

24 **Abstract**

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

42

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

44 **Introduction**

45 Ensuring sustainable agricultural systems with their complex soil-water-plant interactions is an
46 on-going challenge (Foley et al., 2011). To achieve sustainable solutions, innovative research
47 should embrace multi-disciplinary systems and focus on resource-use efficiencies, productivity
48 and profitability - while at the same time address the dynamics of climate change which
49 challenge sustainable crop management and biodiversity (Pi et al., 2021). In this respect, the
50 Earth's critical zone (CZ) plays a major role in exchanges of water, solutes, energy, gases, solids,
51 and organisms among the biosphere, hydrosphere, atmosphere, and lithosphere, which in turn
52 maintains a life-sustaining environment (Chorover et al., 2011; Gordon and Dietrich, 2017; Lin,
53 2010; Rasmussen et al., 2011). Further, and in order to understand the effect of anthropogenic
54 and natural changes, such as those driven by change in land use and climatic variability, on CZ
55 processes, integrated observational (long-term monitoring) and modeling tools are required (Pi et
56 al., 2021; Tetzlaff et al., 2017). This strategy has been shown to be crucial to improve water
57 resources management and for environmental sustainability (Tetzlaff et al., 2017).

58 The inherent complexity of the CZ has led to the establishment of many physically- or process-
59 based model forms (Brilli et al., 2017; Clark et al., 2017; Zhang et al., 2016). These models, in
60 many cases, were developed according to the requirements of the investigated scientific field,
61 such as hydrology, ecology and agriculture. The diverse collection of models makes it difficult to
62 know with any clarity for where and when it is ideal to use a specific model, or a range of
63 alternative but complementary models. To provide clarity for model choice, this paper reviews
64 the application, calibration and validation of models which have been employed or developed for
65 the Chinese Loess Plateau (CLP), and at a variety of spatial scales. The review highlights

66 advantages and disadvantages associated with the described models, together with options for
67 their improvement. Accordingly, a general framework for choosing or developing the most
68 appropriate modeling approach is established, where multiple models should be employed for
69 context and objective comparison. Further, the analytical framework bridges ecosystem services
70 (ES) science (typically conducted through statistical models) with CZ science (typically
71 conducted through the process-based models that are reviewed), where this coupling ensures
72 CLP research has clear societal and policy relevance.

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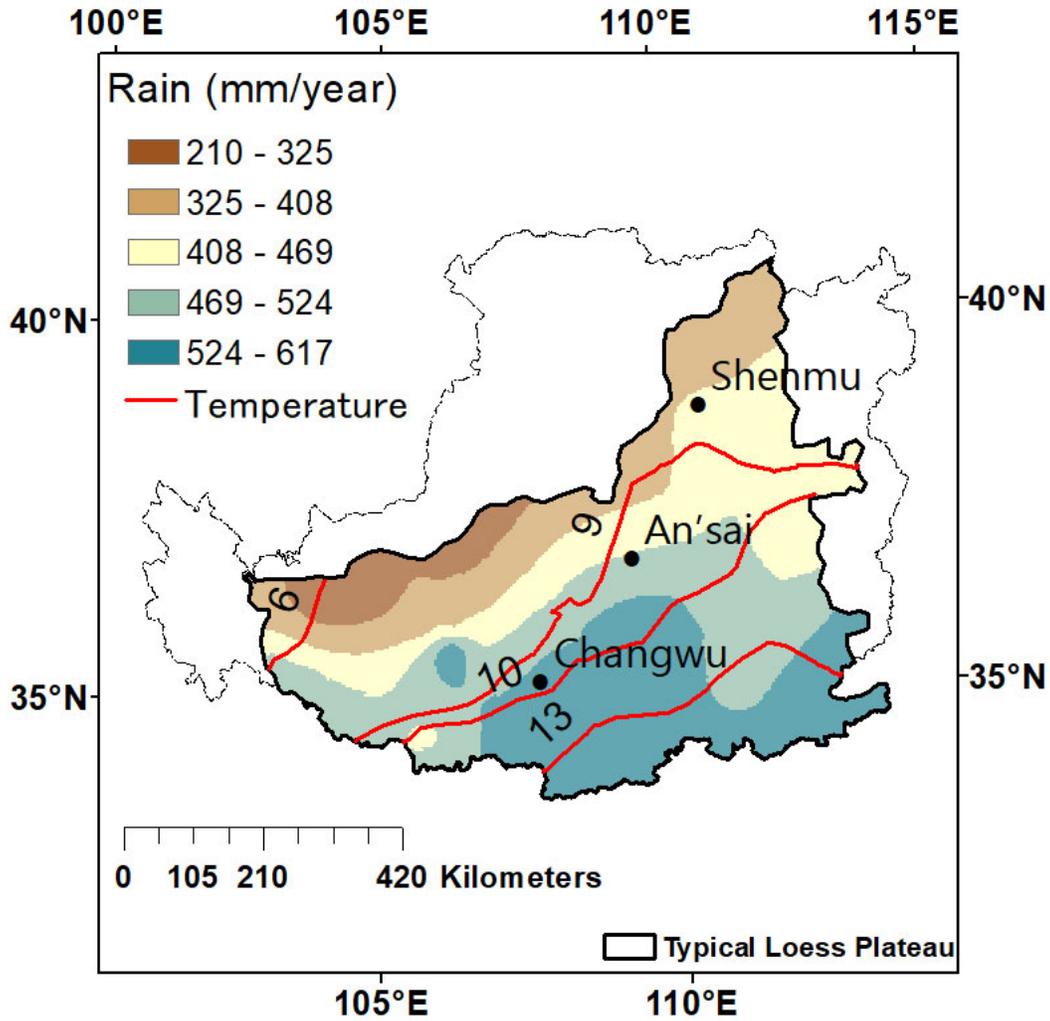
74 **Characteristics of the Loess Plateau**

75 China's Loess Plateau (100°54'-114°43'E and 33°43'- 41°16'N) is composed of arid, semi-arid
76 and semi-humid areas and resides in the middle reaches of the Yellow River encircled by
77 mountains (Figure 1). The main groups of soils formed in loess are silt-loam, loam, silt-clay-
78 loam, sand-loam, silt-clay, and loam-sand soils that are calcareous to the surface (Huang et al.,
79 2010). With an average thickness of 50-200 m, loess soils are highly erodible (Wang et al.,
80 2017). The current ecological state of the region is a result of a combination of factors including
81 climate, soil type and composition, vegetation coverage, and human activities.

82 Rainfall in the plateau typically displays high temporal and spatial variability, with main periods
83 of rainfall from July to September and often in the form of high-intensity rainstorms. Thus,
84 extreme soil erosion is triggered with an increased sediment transport to the Yellow River (Shi
85 and Shao, 2000). Average annual precipitation in the region ranges from 150-750 mm, gradually
86 decreasing from southeast to northwest. Evaporation varies between 1000 to 2000 mm but may

87 exceed 3000 mm in some areas. Annual mean temperature ranges between 6 to 10°C from south
88 to north, while its frost-free period ranges from 185 to 210 days.

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90

91 Figure 1. The Chinese Loess Plateau, shown with geographical
92 variations in mean annual temperature (MAT, °C) and mean annual
93 precipitation (MAP, mm), and the three CZ observatories (CZO).

94

95 In the CLP, the five main land use types are: forestland (25.69%), grassland (25.44%), cultivated
96 land (22.48%), unused land (17.07%), orchards (1.88%), and others (7.44%) (National
97 Development and Reform Commission, 2010). The main crops are wheat (*Triticum aestivum L.*)
98 and maize (*Zea mays L.*), as well as soybeans (*Vigna angularis*), millet (*Panicum miliaceum*),
99 apple orchards, and potatoes (*Solanum tuberosum L.*) (Chen et al., 2007; Huang & Gallichand,
100 2006; Wang et al., 2017). The region is one of China's major producers of winter wheat and
101 spring maize, where the latter is on a constant yield increase with a high yield of about 12 t/ ha
102 (Kang et al., 2003; Liu et al., 2010). Maize is grown in warm and humid valleys and flat areas.
103 Orchard land use varies from apple and kiwi to jujube, pear, grape, and peach fruit crops. The
104 plateau is the largest producer of kiwi fruit and the second largest producer of apple fruit in
105 China (Wang et al., 2017).

106

107 **Vegetation restoration programs**

108 To control soil erosion and improve the ecological environment, vegetation re-generation has
109 been widely applied. This includes extensive tree planting since the 1970s, integrated soil
110 erosion controls at the watershed scale in the 1980s and the 1990s (Xin et al., 2008), and the start
111 of the government-funded 'Grain for Green' (or sloping land conversion, GfG) project in 1999
112 (Lü et al., 2012) that aimed at transforming low-yield slope cropland into grassland/forest (Sun et
113 al., 2015). Vegetation coverage altered land use patterns, and changes in soil organic carbon
114 (SOC) contents and water storage have all been improved by the implementation of these
115 policies (Dang et al., 2014). Chang et al. (2011) indicated that enhanced SOC sequestration was
116 possible through expanding the coverage of grassland and shrub in the northern CLP, together

117 with expanding the coverage of forest in the middle and southern CLP. Yet, the high density
118 planting of exotic tree species, such as black locust (*R. pseudoacacia*), Chinese pine (*P.*
119 *tabulaformis*) and pea shrub (*C. korshinskii*), has been shown to induce soil desiccation and the
120 formation of a dry soil layer (SMC) (Jia et al., 2017). Thus, the effects of vegetation restoration
121 on ES are still unclear, yet this is crucial for gauging the performance of the large-scale
122 ecological restoration programs implemented in this region and in turn, informing policies
123 towards regional socio-ecological sustainability.

124

125 **Monitoring stations**

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

137 measurements include plant properties, soil nutrients and water, canopy size, runoff, soil losses /
138 erosion, water re-distribution in the root zone, and meteorological records.

139

140 **Reviewed models**

141 Various process-based models have been parameterized to simulate the relationship between soil
142 moisture and associated vegetation dynamics for the three main land uses of the CLP – cropland,
143 shrubland and forestland (Zhang et al., 2016). Here, nine models are reviewed in context of their
144 conceptual basis and the model equations that describe the relationships between plants, water
145 and climate (Table 1; Figure 2). Given descriptions are only basic, as many modifications have
146 been applied over time. Further, some modifications are study-specific and are not always
147 embedded in a model’s software or described in its user manual. Most models require similar
148 weather inputs (air temperature, wind speed, global radiation, relative humidity, and
149 precipitation) and are restricted to daily time step calculations (Table 1). Only the SHAW and
150 SWCCV models enable calculations at an hourly time step. The main difference between the
151 nine models is the description of the root water uptake process. Here some models account only
152 for moisture conditions in the soil as the dominant process, while other models include soil
153 temperature and stomatal conductance processes (Table 1). Therefore, detailing *all* model
154 differences is out of scope for this study, where the reader is referred to Brillì et al. (2017) for
155 fuller descriptions of carbon (C) and nitrogen (N) cycles, for most of the study models chosen. A
156 further difference is related to the complexity of the biochemical modeling (‘pools’) component,
157 which can be expressed by the number of model input parameters (Table 1), and where this
158 number might change according to the conditions and vegetation types that are of interest. Given

159 varying levels of model complexity (for example, by the number of parameters) and different
160 (study-specific) validation datasets, comparing prediction accuracy across the study models
161 cannot be objectively reported. Furthermore, no CLP studies have captured information on
162 parameter uncertainty and its consequences for model performance (i.e., via a useful estimate of
163 prediction error). This omission is discussed; addressing it is seen as good practice for future
164 CLP model work. In the following sections, models are reviewed in terms of: (a) plant and soil
165 water interactions; (b) plant and soil nutrient interactions; and (c) plant, soil water and soil
166 nutrient interactions.

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Table 1. Description of the nine soil-plant-atmosphere models that were used for the inter-comparison.

Model name	Dominant processes simulated	Approach to root water uptake	Approach to nutrient uptake	Approach to soil water flow	Time step	Number of input parameters
EPIC (Environmental Policy Integrated Climate)	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).	Function of root depth, soil water content, and an empirical water extraction distribution parameter.	Nutrient uptake is controlled either by plant demand or by the soil nutrient concentration.	Tipping bucket	Daily	22
SHAW (Simultaneous Heat and Water Transfer)	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).	Defined as a pressure head approach, assuming continuity in water potential throughout the plants (soil, xylem of plant, and the leaves of canopy).	Passive uptake – the extraction of nutrients by the roots depends on the concentration of the nutrient in the soil.	Richard's equation	Daily or hourly	10
Biome-BGC	Ecosystem process model that simulates storage and flux of C,	Based on the stomatal conductance.	Nutrient uptake is controlled	Tipping bucket and	Daily	34

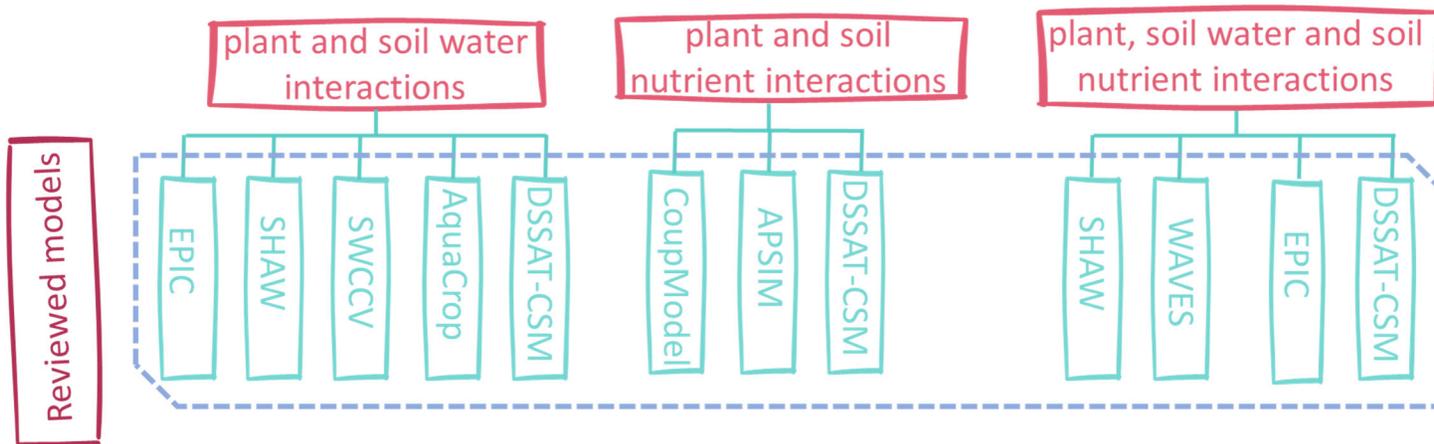
(Bio-Geochemical Cycles)	N and water (White et al., 2000).		either by plant demand or by the soil nutrient concentration.	Richard's equation		
AquaCrop	Crop growth model that simulates the yield response of herbaceous crops to water. Specifically, the model is suited to conditions where water is a key limiting factor in crop production (Hsiao et al., 2009; Raes et al., 2009; Steduto et al., 2009).	Linear root water uptake (Water extraction patterns follow by default the standard 40% ,30% ,20% and 10%).	Nutrient uptake is controlled either by plant demand or by the soil nutrient concentration.	Tipping bucket	Daily	29
CoupModel	Simulation of water flow, heat transfer, solution transport (e.g., chloride) and representation of N and C cycles (Jansson, 2012).	Defined as a pressure head approach, based on the response functions for water content and soil temperature.	Empirical relationships that are related to crop demand and the nutrient state or source (e.g., inorganic or organic).	Richard's equation	Daily	23

DSSAT-CSM	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 .	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.	Tipping bucket	Daily	23
WAVES	Simulates the processes of water, energy, and solute movement among the atmosphere, vegetation, and soil (Zhang and Dawes, 1998).	Described according to a weighting function which depends on the rooting density and availability of soil moisture.	Empirical relationships	Richard's equation	Daily	32
APSIM	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	Various modules, but all plant species use similar physiological principles. Root water uptake is described by an extraction potential, which	The focus of the APSIM is on cropping systems rather than individual crops. No detailed root uptake process.	Tipping bucket and Richard's equation	Daily	21

	grown in temperate and tropical areas (Keating et al., 2003).	depends on soil and crop factors (e.g., Meinke et al., 1993).				
SWCCV	Simulations based on the concept of an equilibrium adjustment of vegetation growth to soil water dynamics and biogeochemical processes (Xia and Shao, 2008).	Described according to a weighting function which depends on the rooting density and availability of soil moisture.	Active nutrient uptake, which is controlled by the Michaelis–Menten function	Tipping bucket	Yearly, daily or hourly	31

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Figure 2. A concept map showing the *key processes that were modeled and the reviewed models*.

172 **Modeling plant and soil water interactions**

173 **Context and background**

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

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

187 From an agriculture perspective, winter wheat monoculture covers 56% of arable land use in the
188 plateau. Therefore, adequate water mass balance assessments for this crop are highly necessary.

189 In areas of the CLP where the total annual rainfall is just under 600mm, water availability is a
190 primary limiting factor for grain yield. Furthermore, winter wheat is sown in mid-September and
191 harvested in early July of the following year, which does not coincide with the rainy season. Soil
192 water storage has a critical role in mitigating the effect of inter-annual variation of precipitation
193 on crop growth. To maximize soil water storage, different approaches are implemented such as

194 to keep the soil fallow during the rainy season (summer) or by limited irrigation practices
195 (Huang et al., 2003; Kang et al., 2002). Maize is another core crop whose growing season of
196 April to September does not match the rainy season (i.e., June to September which provides 50-
197 60% of the annual total rainfall). Shortage of rain water at the early growth stage together with
198 erratic rainfall at later growth stages can reduce maize yield (Zhang et al., 2014). In this respect,
199 conservation tillage together with other field management practices, such as mulching with
200 plastic film, have been extensively applied to improve water use efficiency and thereby stabilize
201 high yields.

202

203 **Model implementation and review**

204 Huang et al. (2006) applied the EPIC model for simulating winter wheat and maize at the
205 Changwu Agro-ecological Experimental Station for a 20-year field experiment. The model
206 performed relatively well in predicting soil water content (SWC) and ET due to ‘accurate’ input
207 values for three key hydrological processes - precipitation, percolation, and runoff. However,
208 runoff (as a component of soil water balance) created computation errors, that affected modeling
209 of subsequent processes, such as yield and contaminant transport. Results were, therefore, only
210 valid for situations where runoff measurements were fully controlled, such as those for terraces
211 with border dykes. Wang and Li (2010) extended the study of Huang et al. (2006) and evaluated
212 EPIC for winter wheat, spring maize, alfalfa, North China milkvetch and small-leaf carmona
213 (*Cameraria microphylla*). EPIC performed well for predicting SWC, yields of winter wheat and
214 spring maize, and dry forage of alfalfa and milkvetch. However, the predictions for small-leaf
215 carmona were poor. A different investigation in the Changwu site, involved the application of the

216 SHAW model to an apple orchard to investigate the effect on soil-water content (Huang &
217 Gallichand, 2006). The study reported apple trees do deplete water eventually, but in this case no
218 specific model sensitivity was reported.

219 Using the SWCCV model, Jia et al. (2019) indicated that an optimal plant coverage or biomass is
220 important for regional water balance, soil protection and vegetation sustainability. Further, a
221 modified Biome-BGC model has been used to simulate the long-term dynamics of actual ET
222 (AET), net primary productivity (NPP) and leaf area index (LAI) for alfalfa, pea shrub, sea
223 buckthorn (*Hippophae rhamnoides*) and black locust (Jia et al., 2019; Zhang et al., 2015).

224 Generally, the modified Biome-BGC performed well in terms of simulating AET dynamics for
225 the four grass, shrub and tree species. As NPP and LAI are linearly related with AET, Biome-
226 BGC is thus similarly suited to simulating NPP and LAI for the same species. The optimal plant
227 coverage (expressed as the maximum LAI) and the optimal SWCCV (expressed as NPP) for
228 different precipitation regions were also quantified to provide a re-vegetation standard index,
229 where this index enables future re-vegetation activities to be objectively guided to ensure a
230 sustainable eco-hydrological environment.

231 The AquaCrop model has been used to simulate both plant (above ground biomass, grain yield,
232 and canopy cover (CC) and SWC characteristics (Zhang et al., 2013). Simulations were
233 performed for winter wheat yield under rainfed conditions, where the model performed well for
234 yield and CC, but not so well for biomass and SWC. The AquaCrop model was sensitive to
235 snowfall, which affected model's performance considerably across key crop development stages.
236 Essentially, it was more important to define when the snow began to melt rather than when it
237 fell. An additional example for improper description of the winter conditions in the CLP is the
238 application of the CERES-Wheat model which is embedded in DSSAT-CSM (Zheng et al.,

239 2017). This model has been applied to facilitate the development of optimal water management
240 practices. Although, simulations for above-ground biomass, LAI, and grain yield were adequate,
241 the model could not properly account for frosting conditions during winter. This resulted in
242 recommending impractical optimized planting dates. Furthermore, the model did not perform
243 well for simulating winter wheat biomass within water stress conditions.

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

260 according to measured retention and unstatuated hydraulic curves or attained by pedo-transfer
261 functions (e.g., Schaap et al. 2001).

262

263 **Modeling plant and soil nutrient interactions**

264 **Context and background**

265 Due to natural drought conditions, intensive human disturbance, and severe soil erosion, the CLP
266 region has the lowest SOC density (SOCD) in China (Yu et al., 2007). Yet, SOC is a key
267 indicator of soil quality and overall soil productivity because of its influence on cation exchange
268 capacity, aggregation, and water retention. Increasing organic C content in the plateau is possible
269 through the re-forestation of degraded soils and ecosystems. Soil C sequestration is vital as it
270 enhances soil fertility while reducing carbon dioxide (CO₂) emissions (Han et al., 2016). SOCD
271 tends to be highest in hilly plateau soils (i.e., areas of high elevation and low temperature) and
272 valley soils (i.e., areas of low elevation and high precipitation). High levels of fine soil particle
273 contents also tend to coincide with high SOCD values. SOCD tends to be higher under cropland
274 than under forest or grassland at the regional-scale of the entire plateau (Liu et al., 2011).

275 Cultivation processes, such as land levelling and terracing, fertilization, tillage, and crop-residue
276 management, tend to increase SOC accumulation in all areas of the plateau, where irrigation
277 mitigates against shortages in rainfall (Liu et al., 2011). Note that there are cases where cropland
278 soils can have lower SOC contents compared to those under forest and grassland (Chen et al.,

279 2007; Dang et al., 2014; Gong et al., 2006; Li et al., 2005; Wang et al., 2001). This occurs in
280 areas that are characterized with relatively homogeneous environments.

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

293

294 **Model implementation and review**

295 It has been suggested that water use efficiency (WUE) and meeting plant N requirements could
296 be improved by plastic film mulching (particularly with black film), together with a controlled
297 fertilizer release for maize, thereby increasing grain yield in the region (Liu et al., 2016). In this
298 respect, mulching and fallow cropping, as part of conventional management practices, and their
299 effect on the water balance and WUE in winter wheat have been evaluated using the CoupModel
300 (Zhang et al., 2007a,b). Model simulations indicated that mulching increased soil water storage,

301 increased wheat transpiration but decreased soil evaporation, thus a higher wheat yield and
302 improved WUE was achieved. Furthermore, water was found to reach deeper horizons resulting
303 in extensive deep percolation in a wet year (Zhang et al., 2007a,b). However, the CoupModel
304 model showed weaker performance when the soil was frozen or partially frozen.

305 N use efficiency is similarly important for sustainable agriculture in arid and semi-arid areas.
306 Zhang et al. (2016) showed a winter wheat sown with a green manure legume crop was able to
307 fix atmospheric N₂ and thereby improve the soil N pool. Cultivation of the green manure in the
308 summer was viewed as a better option than bare fallow. However, simulations from CoupModel
309 indicated that growing green manure in the fallow period without considering optimal harvest
310 times (ca. 30 days before sowing the winter wheat) reduced soil water storage and lowered wheat
311 yields (Zhang et al., 2007a,b). For the North China Plain, the APSIM model has been used to
312 analyze the crop yield and resource use efficiency of wheat-maize systems (Chen et al.,
313 2010a,b,c). For example, APSIM was applied to a alfalfa (lucerne)–wheat rotation system in
314 order to establish best management practice (Chen et al., 2008). The benefits of integrating
315 alfalfa with annual cropping included that of reduced runoff and improved soil water storage
316 (provided a ‘just-in-time’ removal date prior to sowing winter wheat is achieved). Furthermore,
317 alfalfa has been shown to improve the WUE and soil fertility in cropping systems. However, the
318 APSIM model was less successful in simulating the variability of the deep soil water content
319 (Chen et al., 2008). This was attributed to not accounting for the root water uptake from deeper
320 parts of the CZ. Note that there is a degree of uncertainty concerning the benefits of alfalfa to
321 crop yield, due to the extraction of water from deeper soil layers and the development of

322 desiccated layers (Li & Huang, 2008). Thus, future simulations with the APSIM model would
323 have to include a better description of the deep percolation in the CZ.

324 SOM enhances soil chemical and physical characteristics, it is both a nutrient sink and source
325 and it promotes biological activity – thus SOM is a key component of the soil resource base
326 (Craswell and Lefroy, 2001). Fluctuations in the amount, quality and turnover rate of SOM, due
327 to changes in soil management practice, can influence the soil's physical, chemical and
328 biological properties (Haynes, 2000; Jiang et al., 2006). The DSSAT-CSM model has been used
329 to simulate spring maize and winter wheat, providing tolerable levels accuracy for simulations of
330 topsoil SOC and soil organic N (SON) under regular fertilizer application conditions (Li et al.,
331 2015). DSSAT-CSM can similarly be used to investigate the effects of climate change on crop
332 yields and simulate soil nitrate accumulation and leaching under different fertilizer treatments,
333 rainfall conditions, and management practices. Note that the DSSAT-CSM model showed
334 sensitivity to N stress, which effected the model performances.

335 Again, as before, different models use different parameters to simulate the same process, where
336 implementations of multiple models **for the same study** would provide **some** objectivity to
337 simulation accuracy. For example, to describe winter wheat growth using CoupModel, 12
338 parameters were used (Zhang et al., 2007a). Five of these parameters were calibrated (fraction of
339 carbon in leaf reallocated to grain; fraction of carbon in stem reallocated to grain; fraction of
340 carbon in root reallocated to grain; radiation use efficiency and specific leaf area), while the
341 remaining seven parameters were measured and or attained from the literature. In contrast, in
342 DSSAT-CSM, seven parameters were calibrated for winter wheat growth (optimum vernalizing
343 temperature; photoperiod response; grain filling; kernel number per unit canopy weight at
344 anthesis; standard kernel size under optimum conditions; standard, non-stressed mature tiller).

345 The calibrated parameters of both DSSAT-CSM and CoupModel are site-specific and cannot be
346 generalized.

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

357

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

359 **Context and background**

360 In soil-plant-atmosphere systems, plants with their roots provide pathways to transfer water from
361 the soil to the atmosphere. Deep roots re-distribute deep soil water to shallower topsoil layers
362 when the leaf stomata close, which enhances plant water transport efficiency (Lee et al., 2005).
363 For shallow soil layers, which are generally within the root zone, the distributional pattern of the
364 SWC is dependent on land use and topography (e.g., slope gradient and aspect), while
365 infiltration, evaporation, and percolation should not be neglected (Qiu et al., 2001; Xuechun

366 Wang et al., 2013a,b). For each land use type, roots are distributed differently depending on the
367 specific vegetation, which brings about different water uptake and transpiration and hence
368 different soil-water distributions. The soil-water cycle in the soil–plant–atmosphere system is
369 significantly affected by land use, where WUE varies with root density in the different soil layers
370 (Qiu et al., 2001; Wang et al., 2013a,b).

371

372 **Model implementations and review**

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

381 The production of annual crop biomass can be directly proportional to the quantity of radiation
382 intercepted, the amount of water transpired, and the makeup of the nutrients taken up (Gregory et
383 al., 1997). Precipitation, being the major source of available water for dryland crops, needs to be
384 used efficiently to sustain yields and to avoid stored soil water depletion. Availability of soil
385 water directly influences nutrient loss and the rate of mineralization of N from SOM (Gregory et
386 al., 1997). This may result in increased residual N accumulation in the soil after crop harvest,
387 which can degrade environmental quality through increased N leaching into the groundwater and

388 emissions of greenhouse gases, such as N₂O. On the other hand, soils enriched with N through
389 manures and fertilizers can increase crop yields in the presence of abundant soil water that may
390 then result in increased soil-water depletion (Wang et al., 2013a,b). The core task of the CERES-
391 Wheat model was to solve such yield-related problems with respect to determining the main
392 factors that influence yield and to concurrently determine the optimum irrigation and fertilizer
393 management practices, accordingly. The model was applied across the whole Guanzhong region
394 of the Shaanxi province of the CLP, where it simulated the interaction of N, water, and climatic
395 factors in order to evaluate their contributions to wheat yield and associated management
396 strategies (Ji et al., 2014). Note, in a different study, that both CERES-Wheat and DSSAT-CSM
397 inaccurately simulated winter wheat biomass under stressed conditions (Zheng et al., 2017).

398 The influence of vegetative restoration on deep soil–water storage has been the focus of many
399 CLP studies (Chen et al., 2008; Jia et al., 2019; Wang et al., 2013c). Despite reducing soil
400 erosion and water losses, artificial plantings can lead to the formation of dry soil layers which
401 can significantly restrict land productivity (Chen et al., 2008). Fu et al. (2012) tested the SHAW
402 model in a shrubland environment for two shrub species (*Caragana korshinkii* Kom and *Salix*
403 *psammophila*) and observed that increased plant coverage was associated with reduced water
404 storage in the upper soil layers. Water content differed vertically across the soil profile due to
405 differences in root water uptake between the two species; generally, denser shrub coverage
406 increased the degree of soil desiccation. The SHAW model showed a poor performance during
407 the freeze–thaw cycles, since its assumed soil hydraulic properties were inaccurate for a frozen
408 soil. The EPIC model has been applied to forage-crop rotation systems: alfalfa/potato/winter-
409 wheat and was found to reliably capture monthly SWC and the vertical distribution of soil water
410 (Wang et al., 2011; Wang et al., 2013c). The model’s simulation accuracy strongly depended on

411 input parameters such as seasonal rainfall, solar radiation, soil characteristics, and user-defined
412 ET and soil moisture equations (Wang et al., 2011). The EPIC model has proved to be an
413 effective tool to predict soil desiccation, however. Wang et al. (2012) highlighted a decrease in
414 SWC due to the long-term cultivation of a grain crop after alfalfa. Here, the appropriate stand
415 age of alfalfa would be 8–10 years and the appropriate cultivation years for following a grain
416 cropping system would be 16–18 years. Cultivating shallow root crops, such as potato and
417 soybean, has also been recommended to recover soil desiccation after alfalfa (Wang et al., 2012).
418 SWC plays a crucial role in biological and hydrological processes including above and below
419 ground runoff, flooding, solute transportation, soil erosion, plant growth and land-air
420 interactions. Hydrological, ecological and climatic modeling can help understand variation in
421 SWC down the soil profile, which is critical to water management and associated planting
422 strategies (Mendham et al., 2011; Wang et al., 2013a,b,c).

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

429

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

431 Few studies world-wide have fully incorporated ES in the assessment of basin-scale ecological
432 restoration projects where their incorporation could open up opportunities for enhancing benefits

433 to human livelihood and generating public support (Trabucchi et al., 2012). The prevailing
434 quantification methods for ES are usually based on statistical analyses (Fu et al., 2018; Hu et al.,
435 2017; Liu et al., 2019). These ignore system dynamics, and associated uncertainty and feedbacks
436 because of a lack of the mechanistic understandings of the processes involved (i.e. that obtained
437 through physically-based models) (Nicholson et al., 2009). Thus, there is a great urgency to
438 bridge ES science with CZ science through process-based models, to provide research that has
439 clear societal and policy relevance, and with outputs that allow management approaches at
440 different landscape scales to be modified through interventions (Field et al., 2015; Lü et al.,
441 2012; Luo et al., 2019). As described throughout this review, a more comprehensive modeling
442 framework that would account for most dominant spatio-temporal CZ processes is necessary.

443 Particular attention should be given to non-uniqueness or *equifinality*, where very different
444 model structures and/or parameter sets are able to describe some observed behaviors with similar
445 model response (Beven, 2006; Beven and Binley, 2014). It has been acknowledge recently that
446 data-driven models suffer from similar phenomenon (Schmidt et al., 2020). This concept of
447 *equifinality* makes it difficult to define objectively model acceptability. Various methods and
448 techniques have been proposed to identify the ‘best’ model such as the Generalized Likelihood
449 Uncertainty Estimation methodology (Beven and Binley, 1992), the use of the Information
450 Theory to discriminate models (Pachepsky et al., 2006), and a frequency based performance
451 measure (Teegavarapu et al., 2022). Other methods, such as the Diagnostic Efficiency (DE)
452 (Schwemmler et al., 2021), offers the capability to disaggregate the different sources of errors
453 (i.e., the model parameters, the model structure, and/or the input data). By using model
454 ensembles for simulating the same process (e.g., Hassall et al. 2022), one can determine the main
455 error source of the different models. Preceding to the models’ training stage, sensitivity analyses

456 can provide information regarding which parameters and processes are the most important for
457 specific modeled conditions or systems. Sensitivity evaluations can help reduce model
458 complexity and improve efficiency. Local and global sensitivity analyses are possible, where the
459 former is a ‘one at a time’ approach, while the latter considers multiple parameters at the same
460 time (Link et al., 2018; Naves et al., 2020). The local form does not account for interactions
461 between parameters, while the global form does, and as such is computationally intensive which
462 can make it prohibitive in its use.

463 The use of ensemble of model projections to estimate prediction uncertainty, comparable to the
464 suggested approach above, is a common practice in fields such as climate research (Déqué et al.,
465 2007; Reto et al., 2010; Strobach and Bel, 2020) and ecosystem research (Schwalm et al., 2010).
466 This method enables the user to change and test different factors that can affect model
467 uncertainty, such as initial condition, model parameters, spatial/temporal resolution. The
468 simulated results are often considered to provide equal-weighted averages. Thus, it is assumed
469 that the biases of an individual model are partly canceled by averaging all predictions (Reto et
470 al., 2010). This approach might be utilized in soil modeling practices to determine the influence
471 of each model parameter, its uncertainty and its structure on the simulated outputs (e.g., Brown
472 and Heuvelink, 2005; Krishnan and Aggarwal, 2018; Shan et al., 2021). Furthermore, most soil
473 models, as models in other fields (Reto et al., 2010; Strobach and Bel, 2020), are established
474 according to current and recent past conditions (Jasper et al., 2006). Besides the urgent need to
475 calculate uncertainties of models’ predictions, there are uncertainties regarding future conditions:
476 a model calibrated under historic conditions may have questionable validity under future
477 scenarios if the model states differ substantially from those in the calibration period. This

478 challenges, for example, future projections of different ecological systems that might be effected
479 by climate change (McMahon et al., 2009).

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

496

497 **Conclusions**

498 In this review, a multitude of Loess Plateau studies were summarized in order to illustrate the
499 disadvantages and advantages related to the specific process-based modelling approach taken.

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

511 Such a framework has, in part, been established, where some of the process-based models
512 described (typically associated with critical zone science) are coupled with analytical tools
513 (typically associated ecosystem services) that together provide both societal and policy relevance
514 to Loess plateau research. For future studies, the reporting of a given model's suitability and its
515 relative accuracy to alternatives should be promoted, where a common set of model accuracy
516 diagnostics are used to aid comparison across studies and processes. Answers to questions of
517 why a given model was adopted, how well was it calibrated and how well was it validated are

518 crucial to ensure informed management or policy decisions, especially when they involve
519 substantive financial investments.

520

521 **Acknowledgments**

522 We are grateful to the two reviewers for their comments on an earlier version of the manuscript.

523 This work was supported by the Natural Environment Research Council (NERC) Newton Fund
524 and National Natural Science Foundation of China (NSFC) through the China-UK collaborative
525 research on critical zone science (NE/N007433/1, NE/S009094/1, NE/S009159/1 and NO.
526 41571130082).

527

528 **Conflict of interest**

529 The authors declare no conflict of interest.

530

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