A review of models for simulating the soil-plant interface for
different climatic conditions and land uses in the Loess Plateau,
China

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Abstract

Impacts due to climate change, population growth and intensive agriculture continue to be a major concern worldwide. Sustainable agriculture with coherent land management strategies is essential to mitigate against adverse environmental impacts. For the Chinese Loess Plateau (CLP), much research has focused on implementing soil-plant-atmosphere models to inform mitigation initiatives such as large-scale vegetation restoration programs. However, model choice typically depends on measurement availability and specific research questions, where many modeling approaches are established according to site specific data and parameterized via local information, making their generalization elsewhere difficult. Furthermore, in most studies only one modeling approach is selected, and thus its merit is difficult to assess relative to alternatives. Given these challenges, this review examines the capability of models with different level of complexity to simulate water fluxes and nutrient transformations for the CLP. Reviewed models were typically employed under different climate conditions (e.g., snowmelt, soil freezing and thawing) and across different land-uses (e.g., revegetated areas) which reflects the robustness of some models (e.g., for description of vegetation grow), but at the same time illustrates model weaknesses that should be addressed (e.g., water simulations under thawing conditions). On conducting this review, a general framework for choosing or developing the most appropriate modeling approach is established given a study site’s climatic and ecological conditions and research aims.

Keywords: Critical zone observatory; ecosystem services; process-based modeling; semi-arid
Introduction

Ensuring sustainable agricultural systems with their complex soil-water-plant interactions is an on-going challenge (Foley et al., 2011). To achieve sustainable solutions, innovative research should embrace multi-disciplinary systems and focus on resource-use efficiencies, productivity and profitability - while at the same time address the dynamics of climate change which challenge sustainable crop management and biodiversity (Pi et al., 2021). In this respect, the Earth’s critical zone (CZ) plays a major role in exchanges of water, solutes, energy, gases, solids, and organisms among the biosphere, hydrosphere, atmosphere, and lithosphere, which in turn maintains a life-sustaining environment (Chorover et al., 2011; Gordon and Dietrich, 2017; Lin, 2010; Rasmussen et al., 2011). Further, and in order to understand the effect of anthropogenic and natural changes, such as those driven by change in land use and climatic variability, on CZ processes, integrated observational (long-term monitoring) and modeling tools are required (Pi et al., 2021; Tetzlaff et al., 2017). This strategy has been shown to be crucial to improve water resources management and for environmental sustainability (Tetzlaff et al., 2017).

The inherent complexity of the CZ has led to the establishment of many physically- or process-based model forms (Brilli et al., 2017; Clark et al., 2017; Zhang et al., 2016). These models, in many cases, were developed according to the requirements of the investigated scientific field, such as hydrology, ecology and agriculture. The diverse collection of models makes it difficult to know with any clarity for where and when it is ideal to use a specific model, or a range of alternative but complementary models. To provide clarity for model choice, this paper reviews the application, calibration and validation of models which have been employed or developed for the Chinese Loess Plateau (CLP), and at a variety of spatial scales. The review highlights
advantages and disadvantages associated with the described models, together with options for their improvement. Accordingly, a general framework for choosing or developing the most appropriate modeling approach is established, where multiple models should be employed for context and objective comparison. Further, the analytical framework bridges ecosystem services (ES) science (typically conducted through statistical models) with CZ science (typically conducted through the process-based models that are reviewed), where this coupling ensures CLP research has clear societal and policy relevance.

Characteristics of the Loess Plateau

China’s Loess Plateau (100°54´-114°43´E and 33°43´- 41°16´N) is composed of arid, semi-arid and semi-humid areas and resides in the middle reaches of the Yellow River encircled by mountains (Figure 1). The main groups of soils formed in loess are silt-loam, loam, silt-clay-loam, sand-loam, silt-clay, and loam-sand soils that are calcareous to the surface (Huang et al., 2010). With an average thickness of 50-200 m, loess soils are highly erodible (Wang et al., 2017). The current ecological state of the region is a result of a combination of factors including climate, soil type and composition, vegetation coverage, and human activities.

Rainfall in the plateau typically displays high temporal and spatial variability, with main periods of rainfall from July to September and often in the form of high-intensity rainstorms. Thus, extreme soil erosion is triggered with an increased sediment transport to the Yellow River (Shi and Shao, 2000). Average annual precipitation in the region ranges from 150-750 mm, gradually decreasing from southeast to northwest. Evaporation varies between 1000 to 2000 mm but may
exceed 3000 mm in some areas. Annual mean temperature ranges between 6 to 10°C from south to north, while its frost-free period ranges from 185 to 210 days.

Figure 1. The Chinese Loess Plateau, shown with geographical variations in mean annual temperature (MAT, °C) and mean annual precipitation (MAP, mm), and the three CZ observatories (CZO)
In the CLP, the five main land use types are: forestland (25.69%), grassland (25.44%), cultivated land (22.48%), unused land (17.07%), orchards (1.88%), and others (7.44%) (National Development and Reform Commission, 2010). The main crops are wheat (*Triticum aestivum* L.) and maize (*Zea mays* L.), as well as soybeans (*Vigna angularis*), millet (*Panicum miliaceum*), apple orchards, and potatoes (*Solanum tuberosum* L.) (Chen et al., 2007; Huang & Gallichand, 2006; Wang et al., 2017). The region is one of China’s major producers of winter wheat and spring maize, where the latter is on a constant yield increase with a high yield of about 12 t/ha (Kang et al., 2003; Liu et al., 2010). Maize is grown in warm and humid valleys and flat areas. Orchard land use varies from apple and kiwi to jujube, pear, grape, and peach fruit crops. The plateau is the largest producer of kiwi fruit and the second largest producer of apple fruit in China (Wang et al., 2017).

**Vegetation restoration programs**

To control soil erosion and improve the ecological environment, vegetation re-generation has been widely applied. This includes extensive tree planting since the 1970s, integrated soil erosion controls at the watershed scale in the 1980s and the 1990s (Xin et al., 2008), and the start of the government-funded ‘Grain for Green’ (or sloping land conversion, GfG) project in 1999 (Lü et al., 2012) that aimed at transforming low-yield slope cropland into grassland/forest (Sun et al., 2015). Vegetation coverage altered land use patterns, and changes in soil organic carbon (SOC) contents and water storage have all been improved by the implementation of these policies (Dang et al., 2014). Chang et al. (2011) indicated that enhanced SOC sequestration was possible through expanding the coverage of grassland and shrub in the northern CLP, together
with expanding the coverage of forest in the middle and southern CLP. Yet, the high density
planting of exotic tree species, such as black locust (*R. pseudoacacia*), Chinese pine (*P.
tabulacformis*) and pea shrub (*C. korshinskii*), has been shown to induce soil desiccation and the
formation of a dry soil layer (SMC) (Jia et al., 2017). Thus, the effects of vegetation restoration
on ES are still unclear, yet this is crucial for gauging the performance of the large-scale
ecological restoration programs implemented in this region and in turn, informing policies
towards regional socio-ecological sustainability.

**Monitoring stations**

Across the CLP, many spatio-temporal research datasets have been, and continue to be collected,
measuring a wide and impressive variety of processes and elements in the CZ. These datasets
have been used to both parameterize and validate different types of models. Thus, the
performance and value of a given model implementation is often directly dependent on data
availability. Three stations can be identified as ‘first batch’ CZ observatories (CZO): (i) the
‘Shenmu Erosion and Environment Station’, (ii) the ‘Ansai Comprehensive Experimental Station
of Soil and Water Conservation’, and (iii) the ‘Changwu Agro-ecology Experiment Station’
(Figure 1). Crucially, each station is located in one of the three main topographical regions of the
plateau representing a gradient in both rainfall and temperature. At each CZO, treatments of
different vegetative covers and soil and water conservation practices, at some combination of the
plot / slope / watershed / catchment scale were established in the 1980s / 1990s. Their long-term
measurements include plant properties, soil nutrients and water, canopy size, runoff, soil losses /
erosion, water re-distribution in the root zone, and meteorological records.

Reviewed models

Various process-based models have been parameterized to simulate the relationship between soil
moisture and associated vegetation dynamics for the three main land uses of the CLP – cropland,
shrubland and forestland (Zhang et al., 2016). Here, nine models are reviewed in context of their
conceptual basis and the model equations that describe the relationships between plants, water
and climate (Table 1; Figure 2). Given descriptions are only basic, as many modifications have
been applied over time. Further, some modifications are study-specific and are not always
embedded in a model’s software or described in its user manual. Most models require similar
weather inputs (air temperature, wind speed, global radiation, relative humidity, and
precipitation) and are restricted to daily time step calculations (Table 1). Only the SHAW and
SWCCV models enable calculations at an hourly time step. The main difference between the
nine models is the description of the root water uptake process. Here some models account only
for moisture conditions in the soil as the dominant process, while other models include soil
temperature and stomatal conductance processes (Table 1). Therefore, detailing all model
differences is out of scope for this study, where the reader is referred to Brilli et al. (2017) for
fuller descriptions of carbon (C) and nitrogen (N) cycles, for most of the study models chosen. A
further difference is related to the complexity of the biochemical modeling (‘pools’) component,
which can be expressed by the number of model input parameters (Table 1), and where this
number might change according to the conditions and vegetation types that are of interest. Given
varying levels of model complexity (for example, by the number of parameters) and different
(study-specific) validation datasets, comparing prediction accuracy across the study models
cannot be objectively reported. Furthermore, no CLP studies have captured information on
parameter uncertainty and its consequences for model performance (i.e., via a useful estimate of
prediction error). This omission is discussed; addressing it is seen as good practice for future
CLP model work. In the following sections, models are reviewed in terms of: (a) plant and soil
water interactions; (b) plant and soil nutrient interactions; and (c) plant, soil water and soil
nutrient interactions.
Table 1. Description of the nine soil-plant-atmosphere models that were used for the inter-comparison.

<table>
<thead>
<tr>
<th>Model name</th>
<th>Dominant processes simulated</th>
<th>Approach to root water uptake</th>
<th>Approach to nutrient uptake</th>
<th>Approach to soil water flow</th>
<th>Time step</th>
<th>Number of input parameters</th>
</tr>
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<tbody>
<tr>
<td><strong>EPIC</strong></td>
<td>Simulations based on a set of mathematical formulations to describe the physico-chemical processes that occur in soil and water under agricultural management (Williams, 1995).</td>
<td>Function of root depth, soil water content, and an empirical water extraction distribution parameter.</td>
<td>Nutrient uptake is controlled either by plant demand or by the soil nutrient concentration.</td>
<td>Tipping bucket</td>
<td>Daily</td>
<td>22</td>
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<tr>
<td><strong>SHAW</strong> (Simultaneous Heat and Water Transfer)</td>
<td>Simulates soil heat, water, and solute transfer. The model includes the effects of plant cover, dead plant residue, snowmelt, soil freezing and thawing (Flerchinger and Pierson, 1991).</td>
<td>Defined as a pressure head approach, assuming continuity in water potential throughout the plants (soil, xylem of plant, and the leaves of canopy).</td>
<td>Passive uptake – the extraction of nutrients by the roots depends on the concentration of the nutrient in the soil.</td>
<td>Richard's equation</td>
<td>Daily or hourly</td>
<td>10</td>
</tr>
<tr>
<td><strong>Biome-BGC</strong></td>
<td>Ecosystem process model that simulates storage and flux of C,</td>
<td>Based on the stomatal conductance.</td>
<td>Nutrient uptake is controlled</td>
<td>Tipping bucket and</td>
<td>Daily</td>
<td>34</td>
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<tr>
<td><strong>Aquacrop</strong></td>
<td>Crop growth model that simulates the yield response of herbaceous crops to water. Specifically, the model is suited to conditions where water is a key limiting factor in crop production (Hsiao et al., 2009; Raes et al., 2009; Steduto et al., 2009).</td>
<td>Linear root water uptake (Water extraction patterns follow by default the standard 40%, 30%, 20% and 10%).</td>
<td>Nutrient uptake is controlled either by plant demand or by the soil nutrient concentration.</td>
<td>Tipping bucket</td>
<td>Daily</td>
<td>29</td>
</tr>
<tr>
<td><strong>CoupModel</strong></td>
<td>Simulation of water flow, heat transfer, solution transport (e.g., chloride) and representation of N and C cycles (Jansson, 2012).</td>
<td>Defined as a pressure head approach, based on the response functions for water content and soil temperature.</td>
<td>Empirical relationships that are related to crop demand and the nutrient state or source (e.g., inorganic or organic).</td>
<td>Richard's equation</td>
<td>Daily</td>
<td>23</td>
</tr>
<tr>
<td>Model</td>
<td>Description</td>
<td>Methodological Details</td>
<td>Frequency</td>
<td>Duration</td>
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<td>DSSAT-CSM</td>
<td>Simulates crop growth, development and yield as a function of the soil-plant-atmosphere dynamics for over 42 crops (Jones et al., 2003). Also includes CERES-Wheat.</td>
<td>Uses SPAM (a separate module): resolves energy balance processes for soil evaporation, transpiration, and root water extraction. Nutrient uptake is controlled either by plant demand or by the soil nutrient concentration.</td>
<td>Daily</td>
<td>23</td>
<td></td>
<td></td>
</tr>
<tr>
<td>WAVES</td>
<td>Simulates the processes of water, energy, and solute movement among the atmosphere, vegetation, and soil (Zhang and Dawes, 1998).</td>
<td>Described according to a weighting function which depends on the rooting density and availability of soil moisture.</td>
<td>Daily</td>
<td>32</td>
<td></td>
<td></td>
</tr>
<tr>
<td>APSIM</td>
<td>Simulates biophysical processes (including soil processes such as water balance, N and Phosphorus (P) transformations, soil pH and erosion) in farming systems of grain and fibre crops</td>
<td>Various modules, but all plant species use similar physiological principles. Root water uptake is described by an extraction potential, which is empirical. The focus of the APSIM is on cropping systems rather than individual crops. No detailed root uptake process.</td>
<td>Daily</td>
<td>21</td>
<td></td>
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grown in temperate and tropical areas (Keating et al., 2003). depends on soil and crop factors (e.g., Meinke et al., 1993).

<table>
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<tr>
<th>SWCCV</th>
<th>Simulations based on the concept of an equilibrium adjustment of vegetation growth to soil water dynamics and biogeochemical processes (Xia and Shao, 2008).</th>
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<td></td>
<td>Described according to a weighting function which depends on the rooting density and availability of soil moisture.</td>
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<tr>
<td></td>
<td>Active nutrient uptake, which is controlled by the Michaelis–Menten function.</td>
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<td></td>
<td>Tipping bucket</td>
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<td></td>
<td>Yearly, daily or hourly</td>
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Figure 2. A concept map showing the **key processes that were modeled and the reviewed models.**
Modeling plant and soil water interactions

Context and background

In water-limited arid and semi-arid regions, soil moisture and erosion are major factors which limit plant growth and crop productivity (Wang et al., 2013b). During water stress conditions, the ability of the ecosystem to respond depends on the amount of water stored in the soil profile and the plant’s ability to extract it (Jipp et al., 1998). From a regional perspective, land use and topography might also effect soil moisture and provide a useful context (Qiu et al., 2001).

During the government-funded re-vegetation campaigns, fast-growing tree and shrub species were planted in the CLP. Initial growth was often promising, but the soil water quickly depleted, affecting late-stage growth (Chen et al., 2010). Huang et al. (2001) observed a decrease in soil water following planting of apple trees, compared with winter wheat, which could be attributed to the higher evapotranspiration (ET) rate of the former. Similar phenomenon, in which soil water storage declined, was observed at the top 100cm of the soil under different plant types such as grassland, shrub, and forest in the semi-arid hilly area of the CLP (Chen et al., 2010; Jia et al., 2017). This is mainly because the soil water was not able to be fully replenished.

From an agriculture perspective, winter wheat monoculture covers 56% of arable land use in the plateau. Therefore, adequate water mass balance assessments for this crop are highly necessary. In areas of the CLP where the total annual rainfall is just under 600mm, water availability is a primary limiting factor for grain yield. Furthermore, winter wheat is sown in mid-September and harvested in early July of the following year, which does not coincide with the rainy season. Soil water storage has a critical role in mitigating the effect of inter-annual variation of precipitation on crop growth. To maximize soil water storage, different approaches are implemented such as
to keep the soil fallow during the rainy season (summer) or by limited irrigation practices (Huang et al., 2003; Kang et al., 2002). Maize is another core crop whose growing season of April to September does not match the rainy season (i.e., June to September which provides 50-60% of the annual total rainfall). Shortage of rain water at the early growth stage together with erratic rainfall at later growth stages can reduce maize yield (Zhang et al., 2014). In this respect, conservation tillage together with other field management practices, such as mulching with plastic film, have been extensively applied to improve water use efficiency and thereby stabilize high yields.

**Model implementation and review**

Huang et al. (2006) applied the EPIC model for simulating winter wheat and maize at the Changwu Agro-ecological Experimental Station for a 20-year field experiment. The model performed relatively well in predicting soil water content (SWC) and ET due to ‘accurate’ input values for three key hydrological processes - precipitation, percolation, and runoff. However, runoff (as a component of soil water balance) created computation errors, that affected modeling of subsequent processes, such as yield and contaminant transport. Results were, therefore, only valid for situations where runoff measurements were fully controlled, such as those for terraces with border dykes. Wang and Li (2010) extended the study of Huang et al. (2006) and evaluated EPIC for winter wheat, spring maize, alfalfa, North China milkvetch and small-leaf carmona (*Cameraria microphylla*). EPIC performed well for predicting SWC, yields of winter wheat and spring maize, and dry forage of alfalfa and milkvetch. However, the predictions for small-leaf carmona were poor. A different investigation in the Changwu site, involved the application of the
SHAW model to an apple orchard to investigate the effect on soil-water content (Huang & Gallichand, 2006). The study reported apple trees do deplete water eventually, but in this case no specific model sensitivity was reported.

Using the SWCCV model, Jia et al. (2019) indicated that an optimal plant coverage or biomass is important for regional water balance, soil protection and vegetation sustainability. Further, a modified Biome-BGC model has been used to simulate the long-term dynamics of actual ET (AET), net primary productivity (NPP) and leaf area index (LAI) for alfalfa, pea shrub, sea buckthorn (*Hippophae rhamnoides*) and black locust (Jia et al., 2019; Zhang et al., 2015). Generally, the modified Biome-BGC performed well in terms of simulating AET dynamics for the four grass, shrub and tree species. As NPP and LAI are linearly related with AET, Biome-BGC is thus similarly suited to simulating NPP and LAI for the same species. The optimal plant coverage (expressed as the maximum LAI) and the optimal SWCCV (expressed as NPP) for different precipitation regions were also quantified to provide a re-vegetation standard index, where this index enables future re-vegetation activities to be objectively guided to ensure a sustainable eco-hydrological environment.

The AquaCrop model has been used to simulate both plant (above ground biomass, grain yield, and canopy cover (CC) and SWC characteristics (Zhang et al., 2013). Simulations were performed for winter wheat yield under rainfed conditions, where the model performed well for yield and CC, but not so well for biomass and SWC. The AquaCrop model was sensitive to snowfall, which affected model’s performance considerably across key crop development stages. Essentially, it was more important to define when the snow began to melt rather than when it fell. An additional example for improper description of the winter conditions in the CLP is the application of the CERES-Wheat model which is embedded in DSSAT-CSM (Zheng et al.,
2017). This model has been applied to facilitate the development of optimal water management practices. Although, simulations for above-ground biomass, LAI, and grain yield were adequate, the model could not properly account for frosting conditions during winter. This resulted in recommending impractical optimized planting dates. Furthermore, the model did not perform well for simulating winter wheat biomass within water stress conditions.

The descriptions given illustrate that the establishment of a modeling tool for a specific process, under specific environmental conditions, can neglect critical processes. For example, while SWC is typically predicted well by a range of models, there can be errors in runoff assessments due to poor boundary condition definition (i.e., structural error). Further, since it is virtually impossible to construct a ‘super’ model that would include all processes and associated nuances, a modeling framework, using multiple models, is recommended. For example, Huang et al. (2006) (EPIC), Huang and Gallichand (2006) (SHAW) and Jia et al. (2019) (SWCCV) each reported good levels of SWC prediction accuracy, despite implementing different water flow models. Furthermore, given that the soil physical parameters in the above mentioned studies were attained from different sources, SWC prediction can be considered robust. Nevertheless, only concurrent implementations of EPIC, SHAW and SWCC would provide objectivity to this premise. For clarity, the water flow model for EPIC requires the wilting point, field capacity, saturated SWC, and saturated hydraulic conductivity parameters to be estimated from default empirical equations. For SHAW, the Brooks and Corey (1966) hydraulic functions (four parameters) are required, while for SWCCV, the van Genuchten (1980) hydraulic functions (five parameters) is implemented. Parameters for both hydraulic functions of SHAW and SWCCV can be estimated
according to measured retention and unsaturated hydraulic curves or attained by pedo-transfer functions (e.g., Schaap et al. 2001).

Modeling plant and soil nutrient interactions

Context and background

Due to natural drought conditions, intensive human disturbance, and severe soil erosion, the CLP region has the lowest SOC density (SOCD) in China (Yu et al., 2007). Yet, SOC is a key indicator of soil quality and overall soil productivity because of its influence on cation exchange capacity, aggregation, and water retention. Increasing organic C content in the plateau is possible through the re-forestation of degraded soils and ecosystems. Soil C sequestration is vital as it enhances soil fertility while reducing carbon dioxide (CO₂) emissions (Han et al., 2016). SOCD tends to be highest in hilly plateau soils (i.e., areas of high elevation and low temperature) and valley soils (i.e., areas of low elevation and high precipitation). High levels of fine soil particle contents also tend to coincide with high SOCD values. SOCD tends to be higher under cropland than under forest or grassland at the regional-scale of the entire plateau (Liu et al., 2011). Cultivation processes, such as land levelling and terracing, fertilization, tillage, and crop-residue management, tend to increase SOC accumulation in all areas of the plateau, where irrigation mitigates against shortages in rainfall (Liu et al., 2011). Note that there are cases where cropland soils can have lower SOC contents compared to those under forest and grassland (Chen et al.,
Dang et al., 2014; Gong et al., 2006; Li et al., 2005; Wang et al., 2001). This occurs in areas that are characterized with relatively homogeneous environments.

Additional vital soil properties for soil productivity and quality are soil total N (STN) and soil total P (STP) (Comber et al., 2018; Wang et al., 2009; Zhao et al., 2015). Reduction of STN and STP can decrease soil nutrient supply, porosity and soil structure, where the loss of STN and STP by soil erosion, leaching, or rainfall scouring exacerbates the situation (Wang et al., 2009). Soils data from a variety of land use types (cropland, grassland, shrubland, woodland, wasteland and abandoned land) have been investigated where significant differences were observed for soil organic matter (SOM), STN, and nitrate nitrogen (NON) (Gong et al., 2006). Similarly, the spatial homogeneity for STN and STP can change significantly with land use and will broadly decrease in this order: cropland > grassland > shrubland (Wang et al., 2009). Ultimately, the numerous studies concerning vegetation restoration in the CLP displayed the positive effect of vegetation restoration by improving soil quality as stocks of SOC, STN and STP increase with re-vegetational age (Jia et al., 2012).

Model implementation and review

It has been suggested that water use efficiency (WUE) and meeting plant N requirements could be improved by plastic film mulching (particularly with black film), together with a controlled fertilizer release for maize, thereby increasing grain yield in the region (Liu et al., 2016). In this respect, mulching and fallow cropping, as part of conventional management practices, and their effect on the water balance and WUE in winter wheat have been evaluated using the CoupModel (Zhang et al., 2007a,b). Model simulations indicated that mulching increased soil water storage,
increased wheat transpiration but decreased soil evaporation, thus a higher wheat yield and improved WUE was achieved. Furthermore, water was found to reach deeper horizons resulting in extensive deep percolation in a wet year (Zhang et al., 2007a,b). However, the CoupModel model showed weaker performance when the soil was frozen or partially frozen.

N use efficiency is similarly important for sustainable agriculture in arid and semi-arid areas. Zhang et al. (2016) showed a winter wheat sown with a green manure legume crop was able to fix atmospheric N\textsubscript{2} and thereby improve the soil N pool. Cultivation of the green manure in the summer was viewed as a better option than bare fallow. However, simulations from CoupModel indicated that growing green manure in the fallow period without considering optimal harvest times (ca. 30 days before sowing the winter wheat) reduced soil water storage and lowered wheat yields (Zhang et al., 2007a,b). For the North China Plain, the APSIM model has been used to analyze the crop yield and resource use efficiency of wheat-maize systems (Chen et al., 2010a,b,c). For example, APSIM was applied to a alfalfa (lucerne)–wheat rotation system in order to establish best management practice (Chen et al., 2008). The benefits of integrating alfalfa with annual cropping included that of reduced runoff and improved soil water storage (provided a ‘just-in-time’ removal date prior to sowing winter wheat is achieved). Furthermore, alfalfa has been shown to improve the WUE and soil fertility in cropping systems. However, the APSIM model was less successful in simulating the variability of the deep soil water content (Chen et al., 2008). This was attributed to not accounting for the root water uptake from deeper parts of the CZ. Note that there is a degree of uncertainty concerning the benefits of alfalfa to crop yield, due to the extraction of water from deeper soil layers and the development of
desiccated layers (Li & Huang, 2008). Thus, future simulations with the APSIM model would have to include a better description of the deep percolation in the CZ.

SOM enhances soil chemical and physical characteristics, it is both a nutrient sink and source and it promotes biological activity – thus SOM is a key component of the soil resource base (Craswell and Lefroy, 2001). Fluctuations in the amount, quality and turnover rate of SOM, due to changes in soil management practice, can influence the soil’s physical, chemical and biological properties (Haynes, 2000; Jiang et al., 2006). The DSSAT-CSM model has been used to simulate spring maize and winter wheat, providing tolerable levels accuracy for simulations of topsoil SOC and soil organic N (SON) under regular fertilizer application conditions (Li et al., 2015). DSSAT-CSM can similarly be used to investigate the effects of climate change on crop yields and simulate soil nitrate accumulation and leaching under different fertilizer treatments, rainfall conditions, and management practices. Note that the DSSAT-CSM model showed sensitivity to N stress, which effected the model performances.

Again, as before, different models use different parameters to simulate the same process, where implementations of multiple models for the same study would provide some objectivity to simulation accuracy. For example, to describe winter wheat growth using CoupModel, 12 parameters were used (Zhang et al., 2007a). Five of these parameters were calibrated (fraction of carbon in leaf reallocated to grain; fraction of carbon in stem reallocated to grain; fraction of carbon in root reallocated to grain; radiation use efficiency and specific leaf area), while the remaining seven parameters were measured and or attained from the literature. In contrast, in DSSAT-CSM, seven parameters were calibrated for winter wheat growth (optimum vernalizing temperature; photoperiod response; grain filling; kernel number per unit canopy weight at anthesis; standard kernel size under optimum conditions; standard, non-stressed mature tiller).
The calibrated parameters of both DSSAT-CSM and CoupModel are site-specific and cannot be generalized.

Land use type is a key factor to account for, as associated levels of variation in STN and STP directly influence the accuracy of the model’s simulations for soil nutrient status and nutrient movement (Wang et al., 2009). Further, the effect of land uses on soil properties should be expressed by their different behaviors and patterns at various spatial scales. Thus, a key challenge is to apply the DSSAT-CSM model or any other model in this respect, over different spatial scales. While plot scale models tend to be more complex and informative, as spatial (or temporal) scales increase, the applied models are inherently oversimplified, while the value of implementing a plot scale model over an area larger than 1 km² is debatable. Further work is required in this respect, noting that problematic scale issues are inherent to any CZ or ES analysis, whether mathematical or statistical (Comber and Harris, 2022).

**Modeling plant, soil water, and soil nutrient interactions**

**Context and background**

In soil-plant-atmosphere systems, plants with their roots provide pathways to transfer water from the soil to the atmosphere. Deep roots re-distribute deep soil water to shallower topsoil layers when the leaf stomata close, which enhances plant water transport efficiency (Lee et al., 2005). For shallow soil layers, which are generally within the root zone, the distributional pattern of the SWC is dependent on land use and topography (e.g., slope gradient and aspect), while infiltration, evaporation, and percolation should not be neglected (Qiu et al., 2001; Xuechun
Wang et al., 2013a,b). For each land use type, roots are distributed differently depending on the specific vegetation, which brings about different water uptake and transpiration and hence different soil-water distributions. The soil-water cycle in the soil–plant–atmosphere system is significantly affected by land use, where WUE varies with root density in the different soil layers (Qiu et al., 2001; Wang et al., 2013a,b).

**Model implementations and review**

For simulating such processes, the WAVES model has been compared with a simple to implement modified statistical-dynamic model (Huang et al., 2001) based on the Eagleson statistical-dynamic water balance model (Eagleson, 1978). The modifications accounted for seasonal variations of precipitation and soil moisture and their influence on plant transpiration resulting in different computations for soil water properties and water flow. Simulations from the modified model accurately predicted the mean water balance components and the dynamic processes of the mean soil moisture for a specific wheat-fertility-productivity condition (Huang et al., 2001).

The production of annual crop biomass can be directly proportional to the quantity of radiation intercepted, the amount of water transpired, and the makeup of the nutrients taken up (Gregory et al., 1997). Precipitation, being the major source of available water for dryland crops, needs to be used efficiently to sustain yields and to avoid stored soil water depletion. Availability of soil water directly influences nutrient loss and the rate of mineralization of N from SOM (Gregory et al., 1997). This may result in increased residual N accumulation in the soil after crop harvest, which can degrade environmental quality through increased N leaching into the groundwater and
emissions of greenhouse gases, such as N₂O. On the other hand, soils enriched with N through manures and fertilizers can increase crop yields in the presence of abundant soil water that may then result in increased soil-water depletion (Wang et al., 2013a,b). The core task of the CERES-Wheat model was to solve such yield-related problems with respect to determining the main factors that influence yield and to concurrently determine the optimum irrigation and fertilizer management practices, accordingly. The model was applied across the whole Guanzhong region of the Shaanxi province of the CLP, where it simulated the interaction of N, water, and climatic factors in order to evaluate their contributions to wheat yield and associated management strategies (Ji et al., 2014). Note, in a different study, that both CERES-Wheat and DSSAT-CSM inaccurately simulated winter wheat biomass under stressed conditions (Zheng et al., 2017).

The influence of vegetative restoration on deep soil–water storage has been the focus of many CLP studies (Chen et al., 2008; Jia et al., 2019; Wang et al., 2013c). Despite reducing soil erosion and water losses, artificial plantings can lead to the formation of dry soil layers which can significantly restrict land productivity (Chen et al., 2008). Fu et al. (2012) tested the SHAW model in a shrubland environment for two shrub species (Caragana korshinkii Kom and Salix psammophila) and observed that increased plant coverage was associated with reduced water storage in the upper soil layers. Water content differed vertically across the soil profile due to differences in root water uptake between the two species; generally, denser shrub coverage increased the degree of soil desiccation. The SHAW model showed a poor performance during the freeze–thaw cycles, since its assumed soil hydraulic properties were inaccurate for a frozen soil. The EPIC model has been applied to forage-crop rotation systems: alfalfa/potato/winter-wheat and was found to reliably capture monthly SWC and the vertical distribution of soil water (Wang et al., 2011; Wang et al., 2013c). The model’s simulation accuracy strongly depended on
input parameters such as seasonal rainfall, solar radiation, soil characteristics, and user-defined ET and soil moisture equations (Wang et al., 2011). The EPIC model has proved to be an effective tool to predict soil desiccation, however. Wang et al. (2012) highlighted a decrease in SWC due to the long-term cultivation of a grain crop after alfalfa. Here, the appropriate stand age of alfalfa would be 8–10 years and the appropriate cultivation years for following a grain cropping system would be 16–18 years. Cultivating shallow root crops, such as potato and soybean, has also been recommended to recover soil desiccation after alfalfa (Wang et al., 2012). SWC plays a crucial role in biological and hydrological processes including above and below ground runoff, flooding, solute transportation, soil erosion, plant growth and land-air interactions. Hydrological, ecological and climatic modeling can help understand variation in SWC down the soil profile, which is critical to water management and associated planting strategies (Mendham et al., 2011; Wang et al., 2013a,b,c).

EPIC has also been applied to an artificial black locust forest to evaluate biomass and soil desiccation effects; and to an apple orchard (*Malus pumila*), where water and nutrients were reaffirmed as the most important factors that influence yield. Fertilization can also be advantageous in improving WUE and yields of dryland orchards, but conversely, may increase water consumption through transpiration causing soil desiccation because of the deteriorated soil condition (Peng et al., 2017).

**Ecosystem research, critical zone processes and a modeling framework**

Few studies world-wide have fully incorporated ES in the assessment of basin-scale ecological restoration projects where their incorporation could open up opportunities for enhancing benefits
to human livelihood and generating public support (Trabucchi et al., 2012). The prevailing quantification methods for ES are usually based on statistical analyses (Fu et al., 2018; Hu et al., 2017; Liu et al., 2019). These ignore system dynamics, and associated uncertainty and feedbacks because of a lack of the mechanistic understandings of the processes involved (i.e. that obtained through physically-based models) (Nicholson et al., 2009). Thus, there is a great urgency to bridge ES science with CZ science through process-based models, to provide research that has clear societal and policy relevance, and with outputs that allow management approaches at different landscape scales to be modified through interventions (Field et al., 2015; Lü et al., 2012; Luo et al., 2019). As described throughout this review, a more comprehensive modeling framework that would account for most dominant spatio-temporal CZ processes is necessary.

Particular attention should be given to non-uniqueness or *equifinality*, where very different model structures and/or parameter sets are able to describe some observed behaviors with similar model response (Beven, 2006; Beven and Binley, 2014). It has been acknowledged recently that data-driven models suffer from a similar phenomenon (Schmidt et al., 2020). This concept of *equifinality* makes it difficult to define objectively model acceptability. Various methods and techniques have been proposed to identify the ‘best’ model such as the Generalized Likelihood Uncertainty Estimation methodology (Beven and Binley, 1992), the use of the Information Theory to discriminate models (Pachepsky et al., 2006), and a frequency-based performance measure (Teegavarapu et al., 2022). Other methods, such as the Diagnostic Efficiency (DE) (Schwemmle et al., 2021), offer the capability to disaggregate the different sources of errors (i.e., the model parameters, the model structure, and/or the input data). By using model ensembles for simulating the same process (e.g., Hassall et al. 2022), one can determine the main error source of the different models. Preceding to the models’ training stage, sensitivity analyses
can provide information regarding which parameters and processes are the most important for specific modeled conditions or systems. Sensitivity evaluations can help reduce model complexity and improve efficiency. Local and global sensitivity analyses are possible, where the former is a ‘one at a time’ approach, while the latter considers multiple parameters at the same time (Link et al., 2018; Naves et al., 2020). The local form does not account for interactions between parameters, while the global form does, and as such is computationally intensive which can make it prohibitive in its use.

The use of ensemble of model projections to estimate prediction uncertainty, comparable to the suggested approach above, is a common practice in fields such as climate research (Déqué et al., 2007; Reto et al., 2010; Strobach and Bel, 2020) and ecosystem research (Schwalm et al., 2010). This method enables the user to change and test different factors that can affect model uncertainty, such as initial condition, model parameters, spatial/temporal resolution. The simulated results are often considered to provide equal-weighted averages. Thus, it is assumed that the biases of an individual model are partly canceled by averaging all predictions (Reto et al., 2010). This approach might be utilized in soil modeling practices to determine the influence of each model parameter, its uncertainty and its structure on the simulated outputs (e.g., Brown and Heuvelink, 2005; Krishnan and Aggarwal, 2018; Shan et al., 2021). Furthermore, most soil models, as models in other fields (Reto et al., 2010; Strobach and Bel, 2020), are established according to current and recent past conditions (Jasper et al., 2006). Besides the urgent need to calculate uncertainties of models’ predictions, there are uncertainties regarding future conditions: a model calibrated under historic conditions may have questionable validity under future scenarios if the model states differ substantially from those in the calibration period. This
challenges, for example, future projections of different ecological systems that might be effected by climate change (McMahon et al., 2009).

A modeling framework, which can be directly used as a model-based decision support tool (DST), has in part, been developed for the CLP (Hu et al., 2015). This DST provides a platform to explore different management scenarios and to optimally plan them. The DST has four modules: (a) a module for scenario development, (b) the integrated ES model base, (c) the ES trade-off tool, and (d) the multi-objective spatial optimization module based on the fast, non-dominated sorting genetic algorithm-II (NSGA-II). With this DST, scenario testing and optimal decision-making analyses can be performed, considering climate (precipitation and temperature), land cover (vegetation, built-up areas, croplands, etc.) and socioeconomic (population and economic growth) factors. Via different scenarios, the ESs of soil and water and their optimal combinations can be simulated. In turn, adaptive management policy recommendations for vegetation restoration, soil and water resource use, and the payment for ESs for regional sustainability can be derived based on the utility of various trade-off analyses and multi-criteria optimizations. The DST, as with any DST, has the capability to be upgraded and refined. For example, through hybrid modelling strategies where process-based models are combined with statistical and/or machine learning models (Kuhnert, 2014), say to better characterize extreme events (Curceau et al., 2020; 2022).

Conclusions

In this review, a multitude of Loess Plateau studies were summarized in order to illustrate the disadvantages and advantages related to the specific process-based modelling approach taken.
Each study’s model performance was typically bound under different climate, land use, and temporal and spatial scales. Models were categorized in terms of: (i) plant and soil water interactions; (ii) plant and soil nutrient interactions; and (iii) plant, soil water and soil nutrient interactions. In each category, a clear deficiency existed in that research studies typically selected only one modelling approach for analyzing the dominant soil-plant processes. Using only one modeling approach might mislead, say through the indication of only one or the wrong dominant process; and as such, multiple models should be employed for context and comparison. In this respect, the establishment of a modelling framework that includes several models to describe the same process might more accurately highlight prevailing factors, where the use of model ensembles is also possible. The capacity to conduct a sensitivity analysis with respect to model parameter uncertainty should also be included.

Such a framework has, in part, been established, where some of the process-based models described (typically associated with critical zone science) are coupled with analytical tools (typically associated ecosystem services) that together provide both societal and policy relevance to Loess plateau research. For future studies, the reporting of a given model’s suitability and its relative accuracy to alternatives should be promoted, where a common set of model accuracy diagnostics are used to aid comparison across studies and processes. Answers to questions of why a given model was adopted, how well was it calibrated and how well was it validated are
crucial to ensure informed management or policy decisions, especially when they involve substantive financial investments.

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Conflict of interest

The authors declare no conflict of interest.

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