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Coupled Dynamics of Soil Water and Nitrate in the Conversion of Wild Grassland to Farmland and Apple Orchard in the Loess Drylands

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Abstract: Understanding the dynamics of soil water and nitrate in response to typical agricultural crops in dryland ecosystems are crucial for assessing ecological consequences and informing land use planning. This study was conducted in the Changwu tableland, a representative area for agricultural crop cultivation in the Loess Plateau of China. Fifteen soil profiles, including grassland, farmland, and young, mature, and old apple orchards, were sampled to investigate the effects of different land uses on soil water and nitrate dynamics using a "space-for-time" substitution approach. The results showed that the soil water content and nitrate content in farmlands were comparable to those in wild grassland. However, significant differences in soil water were observed below a depth of 2 m in apple orchards, with mature and old orchards experiencing water deficits compared to grassland of 624.9 mm and 690.0 mm, respectively. Moreover, a dried soil layer formed below a depth of 5 m in these orchards. In terms of soil nitrate, the concentration in the 0–5 m depth of apple orchards was significantly higher than that in agricultural land and grassland, and it increased with the age of the orchards. However, below 5 m, the residual nitrate stock per unit depth in apple orchards decreased to levels comparable to grassland and farmland, primarily due to the inhibitory effect of the dried soil layer on downward migration and leaching processes. Furthermore, the relationship between nitrate and soil water at 0–5 m soil depths differed during the conversion from grassland to farmland and apple orchard, with positive and negative correlations observed, respectively. This indicates that water plays a key role in influencing nitrate movement, and distinct hydrological processes occur for soil water and nitrate nitrogen under different land use change conditions. In conclusion, converting grassland and farmland to apple orchards can lead to soil water decline and nitrate accumulation in the vadose zone, posing potential threats to ecosystem sustainability and security in dryland regions. Therefore, implementing appropriate water-fertilizer management practices is crucial for promoting sustainable land use in loess drylands, with potential implications for similar areas worldwide.

Keywords: soil water; nitrate; land use change; vadose zone; loess dryland

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Citation: Lu, Y.; Li, P.; Li, M.; Wen, M.; Wei, H.; Zhang, Z. Coupled Dynamics of Soil Water and Nitrate in the Conversion of Wild Grassland to Farmland and Apple Orchard in the Loess Drylands. *Agronomy* **2023**, *13*, 1711. https://doi.org/10.3390/agronomy13071711

Academic Editor: Shicheng Li

Received: 25 May 2023
Revised: 11 June 2023
Accepted: 25 June 2023
Published: 26 June 2023

1. Introduction

Soil water and nitrogen availability in terrestrial ecosystems have long been a focal point of intensive research, given their critical role in influencing plant growth and productivity [1,2]. This is particularly relevant in drylands, where limited water resources and fragile ecosystems pose significant challenges for sustainable agriculture and forestry practices. With increasing human activity and land use changes in drylands, it is crucial to understand the effects of agricultural crops on soil water and nitrate dynamics, as this can have important ecological consequences.

The Loess Plateau in China is dominated by drylands and has the largest loess deposits globally [3,4]. It supports a significant population through agriculture and forestry, but is also one of the world's most severely degraded regions, which has hindered social and economic development in the area. To counteract this degradation, large-scale afforestation and rehabilitation projects, such as the 'Three North Shelterbelt Development' programme and the 'Grain for Green' project, have been implemented since the 1950s, resulting in a significant change in land use patterns [5]. In particular, since the 1980s, vast areas of cropland have been transformed into apple orchards on the loess drylands, which now cover 25% of the local agricultural land and produce over 25% of the world's apple yield, making it the largest apple cultivation area globally [6]. This transition to apple tree plantations has become one of the primary stages of revegetation to support rural development and increase farmers' income [7,8].

Reforestation and revegetation have shown numerous benefits, including facilitating land development, recovering soil quality, and generating lucrative economic incomes. However, over time, the negative impacts of these practices on the environment have become more apparent. For example, the plantation of apple orchards leads to soil water depletion due to canopy interception, root uptake, and evapotranspiration. Studies have shown that apple orchards have a significant soil water deficit below 2 m compared to farmland [9,10]. Additionally, the overuse of chemical fertilizers and pesticides can result in nitrate accumulation in the soil profile, which moves downward with soil water, degrades groundwater resources, causes eutrophication, and potentially threatens ecosystem and human health due to lower nitrogen use efficiency [11,12]. While research on the impact of land use change and human activities on soil water and nitrate dynamics in agro-ecosystems is extensive, the evolution of soil moisture and nitrate in drylands after drastic agroforestry transformation remain understudied. Specifically, the coupled dynamics of soil water and nitrate after converting wild grassland to farmland and apple orchard are not well understood. This knowledge gap limits our ability to elucidating ecological environment dynamics under changing conditions, which is crucial for the sustainability of ecosystems [1].

The objective of this study was to explore the coupled dynamics of soil water and nitrate in response to the conversion of wild grassland to agricultural crops on drylands. Specifically, we measured fifteen deep soil profiles from wild grassland, long-term farmlands, and young, mature, and old apple orchards in a typical agricultural crops-planting area of the Loess Plateau, employed the "space-for-time" substitution method to (i) characterize the vertical distribution of soil water and nitrate content profiles, (ii) assess the variations in soil water storage and residual nitrate stock across the profiles, and (iii) elucidate the intricate relationship between soil water and nitrate during the transition from wild grassland to farmland and ultimately to apple orchard. The findings will contribute to a better understanding of the ecological consequences of agricultural and forestry practices in the drylands, and provide a scientific basis for land use planning and water-fertilizer management under high quality development of ecological environment.

2. Materials and Methods

2.1. Study Area

The study was conducted in the Changwu tableland, a typical agricultural crops planting area in the middle-southern part of the China's Loess Plateau (35°14′ N, 107°41′ E; Figure 1a). The long-term (1957–2015) average annual temperature, reference evapotranspiration, and precipitation were 9.4 °C, 893 mm, 577 mm respectively [13]. The monthly air temperature and precipitation are in phase synchronization, indicating a typical temperate, semi-humid continental monsoon climate [14]. Rain-fed agriculture without irrigation has been the primary mode of production in the region. While winter wheat and maize were once the main crops, since 2000, 60% of the arable land has been converted into apple orchards, becoming the predominant land use type.

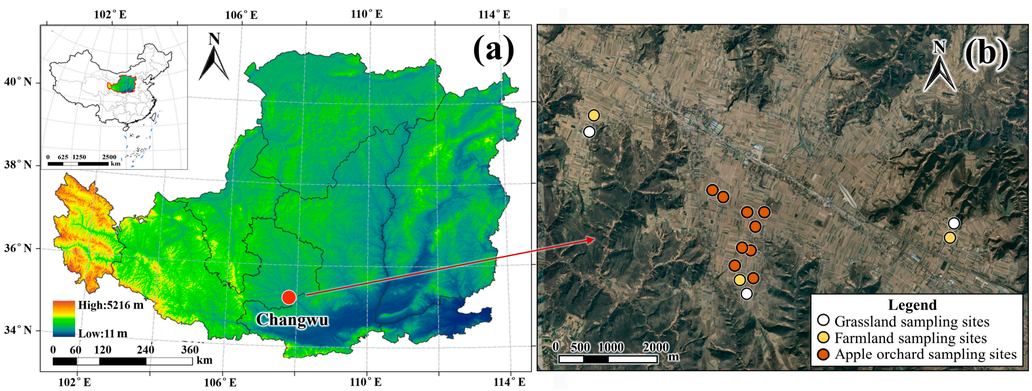

Figure 1. Location of the study area on China's Loess Plateau (**a**), and distribution of the soil sampling sites in the Changwu tableland (**b**).

The area is a typical loess tableland with silt loam soil texture. Due to the loess soil's formation from wind-blown dust deposits [15], the soil horizons are horizontally uniform. Groundwater is located more than 50 m deep in the vadose zone and has little effect on the root zone soil water. The tableland surface is relatively flat, with a slope of less than 0.05, and elevation ranging from 1170 to 1310 m above sea level. However, the edges of the tableland gradually slope to bedrock and have developed deep-cut gullies [13].

2.2. Sampling and Measurement

The study aimed to investigate the changes in soil water and nitrate levels due to land use conversion. To achieve this, we employed a space-for-time substitution approach, which involved carefully selecting spatial locations that represented different stages of land use conversion and extrapolating temporal changes based on the observed spatial variations. A total of fifteen deep soil profiles were selected (Figure 1b), encompassing five distinct land-use patterns. These patterns included natural grasslands (as a control to represent the natural status of soil water and nitrate), long-term farmlands with wheat-maize rotation, and young, mature, and old apple orchards (stand age of around 6–12, 16–20, and 24–28 years old, respectively). The fifteen soil profiles were collected from various sampling sites across the Changwu loess tableland in 2015–2017 (Figure 1b). These profiles were specifically obtained from the central region of each individual plot, employing either a hollow-stem hand auger (6-cm diameter) or a high-power pressure equipment (DPP 100, BJTK Company, Beijing, China), allowing for the collection of soil samples at regular intervals of 0.2 m.

The soil bulk density was determined by the cutting ring method, while soil mass water content was measured by oven drying (105 °C for 12 h) [16,17]. The soil volumetric water content was calculated by multiplying the soil mass water content by the ratio of soil bulk density to water density. The nitrate concentration in soil pore water were measured using ion chromatography (DIONEX ICS-1100, Thermal Fisher Scientific, San Jose, CA, USA) with a relative error of ±3% [13].

The selected apple orchards were planted with the apple tree cultivar "Fuji" (*Malus pumila* Mill.), had a uniform spatial distribution of trees with 3 m between plants in each row and a 3.5-m row space. All sampling sites were flat with no irrigation, and the management practices were similar, including fertilization practices at the same agricultural crops-planting zone. Although there were anomalously wet or hot years, the long-term average annual climate conditions in the area remained relatively stable [9,18]. Given that the changes in soil water and nitrate dynamics under different land uses are cumulative a period of many years, the potential influence of climate variability on the space-for-time substitution approach was found to be negligible in this study. Therefore, the similarity in soil, topography, climate, and management practices among the selected sampling sites satisfies the requirement of the spatio-temporal substitution method, which states that the sites should have similar environmental conditions except for the variables of interest. This similarity allows for an objective analysis of the effects of land use conversion on soil water and nitrate levels.

2.3. Estimations of Soil Water Storage and Residual Nitrate Stock

To qualitatively describe the dynamics of soil water and nitrate in response to the conversion of wild grassland to agricultural crops, indices of soil water storage and stock of residual soil nitrate were calculated.

Soil water storage (*SWS*) in the soil profile is calculated using the following equation:

$$SWS = \sum_{i=1}^{n} (SWC_i \times BD_i \times \Delta Z_i). \tag{1}$$

where SWS is soil water storage (mm), SWC_i, BD_i, and ΔZ_i are the mass water content (g g^{-1}), the bulk density (g cm^{-3}), and the layer thickness (cm) of the *i*th soil layer, respectively.

Residual nitrate stock (*RNS*) in the soil profile is defined by the following formular:

$$RNS = \sum_{i=1}^{n} (N_i \times SWC_i \times BD_i \times \Delta Z_i). \tag{2}$$

where RNS represents residual nitrate stock (kg ha^{-1}), N_i is the nitrate concentration (mg L^{-1}) in the pore water of the *i*th soil layer.

2.4. Z-Scores Analysis

Z-scores, also referred to as standard scores, are a statistical measure that quantifies the distance of a data point from the mean of a distribution in terms of standard deviations [19]. This approach allows for data points from different distributions to be compared on a common scale. In this study, *Z*-scores were calculated to quantify changes in *SWS* and *RNS* across natural grassland converted to farmland and different-aged apple orchards, and the resulting values were cross-plotted to visualize the changing relationships between these variables. The formula for calculating *Z*-scores can be expressed as:

$$Z = \frac{(\overline{X} - \overline{R})}{\sigma_R}. \tag{3}$$

where $\overline{X}$ and $\overline{R}$ represent the mean values of *SWS* or *RNS* in the target objects (farmland and different-aged apple orchards) and reference object (natural grassland), respectively. σ_R represents the standard error for reference object.

2.5. Uncertainty Analysis

Based on the standard error of soil water content and nitrate concentration, the uncertainty of soil water storage and residual nitrate stock can be quantified by the following error propagation analysis of Equation (4):

$$\sigma_y = \sqrt{\left(\frac{\partial f}{\partial x_1}\right)^2 \sigma_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 \sigma_{x_2}^2 + \ldots + \left(\frac{\partial f}{\partial x_n}\right)^2 \sigma_{x_n}^2}. \tag{4}$$

where $\sigma(\cdot)$ represents the standard error of a certain variable, that can be calculated by $SD/\sqrt{n}$, where SD is the standard deviation; and $\partial f/\partial(\cdot)$ represents the partial derivative of f with respect to a certain variable, f is the function of the certain variable.

2.6. Statistical Analysis

An analysis of variance (ANOVA) with a subsequent post-hoc the least significant difference (LSD) test was used to evaluate the differences of variables between different land-use patterns. Treatment differences were considered significant at $p < 0.05$. All statistical analyses were performed using the IBM SPSS Statistics software (IBM SPSS Statistics for Windows, Version 22.0).

3. Results

3.1. Soil Water Content and Nitrate Concentration Profiles

Figure 2a displays variations in soil water content across different land-use types and soil depths. The average water content for the entire soil profile was highest for natural grassland and long-term farmland, both measuring at 0.25 cm^3 cm^{-3}. This was followed by young apple orchards with a soil water content of 0.22 cm^3 cm^{-3}, mature apple orchards with 0.19 cm^3 cm^{-3}, and old apple orchards with the lowest soil water content at 0.18 cm^3 cm^{-3}. Specifically, the shallow soil (0–2 m below the land surface) water contents under different land uses had a certain variation, but the distribution and fluctuation of profiles showed overall similarity. However, below 2 m, the soil water content under shallow-rooted grassland and farmland was significantly higher than that of deep-rooted apple orchards, and the soil water content of apple orchards exhibited a declining trend with increasing stand ages.

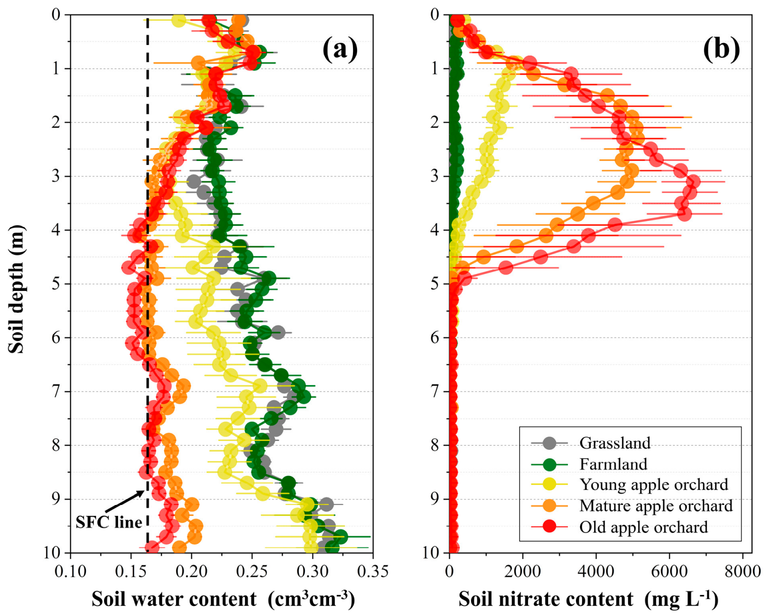

Figure 2. Vertical distributions of soil water content (**a**) and nitrate content (**b**) through the 10-m profile in grassland, farmland and different-aged apple orchards. The error bars represent standard errors of the means (N = 3). The permanent stable field capacity (SFC), which serves as an indicator of a dried soil layer, is defined as 60% of the field capacity.

In Figure 2b, the distribution of soil water nitrate concentration with depth exhibits a parabolic shape, which reflects the history of fertilizer application and suggested that nitrate moves with water mainly in the form of piston flow in the deep vadose zone, despite the land use types. The nitrate concentration in pore-water of the natural grassland profile ranged from 4.61 to 152.9 mg L^{-1}, with an average of 32.7 mg L^{-1}. The nitrate concentration distribution of soil water in farmland was similar to that of grassland, with the values were 60.2 ± 61.1 mg L^{-1} (average ± SD). However, there were clear differences in the nitrate concentrations of soil water among apple orchards and shallow-rooted grassland and farmland. The nitrate concentrations under apple orchards were significantly higher than those of grassland and farmland ($p < 0.05$), and increasing with stand ages. Under all land-use patterns, the nitrate concentration of soil water peaked above 5 m, with an average ± SD of 818.7 ± 285.7 mg L^{-1}, which were higher and more variable than those of 15.6 ± 4.5 mg L^{-1} below 5 m in general.

3.2. Soil Water Storage and Residual Nitrate Stock

The characteristics of *SWS* and *RNS* were similar to soil water content and nitrate concentration profiles across different land use patterns (Figure 3). For grassland and farmland, the *SWS* profiles were similar, with a total water storage of 2481.7 ± 19.9 mm and 2511.2 ± 19.9 mm, respectively, for the 10-m soil profile. However, significant differences in *SWS* profiles were observed below a soil depth of 2 m for deep-rooted apple orchards. The *SWS* decreased by around 271.6, 624.9, and 690.0 mm under the young, mature, and old apple orchards, respectively, in comparison to the *SWS* of shallow-rooted grassland and farmland, indicating a declining trend in *SWS* with increasing stand ages of apple orchards. Furthermore, our variance analysis revealed no significant difference in *RNS* between grassland and farmland ($p > 0.05$), although the accumulation was marginally higher under farmland across various soil depths. However, under deep-rooted apple orchards, *RNS* was significantly higher than under shallow-rooted grassland and farmland, and this accumulation tended to increase significantly with increasing stand ages ($p < 0.05$). Notably, these land use impacts on *RNS* were mainly confined to the 0–5 m soil depth range, with no significant change observed in *RNS* in the soil layer below 5 m due to land use ($p > 0.05$).

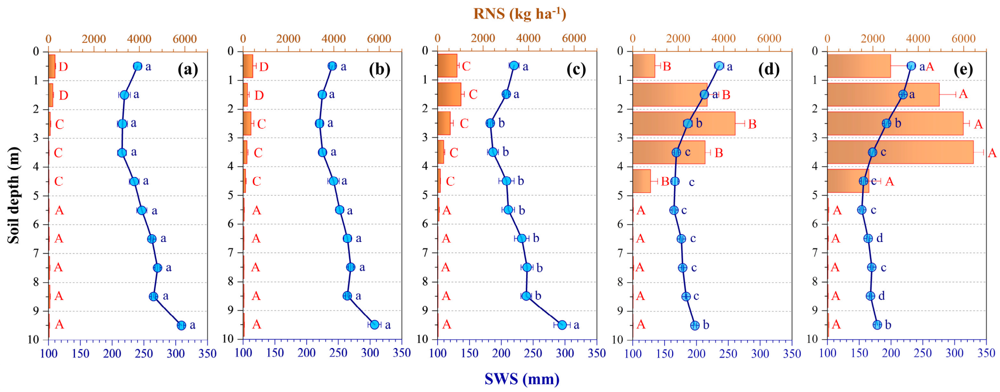

Figure 3. Vertical distributions of water storage and nitrate accumulation in each 1-m layer through the 10-m soil profile under grassland (**a**), farmland (**b**), young apple orchard (**c**), mature apple orchard (**d**), and old apple orchard (**e**). The upper X-axis and orange bars indicate vertical patterns of residual nitrate stock (*RNS*) in each 1-m soil depth, and the lower X-axis and blue-filled circles represent vertical patterns of soil water storage (*SWS*) in each 1-m soil depth. Different upper- and lower-case letters indicate significant differences in *RNS* (mean ± SE) and *SWS* (mean ± SE) among different land-use types within a soil depth ($p < 0.05$), respectively.

3.3. Assessment of Soil Water Storage and Residual Nitrate Stock Changes by Z-Scores

A cross-plot of the Z-scores of *SWS* and *RNS* in natural grassland converted to farmland and different-aged apple orchards is presented in Figure 4. It is evident that the data points of long-term farmland are mostly located in the first quadrants, whereas those of apple orchards are mostly located in the second quadrants. Specifically, the positive and negative relationships between *SWS* and *RNS* are mainly observed at soil depths of 0–5 m under each land use. Within this depth range, the *RNS* increased with increasing *SWS* ($y = 4.56x + 2.52$, $R^2 = 0.59$) from grassland to farmland, while it increased with decreasing *SWS* from grassland to apple orchard. Furthermore, we found that during the transformation of grassland into apple orchard, the *RNS* at soil depths of 0–5 m gradually changed from a low absolute value of slope ($|k|$) and non-significant linear increase in young apple orchard ($|k| = 1.90$, $R^2 = 0.04$, $p > 0.05$) to a high $|k|$ and significant linear increase in old apple orchard ($|k| = 72.58$, $R^2 = 0.41$, $p < 0.05$) with decreasing *SWS*. This suggests that the ratio of *RNS* increasing with the decrease of *SWS* increases with the increase of tree age. However, in the soil depth below 5 m, all data points fall on the X-axis of the horizontal coordinate, indicating that the *RNS* does not change with land use transformation.

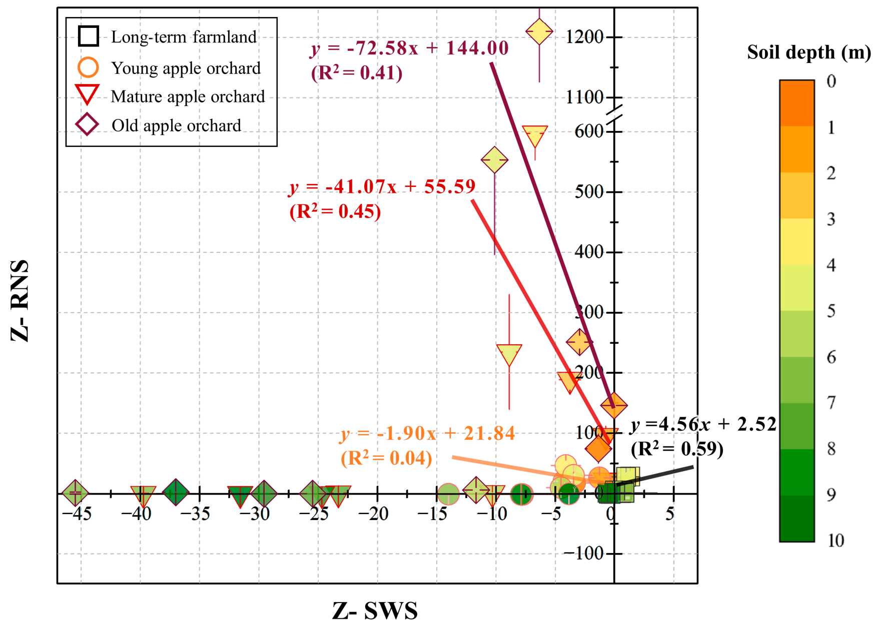

Figure 4. Cross plot of soil water storage (*SWS*) and residual nitrate stock (*RNS*) for each soil depths of farmland and different-aged apple orchards. The black, orange, red, and brown lines represent line regressions between *SWS* and *RNS* at the 0–5 m depths in farmland and young, mature, and old apple orchards.

4. Discussion

4.1. Impacts of Farmland and Apple Orchards on Soil Water in Dryland

Land-use changes often induce alterations in soil water content, as evidenced by previous studies [20]. Our findings reveal that while the shallow soil layer (0–2 m below the land surface) exhibited certain variations in water content across different land uses, the overall distribution and fluctuation patterns showed similarities (Figure 2), with no significant differences observed in the depth-averaged *SWS* (Figure 3). This observation aligns with previous research conducted in the Loess Plateau [21]. We attribute this phenomenon to a combination of factors. Firstly, both deep-rooted and shallow-rooted agricultural crops exhibit limited water consumption within the shallow soil layer of 0–2 m [22]. Moreover, the rapid recharge of rainfall, such as preferential flow and micro-pore flow, primarily occurs within the upper 2 m of the soil profile [13,23]. In contrast, below 2 m, the soil water content beneath shallow-rooted grassland and farmland significantly exceeded that of deep-rooted apple orchards, with the soil water content of the orchards showing a decreasing trend with increasing stand ages (Figure 2). Specifically, the depth-averaged soil water content in young apple orchards (stand age around 6–12 years) was slightly lower than the soil water content of approximately 0.03 cm^3 cm^{-3} observed in the grassland and farmland across the 2–9 m profile (Figure 2). This disparity can be attributed to the relatively lower evapotranspiration rates during the early growth stage of apple orchards [24–26]. As apple trees reach peak production around 17 years [27], a rapid decrease in soil water storage occurs within the orchards. Notably, the water deficit in the 2–10 m soil profile of mature and old orchards reached 624.9 mm and 690.0 mm, respectively (Figure 3). Particularly concerning is the pronounced soil desiccation below a depth of 5 m under mature and old apple orchards, with the soil water content falling below the stable field capacity of around 0.16 cm^3 cm^{-3} (equivalent to 60% of the field capacity [22]), resulting in the formation of a dried soil layer. Consequently, the effects of deep-rooted apple orchards and shallow-rooted farmlands on soil moisture in dryland areas differ significantly. The influence of land use on soil water content increase with depth, highlighting the substantial impact of root water uptake in deep-rooted forested regions.

4.2. Impacts of Farmland and Apple Orchards on Soil Nitrate in Dryland

Land use changes have a profound influence on soil nitrate dynamics [28]. Our findings reveal that the soil nitrate concentration within the 0–5 m soil profile is significantly higher in apple orchards, particularly in mature and old orchards, compared to grassland and farmland (Figure 2). Within the 0–5 m soil depth, the *RNS* shows an increasing trend with the age of the apple orchards. The *RNS* per unit depth ranges from approximately 568 kg ha^{-1} in young orchards to approximately 2547 kg ha^{-1} and 4395 kg ha^{-1} in mature and old orchards, respectively, which greatly exceeds the recommended nitrogen rate of 240–360 kg ha^{-1} [29]. In contrast, the *RNS* per unit depth is much lower in grassland (~114 kg ha^{-1}) and farmland (~251 kg ha^{-1}) (Figure 3). The substantial disparities in soil nitrate content under different land uses are primarily driven by variations in fertilization frequency and dosage [30]. Notably, many farmers, relying on their own experience rather than fertilizer experts' recommendations, apply excessive amounts of nitrogen fertilizer to ensure high apple yields [31]. Consequently, the input of nitrogen fertilizer far surpasses the nutrient output of the orchards (mainly fruit and pruning), resulting in a significant accumulation of nitrate nitrogen in the soil.

It is worth mentioning that the peak nitrate concentration is observed at approximately 1.0 m, 2.5 m, and 3.3 m depths in the soil profile under young, mature, and old apple orchards, respectively (Figure 2). Assuming fertilization occurs after apple planting, the depth of the peak nitrate concentration and the age of the fruit trees imply that the migration rate of nitrate becomes slower as it migrates to deeper depths. Furthermore, when the soil depth reaches 5 m (forming a dried soil layer beneath the soil profile of mature and old apple trees), the *RNS* per unit depth decreases to less than 50 kg ha^{-1}, which is not significantly different from the *RNS* observed in grassland and farmland (Figure 3). These phenomena clearly demonstrate the close relationship between nitrate leaching and soil water dynamics. Nitrate in the shallow soil is more susceptible to continuous precipitation recharge, leading to faster leaching rates. As nitrate migrates to deeper soil layers, it is absorbed and utilized by roots, resulting in increased soil unsaturated conditions and reduced soil water conductivity, thereby slowing down nitrate migration and potentially leading to its accumulation above the dried soil layer.

4.3. Different Relationships between Soil Water and Nitrate under Farmland and Apple Orchards

Soil water conditions varied with land uses, which may affect the transport of nitrate in the vadose zone. Our results show that *RNS* and *SWS* Z-scores have different significant correlations at 0–5 m soil depths in farmland and apple orchard, respectively (Figure 4). These observations confirm the role of water as a key factor influencing nitrate movement in soil [32] and suggest that soil water and nitrate nitrogen may undergo distinct hydrological processes under different land use change conditions.

The positive relationship between *RNS* and *SWS* Z-scores during the conversion of natural grassland to farmland (Figure 4) can be attributed to the high soil water content associated with shallow-rooted cash crops, which facilitates deep drainage and promotes nitrate leaching in the soil [13,33]. This indicates a synergistic relationship between nitrate and soil water in the vadose zone. In contrast, the Z-*SWS* exhibits a negative correlation with Z-*RNS*, with correlation coefficients ranging from −0.20 to −0.64 at soil depths of 0–5 m during the conversion of natural grassland to aging apple orchards (Figure 4). Furthermore, minimal nitrate leaching is observed beyond the 5 m soil depth in apple orchards (Figures 2 and 3). These observations further suggest that when soil water is depleted and a dried soil layer is formed, the soil layer acts as an inhibitory or blocking barrier for the downward migration and leaching of soil water and dissolved nitrate. Consequently, a significant antagonistic relationship between nitrate and water content is established above the dried soil layer in the vadose zone.

4.4. Implications for Land Use Planning and Water-Fertilizer Management in Dryland

The apple industry has gradually become the main source of income for local farmers. However, with the rapid expansion of fruit production, there are some ecological consequences of apple orchard practices in the drylands. In terms of soil water resources, the cultivation of apple trees in drylands has resulted in the excessive depletion of limited soil water reserves, leading to the formation of dry soil layers. Consequently, the sustainable viability of productive apple orchards in loess drylands is generally limited to a span of 25 to 30 years [27]. Furthermore, the injudicious application of fertilizers during apple tree planting has resulted in the excessive accumulation of nitrate in the vadose zone, warranting specific attention. Improper fertilizer usage accelerates soil acidification, diminishes soil polymerization, reduces the permeability coefficient, and compromises microbial activity, ultimately undermining soil productivity [31]. The continuous input of nitrogen fertilizer facilitates the downward migration of nitrate into the deeper layers of the soil. Although the slow movement of accumulated nitrate through the vadose zone, characterized by low water content and deep soil layers, its pollution is difficult to solve, which may have a potential negative impact on soil quality, and eventually reach groundwater, posing a threat to groundwater security. Consequently, the development and implementation of effective countermeasures are pivotal for sustainable soil water and fertilizer practices in loess drylands. Such measures include the adoption of supplemental irrigation techniques and stringent controls on nitrogen fertilizer usage, enabling sustainable land use and facilitating conversions in similar dryland regions globally.

4.5. Study Limitations

In the study, we employed a space-for-time substitution approach to investigate the effects of different land uses on soil water and nitrate dynamics in the loess drylands. By utilizing this approach, we were able to gain insights into the dynamics of soil water and nitrate over time, despite the limited availability of long-term data. We selected specific land use types, including grassland, farmland, and different stages of apple orchards, as representative points along the land use conversion gradient. This allowed us to approximate the temporal changes associated with land use transformation. However, it is important to acknowledge the potential implications of the space-for-time substitution approach on our results. First, this approach assumes that the selected spatial locations are representative of the temporal changes in the studied variables. While we made efforts to ensure the selection of appropriate sites, there might still be inherent variability within each land use category. Second, this approach assumes that the soil conditions remain relatively similar across the different spatial locations representing different temporal stages. However, natural spatial heterogeneity can exist, potentially influencing the observed variations in soil water and nitrate dynamics. Lastly, it is crucial to consider that the space-for-time substitution approach may not capture the fine-scale temporal variability in soil water and nitrate dynamics. Short-term variations, such as seasonal fluctuations, may not be fully captured through this approach, limiting our understanding of the complete temporal dynamics. Despite these limitations, the space-for-time substitution approach provides a valuable framework for inferring temporal changes in soil water and nitrate dynamics, particularly in cases where long-term data are unavailable. It offers insights into the potential effects of land use conversion on soil and water resources, contributing to our understanding of ecosystem sustainability and guiding land use planning decisions.

5. Conclusions

In this study, we systematically investigated the effects of farmland and apple orchards on soil water and nitrate in the loess drylands. The main conclusions are as follows:

1. Comparing the soil water and nitrate content, it was observed that farmland exhibited similar characteristics to wild grassland. However, significant variations in soil water were identified in apple orchards compared to farmland and grassland, particularly below a depth of 2 m. The mature and old orchards showed substantial water deficits

in the 2–10 m profiles, reaching 624.9 mm and 690.0 mm, respectively. Moreover, a dried soil layer was formed at depths exceeding 5 m.

2. The content of nitrate nitrogen in apple orchards within the 0–5 m depth range was considerably higher compared to farmland and grassland. Additionally, the *RNS* exhibited an increasing trend with the age of the apple orchards. However, the *RNS* per unit depth in apple orchards below 5 m decreased to levels below 50 kg ha^{-1}, which was not significantly different from the *RNS* observed in grassland and farmland. This may be attributed to the inhibitory effects of the dry soil layer on the downward migration and leaching of soil moisture and dissolved nitrate.
3. The positive and negative ratios between *RNS* and *SWS* Z-scores at depths of 0–5 m during the conversion of grassland to farmland and apple orchards indicated synergistic and antagonistic relationships of water and nitrate under shallow- and deep-rooted plants, respectively. This suggests that nitrate could move easily with soil water under shallow-rooted plants, while nitrate was more effectively retained in the soil under deep-rooted plants due to larger water deficits.

These findings highlight the complex dynamics of soil water and nitrate influenced by agricultural crops in the loess drylands, emphasizing the importance of considering land use changes and hydrological processes in managing soil moisture and nitrate levels effectively.

Author Contributions: Conceptualization: Y.L. and Z.Z.; Methodology, Y.L. and P.L.; Investigation: Y.L., Z.Z. and H.W.; Data curation: M.L.; Formal analysis: Y.L. and M.W.; Validation: Y.L., M.W. and H.W.; Visualization: Y.L.; Writing—original draft: Y.L. and Z.Z.; Writing—review & editing: Y.L., P.L. and M.L.; Supervision: P.L. and M.L.; Funding acquisition: Y.L. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the National Natural Science Foundation of China (NSFC) grant number [42107068 and 41877017], the China Postdoctoral Science Foundation grant number [2021M692744], and the Fundamental Research Funds for the Central Universities, CHD grant number [300102291303].

Data Availability Statement: The data used to support the findings of this study are included within the article.

Conflicts of Interest: The authors declare no conflict of interest.

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