately delineate the complex transformations and transport of nutrient elements within the soil, thereby enhancing predictions of crop-soil interactions.

5 Conclusions

In this investigation, the ET_0 and LAI were utilized as intermediary variables to enhance a WOFOST-HYDRUS model specifically designed for apple trees, through the integration and refinement of both the WOFOST and HYDRUS-1D models. New phenological parameters for apple tree crop development were established by redefining growth stages, followed by a sensitivity analysis that examined the interaction between state variables and phenological parameters. The subsequent recalibration of these parameters ensured that the outcomes closely reflected the actual growth conditions of apple trees. The model was employed to simulate the leaf area index, yield, and soil moisture content of apple trees across various water deficit treatments. The LD treatment yielded the highest values for both the leaf area index and yield, in contrast to the MD2 treatment, which produced the lowest. The simulation demonstrated high precision for the LAI (with R^2 ranging from 0.8857 to 0.9525 and NRMSE from 8.02% to 14.57%) and for yield (with errors ranging from 6.27% to 9.61%). The WOFOST-HYDRUS model exhibited slightly greater simulation accuracy for shallow soil moisture (R^2=0.8327-0.8452 in the 0-30 cm layer) compared to the deeper layer (R^2=0.7523-0.7963 in the 30-60 cm layer), across diverse water deficit treatments. In summary, the WOFOST-HYDRUS model provides a novel approach for simulating apple tree growth under varying water deficit conditions and for assessing soil moisture dynamics.

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