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Spatial equilibrium model-based optimization for inter-regional virtual water pattern within grain trade to relieve water stress

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ABSTRACT

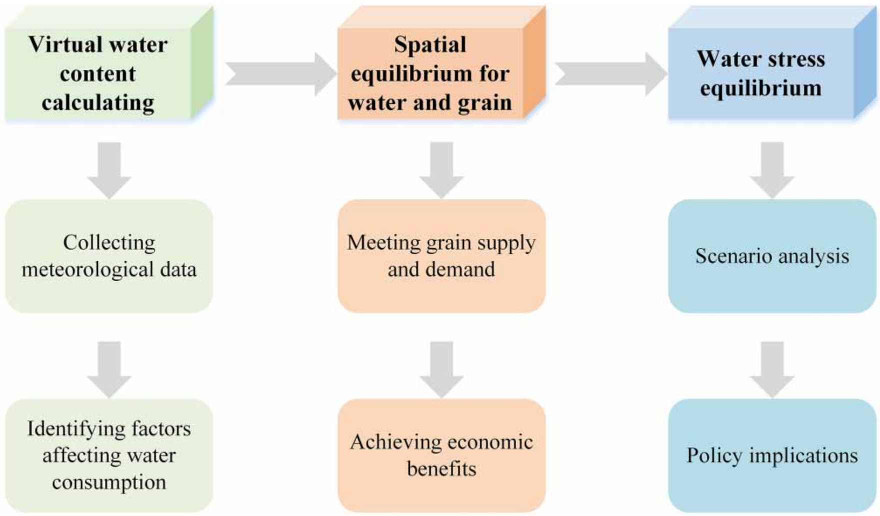
Realizing water usability and management sustainability represents one of the Sustainable Development Goals. Since grain cultivation consumes tremendous amounts of water, the inter-regional grain trade causes virtual water flow, increasing water stress in certain water-scarce regions. As the second-longest river in China, the Yellow River bears increasingly severe water stress. Considering water and food security, this study proposes a spatial equilibrium model (SEM) that combines partial equilibrium theory and transport models to maximize net social revenue and to balance grain supply and demand, thereby optimizing inter-regional grain trade to relieve water stress. According to different natural, technical and social conditions, we conceived five scenarios to predict regional water stress characterized with different water supplies, demographic structures, food demand compositions and water-saving technologies. Our simulation results suggest that the developed SEM can realize spatial equilibrium of food and water resources within the Basin, which is capable of resolving the problem of food demands in regions with varying extents (13%–55%), optimizing inter-regional grain trade and mitigating water stress. Finally, we recommend some constructive policies for different scenarios to relieve water stress.

Key words: food security, inter-regional grain trade, spatial equilibrium model, virtual water, water scarcity, water stress

HIGHLIGHTS

- A spatial equilibrium model is developed to optimize the inter-regional grain trade.
- The inter-regional virtual water flow in the Yellow River Basin is simulated.
- The water stress under different projected scenarios is explored.
- Effective policy recommendations for different scenarios are put forward for agricultural water-saving and alleviating regional water stress.

GRAPHICAL ABSTRACT



1. INTRODUCTION

Performing as the most indispensable natural resource, water occupies its undoubtedly overwhelming priority in the everyday life of mankind, agricultural and industrial production, as well as in balancing the Earth's ecology and sustaining various species of plants and animals living on it. Most of the global freshwater (69%) is used for agricultural production that guarantees human survival and social stability. However, as the modernization of agriculture continues to prosper, the expansion in the farmland to be irrigated is confronted with the ever-increasing crisis of water utilization due to the inherent problem of water scarcity (Yang *et al.* 2007), which has further resulted in the widespread regional stress of water demand, foreign and domestic. It is generally acknowledged that grain cultivation is the most critical sector for agricultural production, which is directly and closely correlated with a nation's food security and the food demand of its whole population. Unfortunately, for a long time the problem of water scarcity has posed a severe threat to the Yellow River Basin (Piao *et al.* 2010; Omer *et al.* 2020), and the people inhabiting in have been suffering with the stress of unevenly distributed regional water and of imbalanced food supply and demand. In order to realize sound and reasonable inter-regional food allocation, while satisfying food supply and demand at a sustainable steady pace, cross-regional grain trade must be expanded across the Yellow River Basin. Serving as a water-intensive product (Hoekstra & Hung 2005), the grain flowing across different regions of a nation will cause the flow of water resources, which is also referred to as the virtual water trade derived from food trade. For the purpose of maintaining a rapidly ever-growing population and providing a more abundant diet, the production of high standard food is inevitably accompanied with expensive of environmental cost (Dalin *et al.* 2015), which will not only decrease the amount of available water used for other purposes but aggravate regional water stress. Therefore, the impact of grain import and export on regional water stress must not be neglected under the background of cross-regional product trading.

Geographer Allan (1993) first introduced the concept of virtual water and defined it as the virtually 'invisible' water embedded in the products. The virtual water can be regarded as a connection among water, food, and trade (Allan 2003). In order to better describe the connections between anthropogenic water consumption and human trade activities, estimating the trading patterns for virtual water is one of the most effective approaches (Zhang & Anadon 2014). By projecting an inter-regional grain trading pattern and calculating the amount of virtual water within grain production, the corresponding virtual water flow can be estimated. The existing methods estimating inter-regional trade can be classified into two categories, i.e., the input–output analysis method and linear programming model. Through comparing certain studies listed in Table 1, we report that the former is commonly used to calculate the trade between different economic sectors, whereas the latter can be applied to diverse commodities more specifically. However, with respect to the grain trade in the Yellow River Basin, not only must the inter-regional delivery cost be minimized, but also the price differences in products and the impact of prices on trade patterns be considered. Furthermore, due to the uneven spatially distributed water resources and the unsound composition of

Table 1 | Comparison of different methods for inter-regional trade flows

		Contents or factors			
Methodologies	**Articles**	**Evaluating inter-regional trade flows**	**Considering transportation costs**	**Research into specified trading goods**	**Considering products' prices**
Input-output analysis	Jiang *et al.* (2015)	√	×	×	×
	Wang *et al.* (2020)	√	×	×	×
Linear programming model	Dalin *et al.* (2015)	√	√	√	×
	Wang *et al.* (2019a)	√	√	√	×
Spatial equilibrium model	Zakharov & Krylatov (2015)	√	√	√	√
	Krylatov *et al.* (2020)	√	√	√	√

food production within the Basin, food export regions confronted with severe water stress will invariably emphasize the problem of water scarcity.

According to the spatial equilibrium model (SEM) developed by the economist Samuelson in 1952, in this study, we establish a tailor-made SEM to optimize the trade of inter-regional food and virtual water, thereby realizing simultaneous spatial equilibrium of food and water stress. Aiming at the objective of maximizing the net social revenue (NSR, the sum of producer surplus and consumer surplus between multiple regions), our proposed model can calculate the optimal flow between regions with minimal delivery cost, and achieve simultaneous equilibrium among multi-regional markets (Krylatov *et al.* 2020). Unfortunately, few studies can be found adopting SEM to assess inter-regional virtual water flow so far. The reason to apply our proposed model to the trade of inter-regional virtual water lies in two factors. Firstly, it helps simulate the inter-regional grain trade pattern, by which the virtual water flow can therefore be obtained. Secondly, since grain is an economic crop, the SEM accounts for grain price and inter-regional delivery cost. Our approach compensates for the deficits of the linear programming model that merely considers delivery cost or distances. In addition, compared with the input–output model, the data engaged in our model are more accessible and time sensitive and can be used with more flexibility under different application scenarios.

Water stress is defined as the shortage of available water suffered by regions as a result of water withdrawal, to which some researchers have already applied the water stress index (WSI) for effective assessment (Huang *et al.* 2019). For instance, agricultural crops are water-intensive products consuming huge amounts of water. With respect to the inter-regional grain trade, the regions exporting crops are confronted with virtual water outflow, thereby causing severe water stress within these areas. Regions importing crops can mitigate local water stress. In this paper, we adopt a WSI based on virtual water flow after equilibrium to reveal the influence on water scarcity. Even though there are studies analysing regional water stress combining with virtual water trade (Feng *et al.* 2014; Zhang *et al.* 2017), however, few studies have focused on how would the virtual water outflow influence the degree of water stress in various scenarios. In the future, China will still be faced with daunting challenges in water management, for which making improvements in water conservation technologies and management governance is the key to food security and water resources (Rodell *et al.* 2018). China's rural population is under a transformation period (Liu *et al.* 2017), which will change the demographic structure of China's cities and towns. Therefore, certain influencing factors that may affect grain demand (Namany *et al.* 2020) include but are not limited to trade uncertainties, changing climatic conditions, fluctuating commodity prices, increasing population, and changing dietary structures, etc. When grain demand varies, the pattern of inter-regional grain trade changes accordingly, which will further change water demand. Regional grain administrations may change the decisions on grain imports and exports, thereby influencing regional water stress.

Considering the aforementioned facts, this paper designs different simulation scenarios for regional water supply, future grain demand pattern, and agricultural water-saving technologies, proposing reasonable water management suggestions based on the water stress caused by virtual water flow. The key contributions of this paper can be summarized as follows. First, this study explores the impact of water scarcity and alleviates water stress by optimizing inter-regional grain trade patterns and virtual water flows. Second, this study establishes an SEM based on grain production and consumption to maximize NSR and estimates inter-regional grain trade, achieving spatial equilibrium in water stress and food trade among regions. Last but not least, this study simulates different scenarios to investigate the effects of different influencing factors on regional water stress. We have presented conductive measures to alleviate regional water stress while offering reasonable suggestions for relevant policies.

2. METHODS

2.1. Study area

The Yellow River is the second-longest river in China, it is 5,464 km long and flows across nine provincial regions, whose geographical locations and contours are presented in Figure 1. The biggest conflict in the Yellow River Basin, where China's main grain-producing area is located, is the shortage of water resources. Due to geographical conditions and other constraints, the regions within the Basin share limited economic connectivity and do not achieve regional synergy of water and food. As the major grain production areas including Henan, Shandong, Nei Mongol and Sichuan provinces, food security and water security in the Yellow River Basin are of crucial priority to China. The amount of available water resources in the Basin will decrease in the future (Piao *et al.* 2010), for which reason this study focuses on the inter-regional grains' trading linkage in the Basin and on the embedded virtual water transport.

2.2. Conceptual framework

Figure 2 illustrates the conceptual framework. First, the virtual water consumed by crops in the Yellow River Basin is estimated using the statistical data from 2019. Then, an SEM is constructed based on grain production and consumption to optimize food trading patterns, to maximize regional NSR and to estimate the consequent regional water stress. Subsequently, a comparison of regional water stress caused by virtual water trade under different scenarios is conducted to propose measures and policy implications to mitigate water scarcity.

2.3. Virtual water content in crops

Virtual water calculation is a critical step laying the foundation for the calculation of virtual water flow caused by inter-regional grain trading, to which the evapotranspiration of a reference crop (ET_0) must be calculated first. According to the

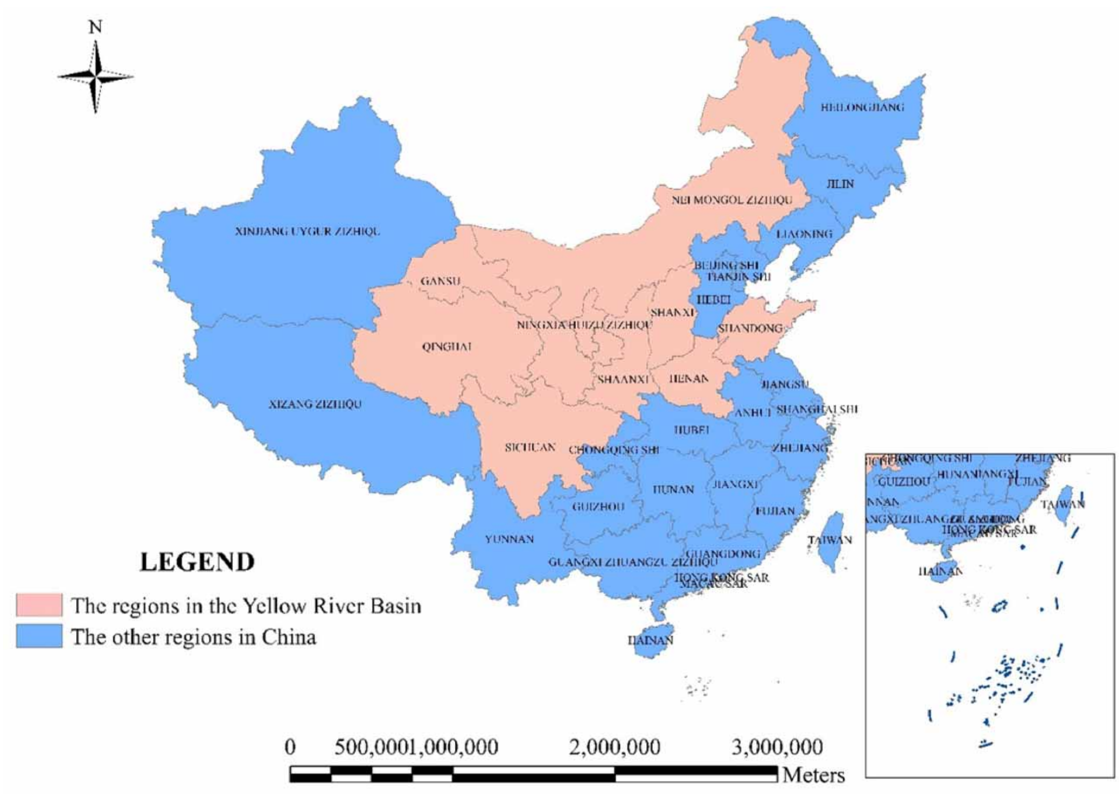


Figure 1 | The regions of the Yellow River Basin by geographical locations.

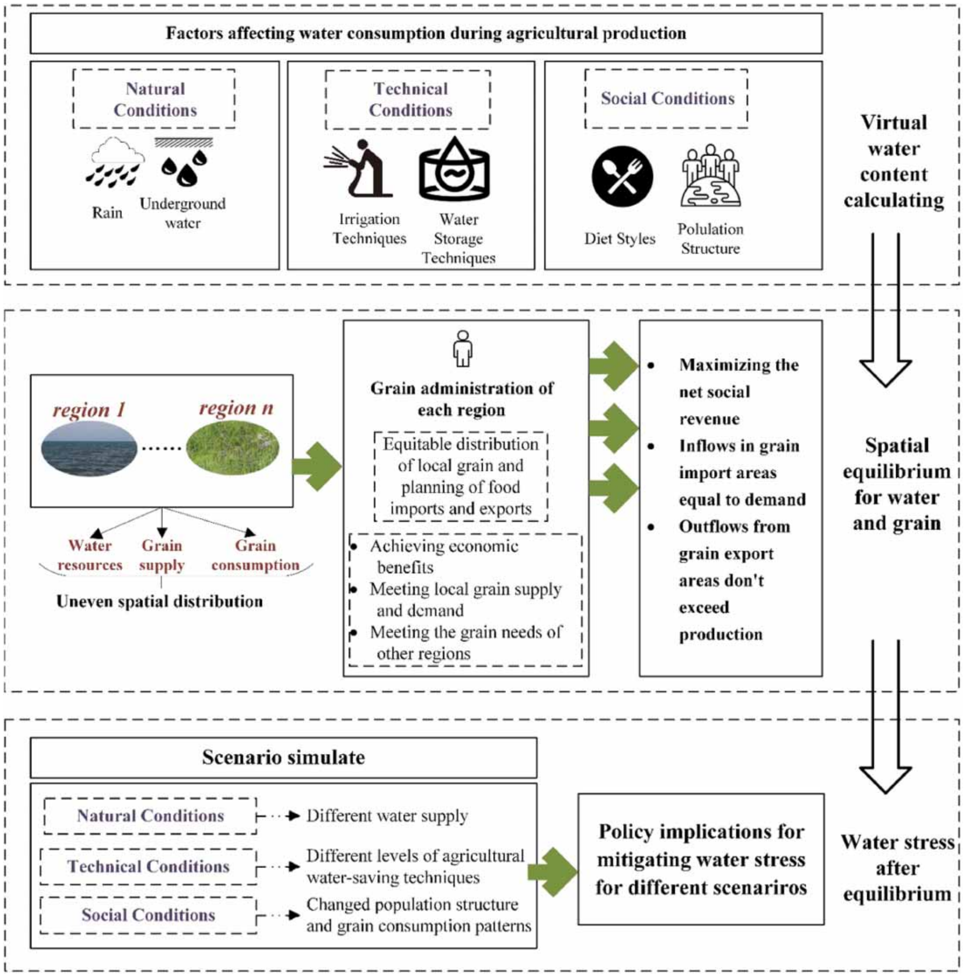


Figure 2 | Conceptual framework for optimizing virtual water flow in grain trade to achieve spatial equilibrium between regional water stress and grain.

standards of Food and Agriculture Organization of the United Nations (FAO), ET_0 denotes the evapotranspiration rate of the referenced surface (www.fao.org). The definition of reference crop is available in the existing study (Hoekstra & Hung 2005). ET_0 is estimated by the FAO Penman–Monteith equation (http://www.fao.org/).

Crop coefficients correct the water requirements of specific general crops:

$$ET_c = k_c \cdot ET_0 \tag{1}$$

where ET_c is the evapotranspiration of a general crop (mm/d), k_c is the coefficient of a specific general crop. Then, the water requirements per unit area of the crop can be calculated during the whole fertility period, which is expressed as

$$CWR = 10\sum_{i=1}^{n} ET_c = 10 \cdot k_c \sum_{i=1}^{n} ET_0 \tag{2}$$

where CWR represents the water requirements per unit area of the crop over an entire fertility period (m^3/hm^2), n is the total days of the crop's fertility period (d).

The virtual water of crops includes blue and green water, and the latter equals the gross virtual water in the crops under rain-fed conditions (Sun *et al.* 2013). The primary crops' virtual water content can be calculated by

$$VWC = \frac{CWR}{CY} \tag{3}$$

where VWC denotes the primary crop's virtual water content (m^3/t), and CY denotes the yield of primary crop per unit area (t/hm^2).

Following the above steps, the total VWC of definite crops in a definite region within their fertility period can be obtained. The total VWC of an area equals the weighted average sum of the VWC of individual crops according to their yields.

2.4. Spatial equilibrium model for inter-regional grain trade and virtual water flow

The inter-regional grains' trading within the Yellow River Basin is estimated by using an SEM, to which the supply–demand situation of inter-regional grain and the inflow–outflow of grains in each region are considered. The assumptions for this SEM are presented as follows:

(1) Complications induced by the process of inter-regional grain trade, such as weather changes, unexpected events, commodity losses, etc., are not considered.
(2) When reaching the spatial equilibrium, the grain trade among the aforementioned nine regions achieves maximum NSR.
(3) The grain supply in each region first considers the demands raised by the remaining regions within the Basin, after which excess supply is then considered to be delivered to other regions of China to calculate the trade flows of the areas within the Basin.
(4) The trade market is perfectly competitive (Wang *et al.* 2019a) without trade barriers among areas.
(5) The modelling process does not consider changes in terms of regional water supply, agricultural water-saving techniques and demographic structure in the year of calculation.

Considering that the NSR generated by inter-regional trade is maximized, the grain consumption of each region is its demand, while the grain production of each region is its supply, the SEM can be expressed as (Yang *et al.* 2002) as follows:

$$\max NSR = \sum_{j}^{n}\sum_{i=1}^{n}(x_{ij}\times P_j) - \sum_{i}^{n}\sum_{j=1}^{n}(x_{ij}\times P_i) - \sum_{i=1}^{n}\sum_{j=1}^{n}(x_{ij}\times c_{ij}) s.t. \begin{cases} c_{ij} = p\times d_{ij} \\ \sum_{j=1}^{n} x_{ij} \le S_i \\ \sum_{i=1}^{n} x_{ij} = D_j \\ x_{ij}, P_i, P_j, c_{ij}, p, d_{ij}, S_j, D_i \ge 0. \end{cases} \tag{4}$$

In the above Equation (4), S_i denotes the grain supply of region i, D_j denotes the grain demand of region j, P_i and P_j are the average retail price of grains, i and j denote the grain export and import regions respectively, c_{ij} denotes the inter-regional delivery cost per unit grain from region i to region j, x_{ij} denotes the amount of grains delivered from region i to region j, p denotes the delivery cost of unit grain per unit distance, d_{ij} denotes the inter-regional distance of rail transportation between region i and region j.

Since the virtual water content varies among regions, the inter-regional grain trade may lead to different virtual water outflow and inflow for the exporting and importing areas. The virtual water outflow (VWF_i^{out}) and inflow (VWF_j^{in}) will be estimated according to the multiplication of the flow of cross-regional grain trade, to which the corresponding virtual water content can be calculated by

$$VWF_i^{out} = \sum_{j=1}^{n} x_{ij}\times VWC_i \tag{5}$$

$$VWF_j^{in} = \sum_{i=1}^{n} x_{ij}\times VWC_j \tag{6}$$

From the perspective of inflow and outflow, a region is defined as a net virtual water outflow area when its outflow exceeds inflow, and the net virtual water outflow (*NVWF*) is defined as the overall output minus the input.

2.5. Water stress index based on virtual water flow after optimization

Based on the existing concept of a WSI, a WSI is developed from virtual water flow (WSI_{vwf_i}) to quantify the impact on regional water resources as a result of the inter-regional grain trade after optimization. The regional water scarcity level is measured by the water stress level (*WSL*).

According to the currently existing studies (Chen *et al.* 2019), the regional water stress is calculated by

$$WSI_{vwf_i} = \frac{NVWF_i^{out}}{WS_i} \times 100\% \tag{7}$$

$$WSI_{u_i} = \frac{WU_i}{WS_i} \times 100\% \tag{8}$$

$$WSL_i = \frac{WSI_{vwf_i}}{WSI_{u_i}}. \tag{9}$$

In the above Equations (7)–(9), WSI_{vwf_i} denotes the WSI resulting from the virtual water output of region i, $NVWF_i^{out}$ denotes the net virtual water outflow concerning the inter-regional grain trade (m^3), WS_i is the upper limit of water resources available to each region under the regulation framework of 'three red lines' for water resources (m^3), WSI_{u_i} denotes the WSI resulting from the agricultural production, WU_i denotes the water consumption in agriculture (m^3).

There are five levels for regional water stress, regions without stress, with slight stress, with moderate stress, and with severe stress (see Table 2).

2.6. Data collection and processing

(1) Meteorological and crop parameters

The data from 232 meteorological stations were collected in 2019 for those nine regions in the Yellow River Basin, which were sourced from the National Meteorological Science Data Centre (https://data.cma.cn/). The total days of the crop fertility period and the crop coefficients were obtained from the results of available researches. As for the regions and crops that had no practical information for reference, the data from the nearest observation sites were used.

(2) Grain production and consumption

The crop yields of all the study regions were obtained from the National Bureau of Statistics Public Data Query Platform (https://data.stats.gov.cn/). As it is difficult to obtain actual grain consumption, the classification method was therefore used to calculate theoretical grain demand in place of actual consumption. The obtained results matched almost precisely the grain consumption projected based on grain reserve. The grain consumption per capita can be categorized into five classes, i.e., consumption of people's food rations, industrial grains, feed grains, seed grains, and grain losses. Each region's total grain consumption was obtained by multiplying the grain consumption per capita by the number of resident populations. Ration consumption and feed grain consumption were further subdivided into urban and rural areas for calculation. The proportion of extra-household consumption for rural and urban residents was calculated at 4 and 12%. Grain consumption coefficients for pork, beef, lamb, poultry, dairy, and aquatic products were 2.50, 0.70, 0.50, 2.70, 0.37 and 1.00, respectively. The loss rate of grain storage was set as 8%.

(3) Grain trade among regions

The prices of the primary crop products were obtained from the 'China Yearbook of Agricultural Price Survey 2020'. The weighted average of the prices of various primary crop products was calculated by taking the grain crop production in each

Table 2 | The levels of water stress

Levels	No stress	Slight stress	Moderate stress	Severe stress
WSL	$\leq$0.2	0.2–0.4	0.4–0.8	$\geq$0.8

region as the weight, which was used to obtain a unified grain price as the average retail price of grain for the SEM. As the grain flow among areas is realized by rail transport, the distance was taken as the number of miles between the railway stations in two capital cities of two regions.

(4) Water utilization data

The upper limit of water resource consumption in each region adopted the objective of total water use control from 'Assessment Measures for Implementing the Strictest Water Resources Management System' issued by the State Council of China (http://www.gov.cn/). The exact regional consumption was obtained from 'China Water Resources Bulletin 2019'.

3. RESULTS AND DISCUSSION

3.1. Virtual water status in 2019

3.1.1. Virtual water content and grain delivery

Table 3 shows the *VWC* of crops and the total *VWC* for each provincial region. In 2019, the virtual water consumption for grain production in the Yellow River Basin was 1.68×10^{11} m^3, accounting for 31% of the total available water resources. Among these three types of crops, wheat has the highest virtual water content. This suggests that under the premise of the same yield, wheat consumes more water than other crops. Serving as a commodity crop with the highest consumer demand, wheat has been confronted with the most serious threat of water shortage. The *VWC* of grains also varies noticeably among regions. The *VWC* for each region listed in descending order is Shaanxi, Henan, Shanxi, Shandong, Qinghai, Gansu, Nei Mongol, Ningxia, and Sichuan. The highest *VWC* region Shaanxi is 2 times and 2.2 times greater than the two lowest virtual water content regions Ningxia and Sichuan. According to the results, noticeable differences exist in *VWC* for classified crops of different regions. One explanation is that different yields and ET_c contribute to various water requirements expressed by Equations (1)–(3). Another reason is that agricultural water supply and comprehensive technical conditions for water saving may differ in terms of regions and crops.

The composition of crop cultivation directly affects regional agricultural water consumption. For the purpose of altering crop patterns to minimize agricultural water consumption, effective policies should be considered as a solution to water-related dilemmas faced by the Basin (Gohari *et al.* 2013).

Grain delivery among regions within the Yellow River Basin in 2019 amounted to 6.77×10^7 t, accounting for 31.6% of the overall grain production in those regions. The region with the highest net export volume of grain was Henan, whose export volume accounted for 27.6% of the region's total production. The two major regions where Henan exports grain were Shaanxi and Sichuan. The top two regions with the highest net exports were Henan (1,848 t) and Nei Mongol (1,120 t), with net exports accounting for 87.7% of the overall exports. The top two regions with the highest net import volume were Sichuan (2,400 t) and Shaanxi (424 t), with their net import volume accounting for 83.4% of the total import volume. Grain net exports and imports of individual region are shown in Figure 3. Within the Yellow River Basin, grain delivery is shifting from regions of high virtual water content to those of low virtual water content, which is in good agreement with the existing studies.

Table 3 | The virtual water content for classified crops (m^3/t)

Regions	Rice	Wheat	Maize	Total
Qinghai	0.0	927.6	477.3	810.4
Sichuan	456.2	1,397.9	457.8	540.2
Gansu	862.1	981.2	533.4	677.7
Ningxia	700.5	1,392.8	447.9	593.5
Nei Mongol	782.0	1,036.1	569.4	606.9
Shaanxi	663.9	2,185.1	636.6	1,190.5
Shanxi	827.3	1,666.3	687.9	877.7
Henan	594.0	1,213.8	556.7	937.8
Shandong	689.6	1,124.8	507.9	814.8

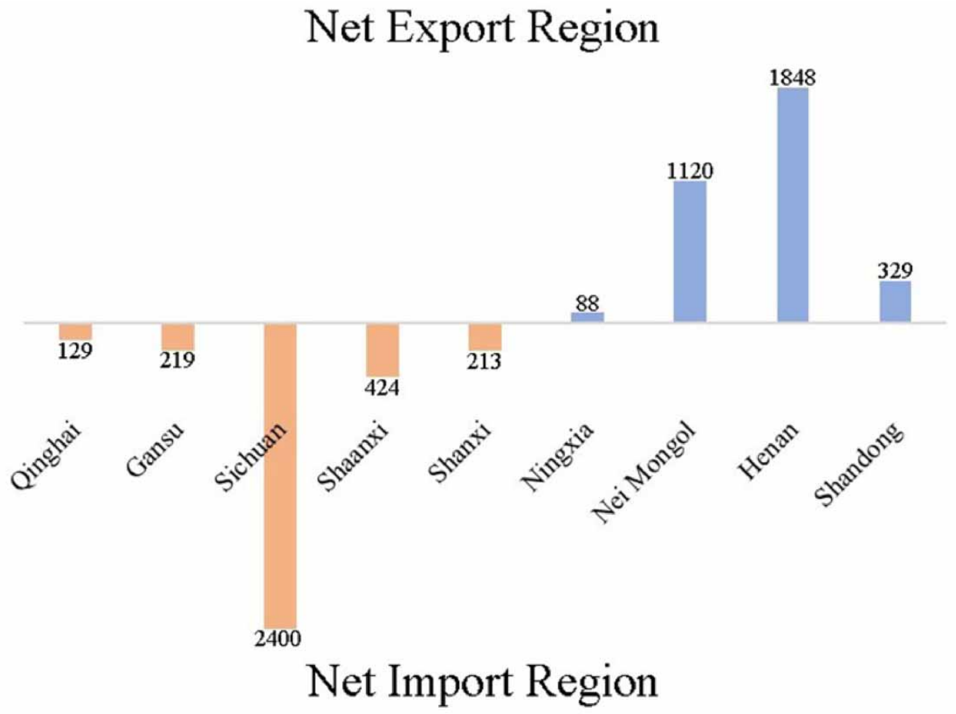


Figure 3 | Net grain export and import of individual region (1×10^4 t).

3.1.2. Inter-regional virtual water flow

The flow of grain among regions of the Yellow River Basin was realized through inter-regional grain supply and demand. Combining the *VWC* of each region, it is feasible to calculate the virtual water flow within these nine regions in the Basin, to which the result is shown in Figure 4.

Figure 3 shows that Ningxia, Nei Mongol, Henan and Shandong are the net grain exporting provinces, suggesting that these provinces are also the net virtual water outflow regions. As explained by Equations (5) and (6), the same amount of grain transfer on the same delivery path results in different virtual water outflow and inflow to the exporting and importing regions, upon which we plotted the virtual water flows from the outflow and inflow perspectives. Figure 4(a) demonstrates the virtual water transferred from the outflow provinces to others, Figure 4(b) illustrates the virtual water imported to the inflow provinces. The volume of virtual water flow among different provinces is shown by different line widths in the chord diagram. A total of 4.97×10^{10} m^3 of virtual water flow was generated among the nine provincial administrative regions in 2019. The province with the largest virtual water outflow was Henan, with a total outflow of 1.73×10^{10} m^3, accounting for 63% of the total outflow volume from all outflow areas, which flew to Sichuan and Shaanxi, respectively. The province having the largest virtual water inflow was Sichuan, with a total inflow of 1.3×10^{10} m^3, accounting for 58% of the total virtual water inflow volume of all inflow areas, whose inflows came from Nei Mongol, Shaanxi, Shanxi and Henan.

Among these nine regions, Henan, Shandong and Nei Mongol were ranked the top three provinces in grain production, while Sichuan was ranked fourth, followed by Shanxi, Shaanxi, Gansu, Ningxia and Qinghai. If grain trade is to be realized with maximum NSR, Henan, Shandong and Nei Mongol must deliver grain to the rest of these regions to ensure the consumption demand of their populations. Intriguingly, as an area with low grain production, Ningxia acts as a grain exporting region, whereas Sichuan province with high grain production is practically a grain importing region. Although this topic involves population size and consumption composition, it is worth exploring whether the trade involved is sound and reasonable, especially regarding the resulting water stress. Furthermore, the virtual water volume transferred from Henan to Sichuan was 1.81×10^9 m^3, from which the amount received by Sichuan was 1.04×10^9 m^3. The above difference between the transferred and received water volume suggests that, although grain trade contributes to water conservation, the water endowment and water stress of each region need further consideration (Zhao *et al.* 2018).

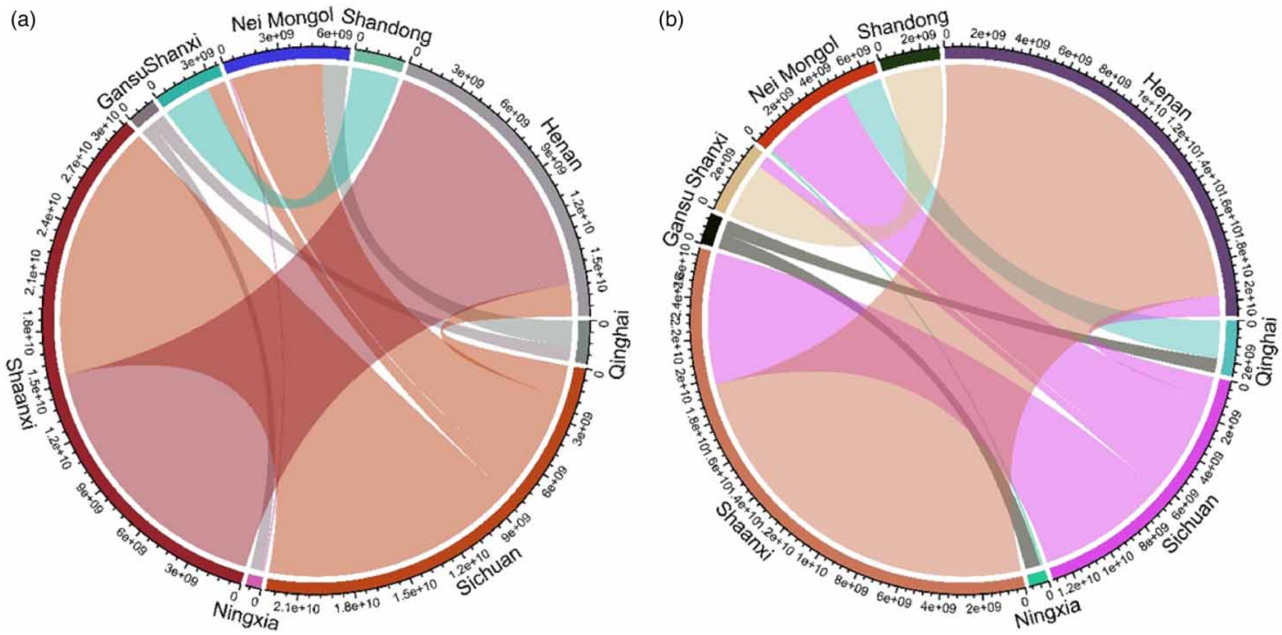


Figure 4 | Virtual water flow within nine regions of the Yellow River Basin in 2019: (a) from outflow perspective; (b) from inflow perspective.

3.2. Scenario analysis

3.2.1. Scenario design

The natural and social environment of the Yellow River Basin will be changing in the future. The former is dominated by climate change, particularly extreme weather conditions that will cause unpredictable precipitation, which may further lead to changes in regional water supply and affect regional water stress. The latter is closely correlated with certain factors such as economic development, rapid population growth and innovative research and development in science and technology, which may bring changes in terms of demographic structure, grain consumption composition, technology advances in agricultural water conservation, and of government policy. Therefore, we conducted different scenario analyses according to the above factors to simulate virtual water transfer and regional water stress.

The basic scenario S0 is the calculated actual situation in the Yellow River Basin in 2019 through SEM and serves as the control group, on which the rest scenario variability settings are based.

The first scenario S1 considers the changes in total regional water supply. Four future stages of water supply for the Yellow River Basin are designed as follows: extreme water abundance, normal water abundance, normal water scarcity, and extreme water scarcity. Based on the water supply over 15 years from 2005 to 2019, the regional water supply was reduced by 50%, shifting from the status of minimum to that of extreme water scarcity, whereas the regional water supply was increased by 50%, shifting from the status of maximum to that of extreme water abundance. The one-third and two-thirds trimesters from extreme water abundance to extreme water scarcity are considered as normal water abundance and normal water scarcity.

The second scenario S2 simulates the impact of different demographic structure and grain consumption composition on regional water stress. According to the forecast of China's total grain demand in 2030 (Yuan *et al.* 2017), the food demand in the Yellow River Basin is estimated to have the same growth ratio, after which a new trading pattern for grains is generated using SEM.

The third scenario S3 represents the mitigation of water stress by technological advances in agricultural water conservation. The National Agricultural Water Conservation Program (2012–2020) has stated the goal of establishing water conservation system to optimize agricultural water consumption. Hence, the technology coefficient ζ_t is used to represent the reduction in water consumption through comprehensive agricultural water-saving techniques throughout the full cycle of crop reproduction, thereby calculating the virtual water savings. ζ_t is defined as the proportion of virtual water consumption for the same unit of grain production under the water-saving technology coefficient being set at the range from 0.1 to 0.9, in which a smaller value denotes greater virtual water saving.

The fourth scenario S4 considers no inter-regional grain trade and thus reduces virtual water transfer, i.e., assuming that all provinces are self sufficient in grain production, the regional water stress caused by grain production is measured by WSI_u.

3.2.2. Water stress under different scenarios

Scenario S0: Based on the estimation of the grain trade pattern in 2019, the embedded water stress is calculated, to which the results are illustrated in Figure 5. In 2019, from the outflow perspective, Henan and Nei Mongol were confronted with more serious water stress as the most prominent virtual water outflow regions. As for regions with inherent shortage of water resources, massive grain export resulted in virtual water outflow, thereby aggravating their water stress. Although Shandong and Ningxia were also regions of virtual water outflow, they had lower water stress, which has been alleviated through virtual water trading. Despite being a region of virtual water net inflow, Shaanxi suffered with severe water stress that was attributed to virtual water outflow and insufficient water supply. For several other regions, virtual water trading relieved regional water stress to some extent. In general, the stress on water resources of the outflow regions was higher than that of the inflow ones, suggesting that the inter-regional virtual water flow does impact the water stress undoubtedly. Suppose the virtual water outflow is used for agricultural production in these regions, under which circumstances not only can the water shortage of these regions be compensated but the corresponding water stress caused by virtual water export be alleviated. Meanwhile, for some of these nine regions, virtual water trading can relieve local water stress to some degree, thereby mitigating water scarcity situations.

Scenario S1: The influence of regional water supply on water stress principally affects the amount of available water for each region, particularly the water for agricultural purposes, which will decrease as the regional water supply decreases. Figure 6 illustrates the level of water stress in the Yellow River Basin under four future scenarios for regional water

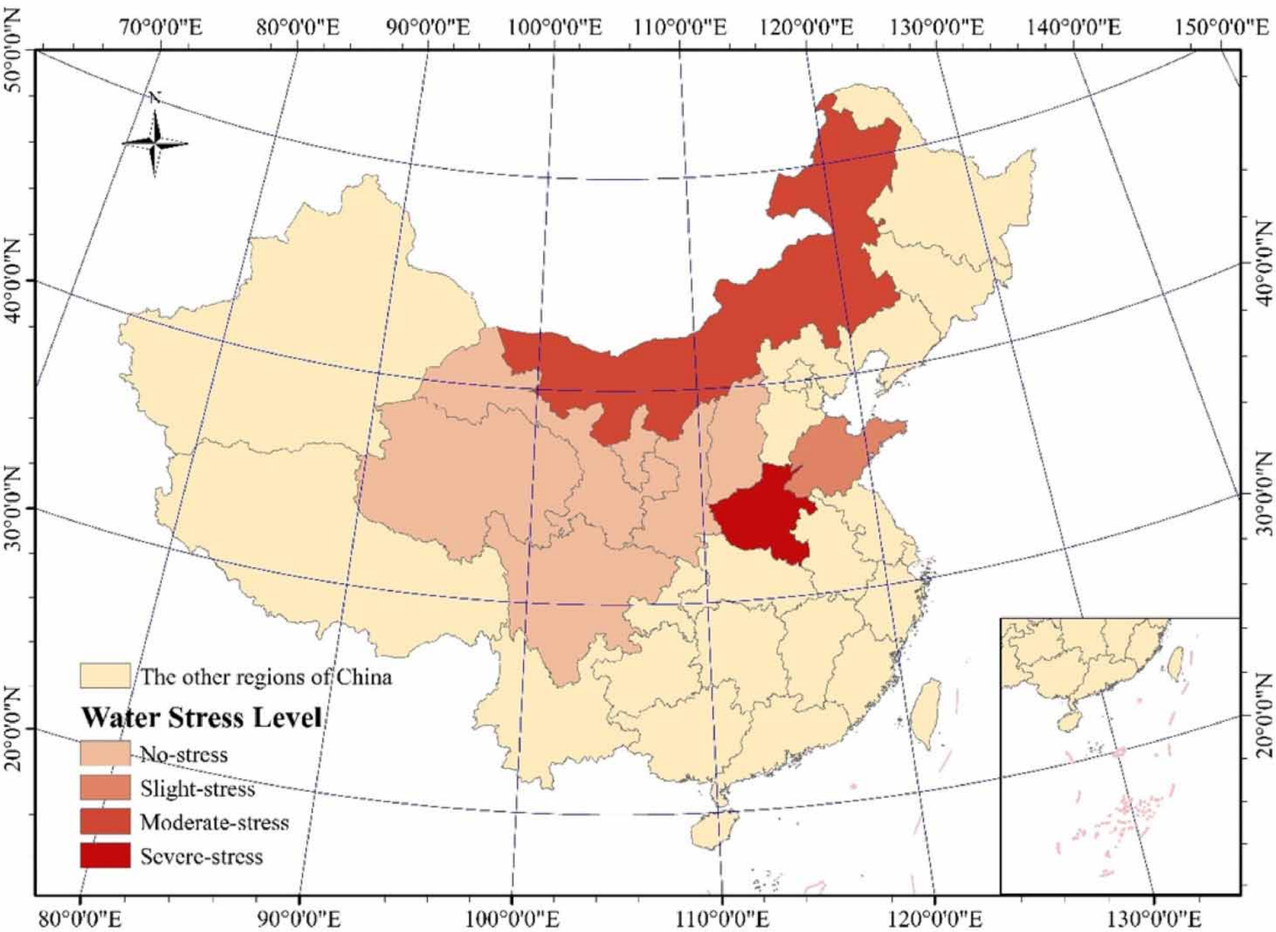


Figure 5 | Water stress level in S0 scenario.

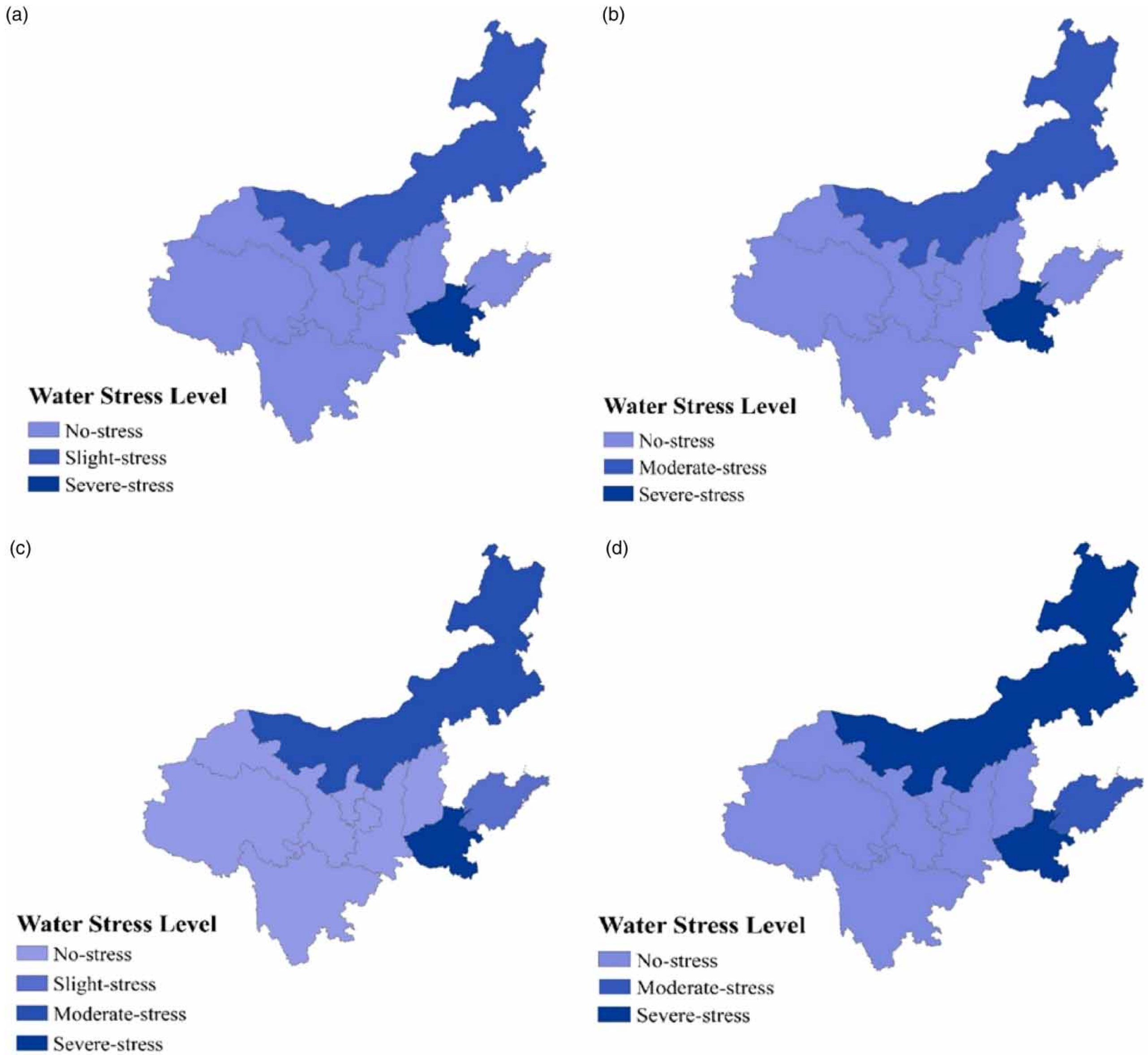


Figure 6 | Water stress level in S1 scenario: (a) extreme abundance; (b) normal abundance; (c) normal scarcity; (d) extreme scarcity.

supply, from which it can be observed that the WSI is positively correlated with the regional water supply. From different statuses of extreme water abundance to extreme water scarcity, the water stress in Nei Mongol varied from slight stress to moderate stress and to severe stress, with an increase of 3.3 times in *WSL*. The status of water stress in Shandong shifted from no stress to slight stress and to moderate stress, with an increase of 3.2 times in *WSL*. The above results suggest that water supply impacts the level of water stress based on the existing food trade pattern. If a region like Henan has been facing water scarcity, exporting the grains with high virtual water content will significantly alleviate its predicament.

Scenario S2: Considering demographic changes, the total food demand in 2030 will exceed 560 million tons, the food production in 2030 will reach 721 million tons, upon which there will be no food crisis theoretically (Yuan *et al.* 2017). When the future grain supply and demand changes, the virtual water flow patterns generated with grain trade change accordingly (see Supplementary Figure S1), to which the resultant regional water stress is shown in Figure 7. In the S2 scenario, Henan and Shandong became net grain exporting regions, contributing 49.83 million tons to the grain trade. From the outflow perspective, the net virtual water outflow from Henan was 3.69×10^{10} m^3, and the net virtual water outflow from Shandong was 8.54×10^{9} m^3. From the inflow perspective, the amounts of virtual water flowing to the remaining seven regions were

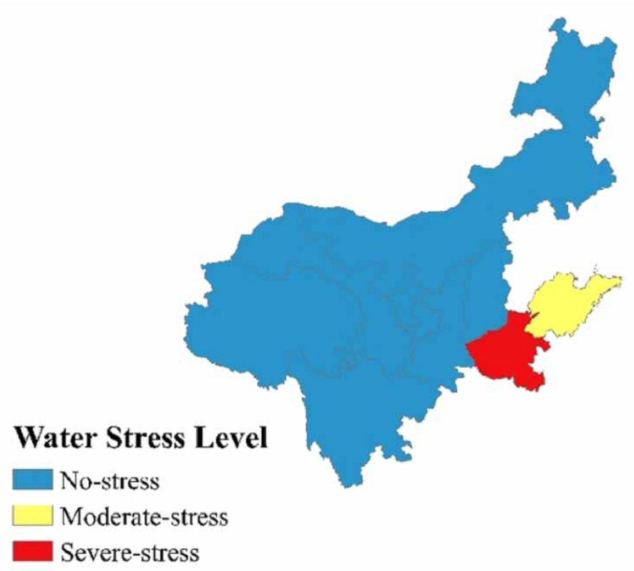


Figure 7 | Water stress level in S2 scenario.

3.81×10^8 m^3 for Qinghai, 6.45×10^9 m^3 for Gansu, 1.42×10^9 m^3 for Sichuan, 1.16×10^9 m^3 for Ningxia, 7.9×10^9 m^3 for Nei Mongol, 1.36×10^{10} m^3 for Shaanxi, and 9.51×10^9 m^3 for Shanxi, respectively. As population and dietary structures change, new virtual water flow patterns may cause higher stress in Henan and Shandong, and lower stress within the remaining seven regions. With the new prediction on grain demand, Shandong became the main grain supply region followed by Henan, causing a more threatening water scarcity to the regions that have already suffered with water shortages. The above results suggest that the central grain-producing regions in China will be confronting with higher water stress as food production and demand change in the future, and the water scarcity in these regions will deteriorate due to food exports, thereby damaging the long-term regional development and food security.

Scenario S3: As the technical coefficient ζ_t increases, producing crops with the same yield that consume more virtual water, thereby increasing the corresponding WSI and WSL (see Figure 8). The severe water stress in Henan can be alleviated to a great extent when its ζ_t is adjusted to less than 0.5. As the region suffering moderate water stress, Nei Mongol needs to adjust its ζ_t to less than 0.4 to eliminate water stress. For the remaining regions, a downward adjustment of the technology coefficient from 0.9 has significant effects in alleviating water stress. The above analytical results suggest that agricultural water conservation has noticeably advantageous impacts on regional water stress, for which reason regions with different water stress level need to adopt techniques that are locally appropriate.

Scenario S4: Supplementary Figure S2 illustrates the comparison between the WSI of agricultural production in S0 and that in S4. The results suggest that, for most regions, either withdrawing from food trading among regions or satisfying their own food demands via local cultivation or both will not be effective in alleviating regional water stress, which may increase the WSI_u for some provinces instead. For those regions suffering water scarcity, if all food demands are satisfied by local agriculture, food crisis may happen due to inadequate agricultural water supply, not to mention the water shortage induced by excessive agricultural water consumption which threatens the everyday function of other industries.

3.2.3. Scenario-driven policy implications

The results of scenario S0 suggest that the virtual water flow of grain trade within the Yellow River Basin are imported from regions with water scarcity to those with water abundancy. In order to reduce the amount and degree of agricultural water consumption, tailor-made rational and flexible pricing mechanisms of agricultural water consumption should be conceived for regions with different water resources. In 2018, the National Development and Reform Commission issued the corresponding policies to further promote comprehensive agricultural water pricing reform in Opinions on Innovation and Improvement of Price Mechanism for Green Development (http://www.gov.cn/). The average effective utilization coefficient of irrigation water in the Yellow River Basin was 0.557 in 2019, suggesting that great potential still exists for water saving.

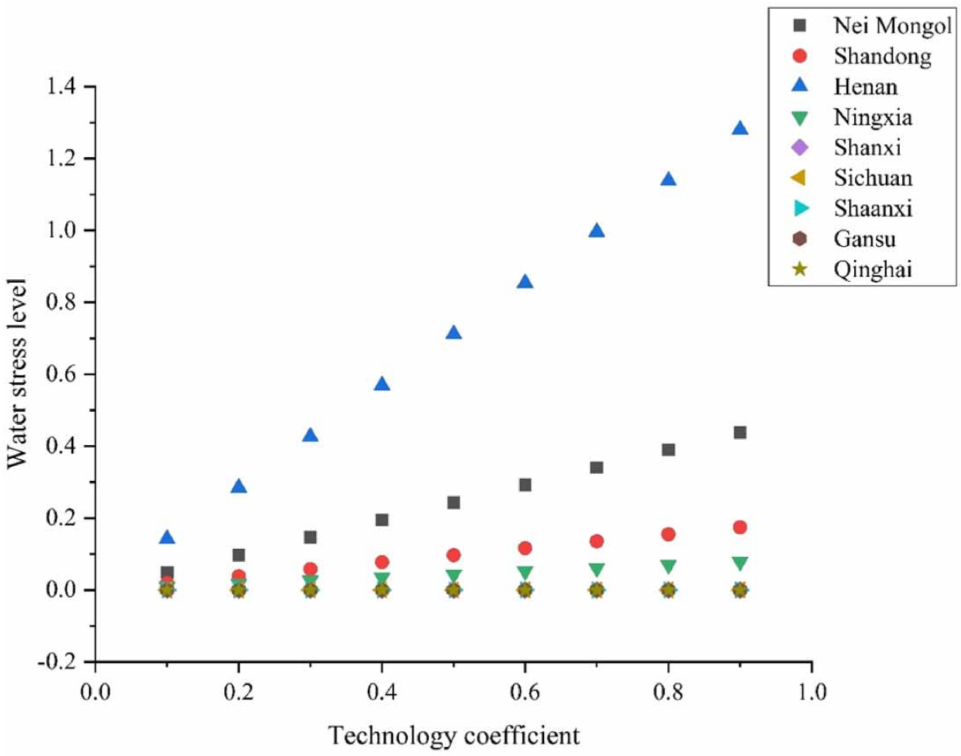


Figure 8 | Water stress level under different technology coefficient.

Differentiated water pricing based on water endowment and agricultural structure of different regions that can effectively alleviate water scarcity in agriculture. Moreover, comprehensive agricultural water price reform is conducive to elevating grain production in quality and quantity with less water resources, thereby guaranteeing food security, while relieving water stress.

Over the past five decades, the observed flow of the Yellow River has declined dramatically, and it is predicted that water scarcity in the Basin would increase in the coming decades (Wang *et al.* 2019b; Omer *et al.* 2020). The results of scenario S1 indicate that water scarcity affects water supply, causing severe regional water stress. In order to ensure adequate agricultural water supply, efficient water storage and retention infrastructures must be constructed, which include but are not limited to strengthening rainwater harvesting and utilization, exploiting and extracting groundwater for irrigation, etc. In addition, developing a model to predict regional water supply based on climate change helps determining the quota for local agricultural water consumption, according to which the agricultural production plan can therefore reduce the stress imposed by water-intensive crops while expanding the planting area of drought-tolerant crops.

Furthermore, scenario S2 has verified that diverse food consumption patterns and demand compositions exist in the aforementioned nine regions, which further leads to different degrees and levels of virtual water transfer and water stress. Therefore, these regions should optimize the composition of grain cultivation in relation to local water and land resources, thus reducing virtual water consumption.

Scenario S3 has proven the validity of improving water-saving techniques in agricultural production, throughout which attention must be paid to elevating water utilization efficiency for grain cultivation. As these regions of Nei Mongol, Henan, Shandong, and Ningxia were already facing water scarcity, it is therefore critical for them to improve relevant irrigation technologies and to implement water conservation regulations in grain production. As stipulated by the 'Outline of the Yellow River Basin Ecological Protection and High-quality Development Plan' (http://www.gov.cn/), local governments and administrations should popularize agricultural water conservation facilities while improving irrigation efficiency. On one hand, it is urgent to advance agricultural water conservancy projects and water-saving facilities to ensure water conservation, on the other hand, minimizing waste in irrigation and increasing the cycling efficiency of water are required. In addition, with respect to those regions exporting virtual water, their water stress would be markedly relieved if they employed the exported virtual water for their own uses. For those regions suffering water shortage and severe water stress, targeted compensative countermeasures should be developed and implemented, such as compensation for water resources and economy, etc.

Scenario S4 highlighted the significance of balancing the relationship between grain import/export and water conservation in agriculture. Different natural conditions such as water endowments, may differ in options for regions on whether to restrict their own agricultural water uses or to alleviate water stress through virtual water trade. Therefore, these nine regions should launch diversified trading programs to resolve contradictions between the above options.

3.3. Advantages and implications of the proposed SEM

Through using an SEM, we solved the problem of inter-regional grain trade in the Yellow River Basin. The simulation model for grain trade has its inherent advantages and benefits, which can be outlined as follows. Firstly, by introducing price factors into the SEM, the NSR within the nine regions was maximized, reaching 8.33×10^{11} million CNY in S0 and 7.38×10^{11} million CNY in S2. Considering the effect of distance, it is more realistic in delivery cost. Secondly, the optimized trade pattern satisfied the demand of each region's grain consumption and fully realized cross-regional grain delivery. With the help of inter-regional trade, in 2019, Qinghai, Sichuan, Shaanxi, Gansu and Shanxi succeeded in local food supply, achieving the percentages 55.18%, 40.69%, 25.62%, 15.89% and 13.52% respectively, of local food supply, by which their food shortages were significantly alleviated. Thirdly, the SEM adopted in this study can be widely applied for diverse food trade plans in specific years and other regions. When the demographic structure of a certain region changes, the residents' preferences for grain consumption differ accordingly. Furthermore, when the composition of grain consumption changes, the optimization of grain trade can be combined with the consumption characteristics of different regions to achieve a new spatial equilibrium.

When the pattern of grain trade reaches spatial equilibrium, the corresponding water stress vanishes. Hence, the SEM can be used to optimize virtual water trade via grain trade, thereby forming targeted countermeasures to upgrade the composition of grain production. As a region with high virtual water content, Henan consumed more water than the other eight regions to achieve the same grain yield. If the grain is exported through trading, a tremendous amount of virtual water embedded in grains will flow out of Henan, which will greatly increase its water stress. However, in contrast with Shaanxi, which also has high virtual water content, the grain production is relatively low. There is no significant virtual water outflow, which would not cause extreme water shortage.

Likewise, as a region suffering with serious water scarcity, Ningxia greatly relieved its water stress through virtual water trading. Therefore, for those regions where water scarcity prevails, adjusting the composition of food production by minimizing high water-consuming crops and/or by importing grains from other regions is an acceptable alternative, through which water stress problems can be counterbalanced by sufficient grain supply (Ren *et al.* 2018). In addition, the food export quota in water-scarce regions should be reduced, especially against agricultural products with high virtual water content. If the virtual water in certain regions is exported rather than used by the region itself, water-scare situations will not be eased.

Rational planning of grain trade patterns is closely inter-correlated with regional and national food security. As the economy grows, people's living standards further improve, affecting the composition of grain consumption (Samireddypalle *et al.* 2019), which therefore launches diversified demands for grain crops and requires stable food supply. According to our analytical results from the Yellow River Basin, although inter-regional grain trade can balance grain supply spatially, unevenly distributed regional water resources impose encumbrance on spatial equilibrium. Meanwhile, in order to defend the bottom red line of China's agricultural industry security, the grain self-sufficiency rate must be steadfastly and consistently kept above 95%. This means that, in the future, the trade-off between food demand composition and grain production increase must rely on self production, which consumes large amounts of water resources, posing a challenge for water security and a threat to food security.

4. CONCLUSIONS

Based on CROPWAT8.0 and an SEM in virtual water research, for the first time, we estimated the virtual water flow embedded within grain trade in the Yellow River Basin in 2019 with grain supply–demand excluding the importing and exporting trade. We also maximized the NSR in simulations. Considering the natural conditions of regional water supply, the technical indicators of water conservation levels, and the social factors of demographic structure and food consumption composition, we designed diverse scenarios for alleviating regional water stress, in which we assumed that no grain trade existed among regions. Our study results suggest that different regions should develop tailor-made policies to optimize virtual water flow patterns while considering their own water resource endowment and grain cultivation composition to relieve water stress and to protect water security.

Despite these findings of our study, however, certain disadvantages still exist, which may pose positive impact or detrimental influence potentially on corresponding problems. Some of them derive from two sectors: sampling validity, exogenous and endogenous uncertainty. A small amount of the uncertain samples may be induced by less accurate statistical data such as food prices for S0 and water supply data for S1. The latter disadvantage may be attributed to scenario settings, to which the exogenous uncertainty may arise from climate and precipitation changes, affecting the food trade model in scenarios S3 and S4, while the endogenous one may originate from human behaviour or environmental evolution. Specifically, those uncertainties exist in demographic structure and dietary pattern of the population in S2, or in alternatives between importing/exporting grains and conducting water savings in S4, all of which constitute the theoretical presumptions for this study.

Grain trade is a highly sophisticated human endeavour that correlates closely with policies and social realities. In order to establish a sound virtual water trade pattern, various practical factors must be considered. Although the purpose of SEM is to maximize NSR, the objective of this optimization may not be applicable under certain extreme conditions. If severe climate change happens or tragic catastrophe occurs, the final goal would be to satisfy the victims' food demands and to maintain social stability, which is far beyond the simulation capacity of SEM. Our future research interest will be focusing on the impact of various parameters of SEM on virtual water trade, paving the way for the mitigation of regional water stress under different hydro-climatic environments.

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DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

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