## **General comments**

This paper investigates the effect of plant mixture on water cycle process. The authors perform a meta-analysis, using 1631 paired observations (monocultures-mixtures) from 88 published studies. They conclude that, compared to monoculture, plant species mixtures can promote positive hydrological processes by improving plant water use and reducing unproductive water consumption. Given the relatively fewer information on hydrological processes in relation to plant mixture in previous studies, compared to biomass and soil properties, the study is of great interest.

However, the descriptions of statistical analyses are incomplete, and the explanations of how to analyze the effects of mean annual precipitation and temperature on the relationship between plant mixtures and water cycling, as well as the roles of other influencing factors, are unclear.

In the discussion, the mechanisms underlying the impact of plant mixtures on hydrological processes are mainly attributed to complementarity and interspecific facilitation, with selection effects and complementarity effects also mentioned. These theories form the foundation for understanding the relationship between biodiversity and ecosystem functions. However, the article does not effectively integrate these theories with the research results.

Response: Thank you very much for your time and constructive comments on our paper. We have read through comments carefully and have made modifications. Please see the following point-by-point replies for details.

However, the descriptions of statistical analyses are incomplete, and the explanations of how to analyze the effects of mean annual precipitation and temperature on the relationship between plant mixtures and water cycling, as well as the roles of other influencing factors, are unclear.

Response: Thank you for your comment. We will add descriptions of statistical analyses as follows in the text (Line 135-142).

"To analysis the impact of MAT and MAP on the changes in water cycling caused by plant mixtures, we incorporated terms for MAT and MAP into Equation 3 (Peng & Chen, 2021). The optimal model was selected based on the AIC values. Ultimately, this allowed us to determine the variations in the effects of MAT and MAP on plant mixtures at different soil depths.

To examine whether the species mixture effects changed with influencing factors such as ecosystem type, management practices, seeding pattern, fertilizer use or plant type—we conducted an analysis using the linear mixed-effects model as follows:

$$\ln RR = \beta_0 + \beta_1 \times F + \pi_{study} + \varepsilon$$

(4)

where  $\beta_s$  are the coefficients to be estimated, *F* is the influencing factor, other implications as previously mentioned,  $\pi_{study}$  is the random effect factor of the study, and  $\varepsilon$  is the sampling error."

In the discussion, the mechanisms underlying the impact of plant mixtures on hydrological processes are mainly attributed to complementarity and interspecific facilitation, with selection effects and complementarity effects also mentioned. These theories form the foundation for understanding the relationship between biodiversity and ecosystem functions. However, the article does not effectively integrate these theories with the research results.

Response: Thanks for your time and constructive comments. We will reorganize section "4.1 Effect of plant mixture on the water cycle and the underlying mechanism" as follows in the text (Line 225-275).

"The effects of plant mixtures on ecosystem functioning are multifaceted. Here we review the underlying mechanisms systematically that contribute to biodiversity and ecosystem functioning (BEF), which a particular focus on studies related to the water cycle. Our results demonstrated the beneficial effects of plant mixtures on the water cycle, as it can maintain soil moisture content comparable to that of monocultures while increasing productive water consumption (Li et al., 2021; Schaub et al., 2020). Complementarity was the most prevalent explanation for the positive effect of plant mixtures (Figure 11) (Döring & Elsalahy, 2022; Barry et al., 2019). Numerous studies have confirmed that temporal and spatial niche differentiation among various species facilitates resource partitioning (Figure 11 R1) (Barry et al., 2019; Freund et al., 2021; Guimarães-Steinicke et al., 2022). We observed that plant mixtures had a slight effect on the whole soil profile. However, with increasing soil depth, these mixtures consume more water than monocultures (Figure 3). Deep-rooted species may deplete more soil water in the mixture plots, despite the fact that more water entered the soil during rainfall events (Lange et al. 2019). This is consistent with the finding of Kimberly et al. (2019), who showed that plants in more diverse assemblages adjust their soil water uptake to the deeper layers (30 and 60 cm). Plant mixtures increase soil water consumption and occur more frequently in areas with lower annual rainfall (Figure 6). Insufficient surface water forces deep-rooted species in mixed communities to alter their root morphology and absorb more deep soil water (Zhao et al. 2023). The impact of plant mixtures on soil water is a comprehensive reflection of multiple water cycling processes, such as increase canopy interception of water, reduce rainfall kinetic energy, and consequently reduce throughflow and runoff (Figure 2). Additionally, they may enhance soil water-holding capacity by changing soil properties, allowing more water to enter the soil during rainfall events (Gong et al., 2022; Lange et al., 2019).

Facilitation, which occurs through the alteration of the abiotic properties of the environment by cohabiting species, is crucial to the maintenance of BEF, through abiotic feedback (Barry et al., 2019). Deep-root species not only use deeper water sources, but also promote the availability of water for adjacent species through hydraulic redistribution (Figure 11 R2) (Bayala & Prieto, 2020; Hafner et al., 2021; Oram et al., 2018). Plant mixtures showed increased WUE, infiltration rate and decreased evaporation (Figure 2), which confirms the positive plant and microclimate facilitation in mixed plants (Ren et al., 2019). This abiotic factor facilitation may be a crucial factor in improving soil carbon, nitrogen, and phosphorus content, as well as microbial turnover rates (Prommer et al., 2020). Suitable microclimates resulting from mixed plantations also promote a healthy water cycle (Figure 11 A1, A2) (Aguirre et al., 2021). A dense canopy, for example, absorbs more radiation and enhances plant

transpiration, maintaining lower vegetation surface temperature, and reducing the inhibitory effect of high temperatures on transpiration (Guimarães Steinicke et al., 2021).

Biotic facilitation from other trophic levels is also an important factor in the water cycle, although it has not been quantified in this study (Figure 11 B1, B2) (Schöb et al., 2018; Yu et al., 2021). Biotic feedback may enhance the performance of plant mixtures by inhibiting the establishment of enemies and promoting the recruitment beneficial mutualists. The interaction among trophic levels could also facilitate contrasting functional performance in mixtures relative to monocultures (Homulle et al., 2022; Yu et al., 2022).

Selection effect may be another mechanism explaining the positive effects of plant mixtures (Loreau & Hector, 2001). The "selection effect" refers to the likelihood that higher function species are present. For example, shrubs may be more important than trees in reducing runoff. Thus, assemblages containing a higher proportion of shrubs will have lower levels runoff than those with less shrubs (Jie et al., 2008). Selection and complementarity effects often occur simultaneously in diverse biological systems, with their dominance being determined by season and environmental context (Zhang, Gao et al., 2021). Positive interactions between different species do not always exist. When selection effects predominate, monocultures may outperform plant mixtures (Wang et al., 2021). The plant morphology of dominant species in the biodiverse communities has a significant impact on the water cycle, including canopy structure, plant height, and leaf size, which further impact throughfall (Bordoloi & Ng, 2020). Species with different functional traits are more likely to promote each other's performance, where species with the same functional traits are more likely to compete with each other (Bongers et al., 2021; Guiz et al., 2018). For instance, Ding et al. (2015) reported that agroforestry systems generated more runoff than monocultures because the cropseeding disturbance of the soil surface. Another important influencing factor is interspecific competition, which may result in poorer plant performance in mixtures relative to monocultures (Mahaut et al., 2019). Furthermore, species interactions are influenced by environmental factors and genetic evolution, which can promote the complexity of interactions (Schöb et al., 2018)."