




Developing a National-Scale Hybrid System Dynamics, Agent-Based, Model to Evaluate the Effects of Dietary Changes on the Water, Food, and Energy Nexus

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Abstract

The pressing issue of the impact of changing agricultural policies on the water, food, and energy nexus is of utmost importance in today's world. This issue is particularly critical in countries currently grappling with a severe water crisis. This work develops a national-level water, food, and energy (WFE) nexus model using a combination of system dynamics modeling (SDM) and agent-based modeling (ABM). The WFE model focuses on water resources, with agriculture being the primary user. A model agent was designed for agriculture which includes a variety of agricultural products with varying yields, blue water and greywater consumption, energy consumption, and land area under cultivation for each crop. This paper's systems dynamics model is intended for application to meet the nutritional needs of a country's population by balancing water and energy resources and consumption while maintaining food security. The model's application covers two scenarios in Iran, a country under severe water stress. The first scenario involves nutrient supply based on the current diet, while the second scenario suggests a lacto-ovo diet. The outcomes of this study reveal that both scenarios can lead to water and energy savings. For example, the implementation of Scenario 1 and 2 can reduce the groundwater storage deficit that occurred during the five-year study period by approximately 65% and 85%, respectively. Furthermore, based on the high volume of water saved in both scenarios, the increase in the volume of greywater is deemed neither significant nor hazardous. Considering new policies of agricultural production can lead to a new balanced diet in terms of nutrients and energy, which can impact the achievement of sustainable WFE resources. The findings of this research could prove beneficial for national policymakers who seek to promote sustainable WFE resource management.

Keywords System dynamics · Agent-based Model · Lacto-ovo vegetarian diet · Food security · Water-food-energy nexus

1 Introduction

Water scarcity leads to food insecurity, which causes political unrest and social upheaval. The challenge confronting humanity is to make use of water resources to sustain food production while preserving natural ecosystem services. It is known that water and food security are interrelated topics (Rockström et al., 2001; Kheirinejad et al. 2021b). Meanwhile, urbanization, population growth, increasing living standards, climate change, globalization, and political instability are other criteria that influence food security (White et al. 2007; De Laurentiis et al. 2016). Previous studies have proposed approaches to achieve water, food, and energy security. Rosegrant et al. (2003) argued that political reform and judicious increasing in investments can improve food security, especially in developing countries. Brauman et al. (2013) reported increasing crop water productivity through management interventions that achieve food security and water sustainability by reducing the amount of water required for crop production.

On the one hand energy provision is linked to food security. On the other hand, food production plays a role in energy production and energy consumption (Kheirinejad et al. 2021a). Food production is mainly dependent on nonrenewable (fossil-fuel) energy in industrialized countries (Loáiciga 2011). For instance, the United States utilizes 10 calories of fossil fuel energy to produce one calorie of food energy (Gould and Caplow 2012). The competition for land in the search for food security and energy security is another key challenge to the worldwide development of renewable energy resources. The generation of electricity using biomass and solar energy is an example that promotes land competition for these systems' implementation (Nonhebel 2005; El-Mashad and Zhang 2010). Expanding on prior research that highlights land's role in the food and energy nexus (Akbar et al. 2023) assessed the climate impact of using fossil fuels in farming and propose a water-food-energy-land-climate nexus index.

Taking everything into account, ensuring food security involves finding equilibrium between the increasing demand for food and the Earth's finite ability to supply it. The solution to this dilemma lies in focusing on both the production and consumption sides, relying on a WFE nexus approach. De Laurentiis et al. (2016) discuss and review the potential of dietary changes (with focuses on nutrient-rich diets) within the WFE nexus framework as a promising approach to attain food security and sustainability. To achieve dietary shifts the latter authors suggested consuming seasonal products, balancing energy inputs and expenditures, and reducing the consumption of high-burden products. Furthermore, Core (2020) argues that a global shift toward more sustainable and water-efficient diets is essential to reduce water usage and cope with climate change and water scarcity. Such a shift is necessary to enhance food, water, and nutrition security. A WFE nexus approach takes into account the water and energy resources involved in food production. Implementing a WFE nexus framework is crucial for assessing the feasibility of altering dietary patterns in favor of sustainability. Nevertheless, it seems that a model tailored specifically for this objective has not yet been established.

The importance of modeling the effects of changing dietary habits on the WFE nexus is supported by the fact that food production consumes a significant amount of water worldwide, accounting for 70% of global freshwater withdrawals and 90% of freshwater consumption (Shiklomanov 1998; Johnson et al. 2001). Also, food production accounts for 30% of worldwide energy usage. There are complex interdependencies that exist between

the WFE resources (Scanlon et al. 2017), and improvement in the societal understanding of the WFE nexus has revealed its complex feedbacks. Therefore, developing the capacity to simulate and evaluate the complexities that underlay the WFE is essential for balancing the supply and demand of water, food, and energy (Kheirinejad et al. 2022). Deep understanding of the causal relationships between multiple variables that affect the WFE components is imperative for their effective management (Ghorbany et al. 2022, 2023). SDM is a suitable approach for considering these interrelationships and providing a comprehensive assessment of the WEF nexus.

Previous studies have reported various frameworks using SDM to assess the dynamic behavior of the WFE nexus (Akhtar et al. 2013; Sohofi et al. 2016; Smajgl et al. 2016; Sušnik et al. 2018; Bakhshianlamouki et al. 2020; Ravar et al. 2020; Elsayed et al. 2020). SDM provides a framework for understanding the feedback mechanisms inherent to the WFE nexus, but it does not necessarily lead to spatial decision-making (Bazzana et al. 2020). SDM is based on the premise that system dynamics are the result of stock accumulation, and each stock is composed of homogeneous elements. It is possible to take into account the differences between elements by adding new stocks that have the desired characteristics. Adding new stocks, however, may greatly increase system complexity that may be best handled by introducing structural and functional changes that modify the overall system structure. ABM, on the other hand may capture the properties of system elements while preserving its structure (Ding et al. 2018). One of the advantages of ABM is that it can represent systems in great detail by introducing multiple agents. In fact, agent-based modeling has been applied to modeling and analyzing the WFE nexus for various purposes. Khan et al. (2017), for instance, applied ABM to simulate the effects of water resources decisions on the water, food, energy, and environment nexus at the watershed scale. Their approach allows for a more detailed spatial investigation of the WFE nexus. Modeling the WFE nexus at the urban scale has been accomplished with a combination of ABM and NetLogo. Specifically, the model of sustainable urban development reported by Li et al. (2017) considered three agents and their decision-making behaviors. These three agents were the household, the firm, and government agents, which constitute an environmental system for the analysis of the urban WFE nexus with the ABM. ABM was applied to the WFE nexus by combining it with multi-objective optimization accounting for the spatial and temporal dependencies of the WFE nexus related to energy derived from food waste (Falconer et al. 2020).

The two modeling methods, i.e., ABM and SDM, each have their advantages and disadvantages. Clearly, by integrating their strengths, a model that leverages their advantages can be developed. Nikolic et al. (2013) combined SDM and ABM in the context of integrated water resource management considering spatial and temporal variabilities. Bazzana et al. (2020) applied combined SDM and ABM to the analysis of land use allocation and its effect on the WFE nexus in Ethiopia.

Despite the other investigation in water resources studies that consider the individual aspect of WEF (Akbari-Alashti et al. 2014; Beygi et al. 2014; Bozorg-Haddad and Mariño 2011; Bozorg-Haddad et al. 2007, 2009a, b, 2010a, b, 2013, 2015, 2016, 2017; Fallah-Mehdipour et al. 2011, 2013a, b; Karimi-Hosseini et al. 2011; Orouji et al. 2014; Sabbagh-pour et al. 2012; Soltanjalili et al. 2011), this study combines SDM and ABM to simulate the complex feedbacks of the WFE nexus at the macro (national) level. This study focuses primarily on improving the water resources balance; therefore, it simulates the agricultural sector with great detail because it is the sector with the largest freshwater consumption in

many countries, middle eastern ones being a case in point. The WFE nexus' dynamic system is enhanced by adding agents for modelling the water and energy consumption in different agricultural sectors (farming, gardening, and animal husbandry). This approach addresses a notable gap in the current WFE nexus modeling efforts, which often lack an inclusive and user-friendly simulation tool specifically designed for the food subsystem with a focus on crop production (Akbari Variani et al. 2023). Agricultural products have heterogeneous characteristics that are taken into account with ABM. Policy changes can be assessed by combining SDM with ABM while preserving the overall structure of a dynamic system. Two agents are created in this study to simulate system dynamics, one representing the current WFE situation, and the other representing a dietary change scenario. It is crucial to recognize that policies aimed at modifying crop patterns and dietary habits should first be crafted and scrutinized at the national level prior to regional implementation. This approach stems from the intricate nature of the WFE nexus, which intertwines aspects of WFE security, necessitating a coherent national strategy to ensure regional success. Accordingly, our study introduces a framework designed for analyzing the WFE nexus on a national scale. The need for such a framework is further emphasized by the scarcity of research addressing the WFE nexus at global and national levels compared to regional studies. Gao et al. (2023) note the increased complexity and challenges in data accessibility as one moves from regional to broader scales. This gap in research underscores the significance of our national-level model as a vital tool for addressing these expansive challenges effectively. In addition, our review of the literature indicates that models that incorporate dietary changes within the WFE nexus are lacking. This study addresses this knowledge gap by developing and evaluating a model to evaluate the effect of dietary changes on the WFE nexus at the national scale. The model's outputs serve as the basis for informed decisions that can be made regarding food security and vital resource management. This is crucial considering that overuse and inefficient use of natural resources have led to environmental damage, sometimes irreversible (Amjad Makhdum et al. 2024).

2 Methodology and Model Structure

Water resources are key components of the WFE nexus, which is why this work models renewable and non-renewable water resources in detail. Water allocated to humans and the environment involves supply and demand factors. On the demand side improving the efficiency of water use and water conservation are well-known means to reduce water use. The comparison of consumption-based and production-based nexus approaches may lead to findings underscoring the suitability of adopting consumption-based methodologies in future nexus modeling and governance efforts (Huang et al. 2021). This work considers demand-side scenarios that constitute water use, especially in the agricultural sector, which accounts for most of the freshwater use in many countries. Agriculture accounts for 70% of global freshwater withdrawals, on average. Food production has increased by more than 100% in the last 30 years. The Food and Agriculture Organization (FAO) estimates that about 60% more food will be needed by 2050 to meet the food requirements of an expanding world population (FAO, 2017). Two diet scenarios are herein considered in our assessment of the WFE nexus in this application. One scenario (Scenario 1) proposes a modified, yet, suitable, diet based on products chosen from among those that make up the current diet, and

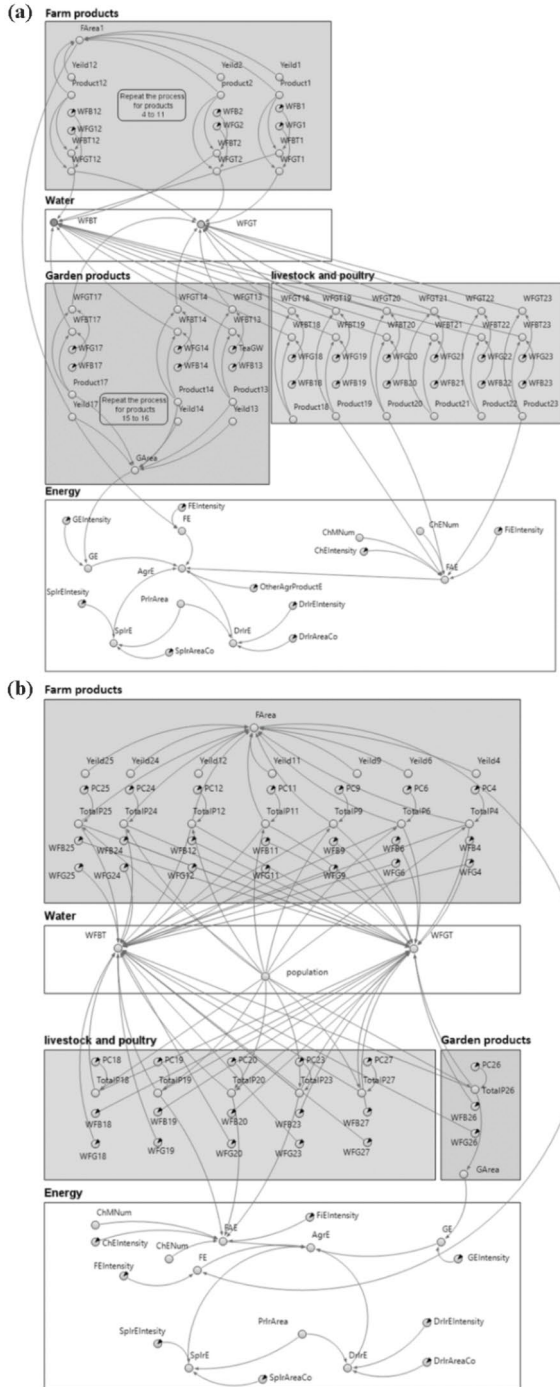
the second (Scenario 2) proposes a diet based on lacto-ovo products (i.e., vegetables, eggs, and dairy products, but not meat). The diet associated with the first scenario is the desired food basket proposed by the health authorities (which in the case of the application example is the Ministry of Health in Iran), which may be a modified version of the current diet of most people in a given country. The lacto-ovo diet would eliminate meat and replacing it with alternative foods that satisfy nutritional requirements. The American Heart Association advises that the lacto-ovo diet meets basic nutrient needs (Pimentel and Pimentel 2003).

The agent based (AB) and SD models were combined in this work to simulate management scenarios in the WEF nexus. Combining SD and AB modeling overcomes their individual limitations (Ding et al. 2018). SDM allows the highest level of abstraction and ABM can take into account the variable nature and scale of system elements (Silva et al. 2011). SDM ignores the effects of heterogeneous mixing because each stock is made up of homogeneous elements, whereas heterogeneous elements can be easily created with ABM (Ding et al. 2018). For example, in this paper's model one stock was defined for the energy sector, in which all types of energy are homogenized according to their heat requirements. In the case of water resources the inflows and outflows are homogeneous and are represented by their water volume, and these items are simulated with SDM. Homogenization of crop products in the agricultural sector is possible through their caloric nutritional content. The yield, blue, and greywater footprints per ton of produce and the energy used in the production process are characteristics specified for each type of agricultural product. Because of the heterogeneity inherent in the water and energy inputs the stock and flow approach has not been previously implemented to model the food sector.

The WFE nexus' feedbacks between water, food, and energy systems were modeled at the macro or national level with SDM, as shown in Fig. 1. Figure 1 shows the water and energy resources affect all sectors. The critical situation of water resources is addressed by considering all the sectors consuming water and the policies that govern water use under the current situation and under scenarios 1 and 2. Energy used by the transportation, domestic, public, and commercial sectors under current situation is used to calculate the total energy input. The water used by various energy carriers does not change in the scenarios considered in this work. The feedbacks involving water and energy are respectively represented with solid and dashed lines in Fig. 1.

A micro-level approach was developed to address the water-intensive agricultural sector (or the food sector) via an AB model that features two agricultural agents. The AnyLogic software offers all the benefits of the object-oriented method for SDM. In addition, it is possible to design complex models in a hierarchical fashion in which it is logical to add parts of stocks and flow diagrams to different types of agents and show only their interface variables as input or output in the dynamic system. The dynamic components of the system can be structured into a variety of agents and then parameterized, organized into different structures, and reused. This feature of the software as a modeling platform allows the insertion of nexus causal relationships in a dynamic system, which is defined as the main agent. A separate agent was defined for the agricultural sector because the information and feedbacks involved, and special parameters of the agricultural agent were used in the main agent (nexus dynamic system). Only one agent is called in each simulation run by the dynamic system and its parameters (water use, energy consumption, and gray water use) are applied. One agent is designated for current conditions (Fig. 2a), and another for the scenario conditions (Fig. 2b). A noteworthy point here about Fig. 2 is that the variables

Fig. 2 Agents designed for the agricultural sector: **(a)** for current situation **(b)** for scenarios



2.1 Water Balance

This work combines SDM and ABM to obtain the balance of surface water and groundwater resources within the framework of the WFE nexus. The equations of balance for surface and groundwater resources prescribe that changes in the volume of surface water and groundwater resources depend on their inputs and outputs. The changes in storage volume based on inputs and outputs are summarized in Fig. 3. It is noteworthy that Kheirinejad et al. (2022) proposed a model that considers the effects of reducing per capita water and energy consumption within the framework of the WFE nexus. The water-balance equations for surface water and groundwater resources are given respectively by Eqs. (1) and (2):

$$\delta SW_t = f(Pre_t, Dr_t, OCSW_t, DomWN_t, IndWN_t, AgrWN_t, WE_t, WEIF_t, AgrSWCo_t, DomSWCo_t, IndSWCo_t, Fo_t) \tag{1}$$

$$\delta GW_t = g(Pre_t, Dr_t, OCGW_t, DomWN_t, IndWN_t, AgrWN_t, AgrGWCo_t, DomGWCo_t, IndGWCo_t, Fo_t) \tag{2}$$

in which δSW_t = the change in surface water storage during period t; δGW_t = change in groundwater resources during period t; f and g denote numerical functions that calculate respectively the surface and groundwater balances; Pre_t = the precipitation during period t, $OCSW_t$ = the difference between the volume of surface inflows and that of outflows through the land border of the country during period t, $OCGW_t$ = the difference between the volume of groundwater inflows and that of outflows through the country's border dur-

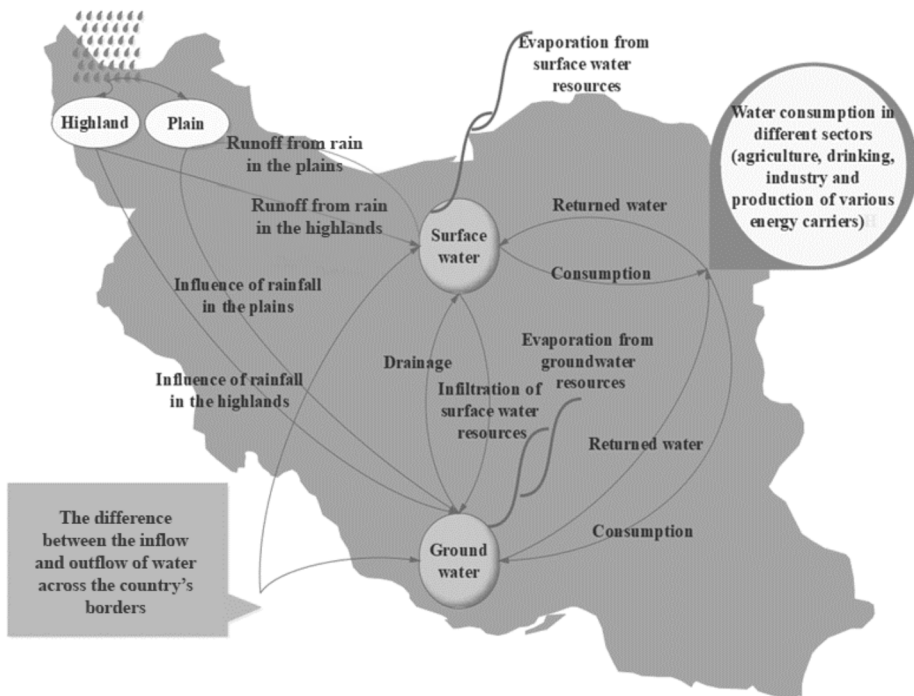


Fig. 3 Schematic of water resources and water use-feedbacks

ing period t , Dr_t = the drainage of groundwater resources to surface water resources during period t , $DomWN_t$ = the volume of gross water use in the residential sector during period t , $IndWN_t$ = the volume of water use in the industrial sector during period t , $AgrWN_t$ = the volume of water use in the agricultural sector during period t , WE_t = the volume of water required to produce various types of energy carriers (except those included in the industrial sector) in the current situation during period t , Fo_t = the volume of discharge of springs to surface water sources during period t , $AgrSWCo$ = the percentage of agricultural water use supplied by surface water sources, $IndSWCo$ = the percentage of industrial water use supplied by surface water sources, $DomSWCo$ = the percentage of residential water use supplied by surface water resources, $AgrGWCo$ = the percentage of agricultural water use supplied by groundwater resources, $IndGWCo$ = the percentage of industrial water use supplied by groundwater resources, $DomGWCo$ = the percentage of residential water use supplied by groundwater resources, and $WEIF_t$ = the volume of water saved due to energy savings according to the two alternative dietary scenarios during period t .

The methods of calculating water and energy use in the agricultural sector are described in Sect. 2.2 and 2.3, respectively.

2.2 The Agricultural Water Requirement

The concept of blue water footprint (in which blue water represents the volume of surface and groundwater used for the production of a good) is applied in the calculation of the volume of water withdrawal and use in the agricultural sector. The concept of greywater footprint (whereby greywater constitutes the volume of fresh water needed to assimilate the pollutants load based on the existing standards for ambient water quality) was applied in the assessment of the environmental water requirements (Mekonnen and Hoekstra 2010). Calculations of the agricultural water requirements are performed with Eq. (3) through (5). It should be noted that the $Product_{i,t}$ variable in the current situation is equal to the total weight of each agricultural product in a period for which information is available. However, the $Product_{i,t}$ variable is replaced by the $TotalP_{i,t,s}$ variable when the model simulates the conditions under the scenarios, which is discussed in Eq. (17).

$$WFBT_t = \sum_{i \in A} WFB_i \times Product_{i,t} \tag{3}$$

in which $WFBT_t$ = the total volume of water use by the chosen agricultural products during period t , $Product_{i,t}$ = the amount of agricultural product i during period t (tons), and WFB_i = the water intensity of agricultural product i (cubic meters per ton). $WFBT_t$ was calculated under the dietary Scenarios 1 and 2 described above and in the current situation. It should be noted that in the first agent of agricultural sector the $WFB_i \times Product_{i,t}$ is abbreviated to $WFBT_{t,i}$ (Fig. 2a).

Several agricultural products were selected to calculate the water and energy requirements of the agricultural sector.

These products constitute a major share of the country’s agricultural production and make up most of the country’s food basket.

Parameters $OtherAgrWN$, $OtherAgrGW$ and $OtherAgrProductE$ are introduced to take into account the water use, greywater use, and the energy requirements of other agricultural products.

The latter parameters are used to calibrate the SD-AB model of the WFE nexus, and their values for the current situation are presented in Sect. 4. Their values under Scenarios 1 and 2 are equal to zero. The volume of water withdrawal during period t ($AgrWN_t$) (gross consumption) is calculated with Eq. (4):

$$AgrWN_t = WFBT_t \times \frac{1}{R_{Agr}} + OtherAgrWN \quad (4)$$

in which R_{Agr} = the irrigation efficiency, $AgrWN_t$ = the total volume of water uses by the agricultural sector during period t , and $OtherAgrWN$ = the gross consumption volume of other agricultural products. The irrigation efficiency equals the ratio of the water used for beneficial evapotranspiration to the water withdrawal for irrigation (Mekonnen and Hoekstra 2011).

The greywater footprint of agricultural products was obtained from Mekonnen and Hoekstra (2010, 2011). Equation (5) calculates the total greywater use by the agricultural sector:

$$WFGT_t = \sum_{i \in A} WFG_i \times Product_{i,t} + OtherAgrGW \quad (5)$$

in which WFG_i = the volume of greywater required to produce one ton of product i (cubic meters per ton), and $WFGT_t$ = the total volume of greywater during period t , and $OtherAgrGW$ = the greywater requirement of other agricultural products. It should be noted that in the first agent of the agricultural sector the $WFG_i \times Product_{i,t}$ is abbreviated to $WFGT_{t,i}$ (Fig. 2a).

2.3 The Agricultural Energy Requirement

Energy use by the agricultural sector includes the expenditure of natural gas, kerosene, electricity, and other energy carriers by agricultural machinery, poultry farming, and other activities. Most of the energy use by the agricultural sector (more than 80%) is by poultry farming, water pumping, agricultural machinery (agriculture and horticulture), fisheries, and aquaculture. This study calculates energy use in each of the agricultural sub-sectors using Eq. (6) through (12). The remaining energy use was attributed to other products. The total energy uses by the agricultural sector, except that related to groundwater pumping, was calculated with Eq. (13). Water withdrawal by wells for agricultural and industrial use was calculated with Eq. (14), and the use of energy to pump groundwater for agriculture and industry is given by Eq. (15).

The energy intensity in the farming and gardening sub-sectors was calculated in terms of their areas under cultivation. The area under crop cultivation was calculated based on crop yields. The energy use by the pressurized irrigation sector requires the total area under cultivation which was calculated with Eq. (6) through (8). The energy required in the farming and gardening sub-sectors (excluding water pumping) is estimated using Eqs. (6) and (7).

$$GArea_t = \sum_{i \in G} Product_{i,t} \times Yeild_{i,t} \tag{6}$$

in which $GArea_t$ = the area of gardens during period t (hectares), $Product_{i,t}$ = the amount of agricultural production i during period t (tons), $Yeild_{i,t}$ = the yield of crop i during period t (tons per hectare), and set G = the subset of garden products.

$$FArea_t = \sum_{i \in F} Product_{i,t} \times Yeild_{i,t} \tag{7}$$

in which $FArea_t$ = the area of farmlands during the period t (hectare) and set F = the subset of crops.

$$FE_t = FArea_t \times FEIntensity \tag{8}$$

in which FE_t = the energy required by the farm sub-sector during period t, and $FEIntensity$ = the intensity of the farm sub-sector energy use excluding water pumping energy use (MWh per hectare).

$$GE_t = GArea_t \times GEIntensity \tag{9}$$

in which GE_t = the energy required for the garden sub-sector during period t, and $GEIntensity$ = the intensity of energy use of the garden sub-sector excluding energy for water pumping (MWh per hectare).

The farm animal sub-sector includes energy use by the poultry and aquaculture sectors. The energy use was calculated according to the number of chickens produced and the weight of fish production. The weight of chicken production is converted to the number of chickens by applying a coefficient in each year. Energy use in the farm animal sector is estimated with Eq. (10):

$$FAE_t = Product_{23,t} \times FiEIntensity + (Product_{20,t} \times ChENum_t + Product_{19,t} \times ChMNum_t) \times ChEIntensity \tag{10}$$

in which FAE_t = the energy use in the farm animal sector in period t; $FiEIntensity$ = the energy intensity of the aquaculture sub-sector (MWh per ton), $ChEIntensity$ = the energy intensity of the poultry sub-sector (MWh per Number), $ChENum_t$ = the ratio of the number of laying hens to the weight of eggs produced by them during period t; $ChMNum_t$ = the ratio of the number of broilers to the chicken meat weight during period t; $Product_{23,t}$ = the mount of fish production (ton), $Product_{20,t}$ = the amount of laying hen production (ton), and $Product_{19,t}$ = the amount of broiler production (i.e., chicken brooding operation, in tons).

Energy use by the pressurized irrigation sub-sector has two components: sprinkler and drip irrigation. The area of irrigated land for each irrigation method was calculated. The total energy use in this sector was calculated with Eqs. (11) and (12) by applying the intensity of energy use per hectare of land irrigated by drip and sprinklers. The average area

under cultivation corresponding to current situation and two alternative dietary scenarios during the period under study is calculated with Eq. (11):

$$SpIrE_t = PrIrArea \times SpIrAreaCo \times SpIrEIntensity \quad (11)$$

in which $SpIrE_t$ = the total energy required for sprinkler irrigation during period t, $PrIrArea$ = the area of agricultural land under pressurized irrigation, $SpIrAreaCo$ = the percentage of land area equipped with pressurized sprinkler irrigation, and $SpIrEIntensity$ = the energy intensity under sprinkler irrigation (MWh per hectare).

$$DrIrE_t = PrIrArea \times DrIrAreaCo \times DrIrEIntensity \quad (12)$$

in which $DrIrE_t$ = the energy required by drip irrigation during period t, $DrIrAreaCo$ = the percentage of land area equipped with pressurized drip irrigation, and $DrIrEIntensity$ = the energy intensity of drip irrigation (MWh per hectare). The energy use by the agricultural sector (except for the pumping of water from wells) during period t is calculated as follows:

$$AgrE_t = FE_t + GE_t + FAE_t + SpIrE_t + DrIrE_t + OtherAgrProductE \quad (13)$$

in which $AgrE_t$ = the energy use by the agricultural sector (except for the pumping of water from wells) during period t and $OtherAgrProductE$ = the energy use of other agricultural products.

Water pumping by wells for agricultural and industrial use of groundwater is given by Eq. (15):

$$VW_t = IndGWDCo_t \times IndWD_t + AgrGWDCo_t \times AgrWD_t \quad (14)$$

in which VW_t = the volume of gross agricultural and industrial use of groundwater during period t. The energy uses by pumps to supply groundwater for agricultural and industrial uses during period t is calculated with Eq. (15):

$$PumpGwED_t = (Well \times VW_t \times EV \times EWIntensity) + (Well \times VW_t \times DV \times DWIntensity) \quad (15)$$

in which $PumpGwED_t$ = the energy use by pumps to supply groundwater for agricultural and industrial uses during period t, $Well$ = the percentage of groundwater withdrawn by wells, EV = the percentage of groundwater withdrawn by electric wells, DV = the percentage of water withdrawn by diesel wells, $EWIntensity$ = the energy intensity of electric wells (MWh per cubic meter), and $DWIntensity$ = the energy intensity of diesel wells (MWh per cubic meter).

$$TAE_t = AgrED_t + PumpGwED_t \quad (16)$$

in which TAE_t = the energy use by the agricultural sector during period t.

The quantification of the effects of the dietary Scenarios 1 and 2 on the WFE is made with the following equation:

$$TotalP_{i,t,s} = Population_t \times PC_{i,s} \times 0.000365 \quad (17)$$

in which $PC_{i,s}$ = the daily capita supply of basic food products by the diet Scenarios (= 1 or 2) (grams per person per day), $TotalP_{i,t,s}$ = the amount of product i under Scenarios (= 1 or 2) during period t ; the population during year t .

The difference between the energy use under each scenario and in the current situation is calculated with Eq. (19):

$$DeltaE_t = TAE_t^0 - TAE_t^S \quad (18)$$

in which $DeltaE_t$ = the difference between the energy use in each scenario and the current situation during period t , TAE_t^0 = the energy use under current situation during period t , and TAE_t^S = the energy consumed under scenarios (= 1 or 2) during period t .

The water saved was computed using Eq. (19). It was assumed that if more energy were needed under each scenario the share of energy exports would be reduced and used to implement the scenario (this was not the case in this study's application).

$$iffunc_t = \text{if } (DeltaE_t > 0) \{ \text{return } DeltaE_t ; \} \text{ else } \{ \text{return } 0 ; \} \\ WEIF_t = iffunc_t \times avWE \quad (19)$$

in which $iffunc_t$ = the amount of energy saved during period t , and $avWE$ = the water intensity of energy (cubic meters per MWh).

3 Case Study Area

Iran was selected as the study area to evaluate the performance of the developed approach. The country is located in southwestern Asia between latitudes 25° and 40° North, and longitudes 44° and 63° East. Iran covers a total area of 1.75 million km². The average annual rainfall equals 250 mm, which is one-third of the world's average precipitation and one half of the average precipitation of Asia. About 90% of the country is classified as arid or semi-arid. Iran faces threats to its water security, which makes an ideal test case for this paper's methodology. Iran has large energy resources and high water demand. Agriculture accounts for the largest share of water use.

This study was based on data for water years 2010/2011 through 2014/2015. The water year describes a period of 12 months beginning October 1st of any given year and ending September 30th of the following year. Pertinent water data are cataloged by water year. This work obtained the necessary data from the Ministry of Energy (20102015a, b–2014), the Statistical Center of Iran (2016), the Ministry of Industry, Mines, and Trade (2011), and Gadonneix et al. (2010).

Table 1 Blue and greywater use per ton of product

Row	Kind	Product	Water consumption in Iran per ton of product produced (cubic meters)		
			Greywater	Blue water	
1	Farm products	Industrial crops	Sugar cane	12	22
2			Sugar beet	46	346
3			Soy	45	81
4		Cereals	Wheat	249	737
5			Barley	219	73
6			Rice	330	2,267
7			Corn	324	552
8		Vegetables	Tomato	23	284
9			Potato	35	255
10			Onion	22	265
11			Other vegetables	38	188
12		Legumes	Bean	470	1,451
13	Garden products		Oranges and tangerines	43	497
14			Apple	48	775
15			Grape	80	0
16			sour lemon	38	440
17			Tea	507	7,256
18	Production of protein products - livestock and poultry		Milk	194	356
19			Chicken meat	838	1,614
20			Egg	697	1,320
21			Beef	539	1,208
22			Mutton and goats	67	429
23			Fish	440	740

Table 2 Total observed agricultural energy uses in Iran (TWh)

Water year	2010	2011	2012	2013	2014
Agriculture	77.6	79.4	82.6	84.9	86.4

3.1 Agriculture

Twenty agricultural products were identified in the agricultural sector (see Table 1) that account for a major share of Iran's agricultural production and its food basket. The products listed in Table 1 were classified into six groups and their blue and greywater footprints were obtained (Deputy of Infrastructure Research and Production Affairs 2015; Yuan et al. 2017). The average irrigation efficiency was estimated at 36% and 43.8% for the water years 2010/2012 and 2012/2015, respectively (Abbasi et al. 2016). The average irrigation efficiency for the five-year study period was 40.68%.

The energy use by the agricultural sector is listed in Table 2 (Ministry of Energy 2015b). These data were used for calibration. The average energy use by the poultry farms was

1.64 L of diesel per chicken in 2009. The average diesel intensity (excluding water pumping consumption) was 92.6 L of diesel per hectare of cultivated land in 2009 (Amidpour 2014). The diesel intensity depends on agricultural mechanization, working width, the type of machinery, and the price of energy.

The garden sub-sector had an energy intensity equal to 51 L of diesel (equivalent) per hectare in 2009 (Amidpour 2014). The fisheries and aquaculture sub-sector rely on diesel fuel and electricity as main sources of energy, having an energy intensity of 416 L of diesel (equivalent) per ton of aquatic product in 2009 (Amidpour 2014). Livestock breeding has a very small share (less than 3%) of the total energy consumption of the agricultural sector (Amidpour 2014). Consequently, breeding is not included in the model simulations due to its low share of energy consumption and the paucity of data livestock. Data for various agricultural sub-sectors such as product weight, the yield of selected agricultural products, and product ratios were obtained from the agricultural yearbook (Ministry of Agriculture, 2010–2014).

3.1.1 Energy Use by Pressurized Irrigation

Pressurized irrigation is powered by diesel and electric pumps. The energy required to power Wheel Move (gasoline), Center Pivot, and Linear Move (electricity) systems was low enough to be ignored (Energy Information 2014). Over 50% of the total area under pressurized irrigation in Iran is served by sprinklers and the remaining 50% by drip irrigation in 2009 (Energy Information 2014). The average duration of drip and sprinkler irrigation was eight hours daily, each applied during 200 days and 120 days, respectively. Therefore, the annual number of working hours was 1,600 h for drip irrigation and 960 h for sprinkler irrigation. Table 3 lists the amount of energy use by both irrigation methods and the two types of pumps (i.e., electric pumps and diesel pumps). 75% of the energy required for secondary pumping in pressurized irrigation (drip and sprinkler) was supplied by electric pumps, and the rest by diesel pumps. These percentages were assumed to be constant over the study period. Therefore, the energy use by drip and sprinkler irrigation was calculated to be 1.088 and 1.44 MWh per hectare, respectively (Iranian Fuel Conservation Company 2006). The area of agricultural land under pressurized irrigation is equal to 2.043 million hectares.

3.1.2 Energy Use by Water Wells

The following steps were taken to estimate the energy use by diesel and electric pumps. The average electricity use by each well was obtained by dividing the electricity consumption of agricultural wells by the number of agricultural wells that had access to electricity. Next, the amount of energy use per cubic meter of extracted water was calculated by dividing the energy use of each well by the amount of water withdrawn. The National Iranian Oil Refining and Distribution Company collected data on diesel fuel use by agricultural wells in 16 areas under its service. The data established that the average use of diesel by agricultural wells was about 5,626 L per year. The average electricity required to withdraw one

Table 3 Energy required for pressurized irrigation per hectare per hour

Irrigation method	Pump type	
	Diesel (L)	Electric (KWh)
Electric (KWh)		
Drop irrigation	0.16	0.35
Sprinkler irrigation	0.36	0.77

cubic meter of water by agricultural wells (deep and semi-deep) was about 0.7 kWh. The amount of diesel fuel consumed to extract a cubic meter of water by agricultural wells was about 0.07 L. 57% of the wells were electric-powered and the remainder were diesel-powered (National Iranian Oil Refining and Distribution Company 2009; Ministry of Energy, 2003–2011).

3.2 Industry

Industry has the lowest share of the water abstraction, which was 2.74 billion cubic meters during the study period. This was based on calculations of the average resource availability and use in 2009 (Ministry of Energy 2015a). It should be noted that 87% of the groundwater extracted to meet industrial and agricultural demands was withdrawn by wells (Ministry of Energy 2015a). Moreover, the average water use for energy production was estimated at 2.45 cubic meters per MWh (World Energy Council, 2010; Ministry of Energy 2015b).

Table 4 lists the per capita daily consumption of various food products which provide the necessary energy and nutrients corresponding to the modified diet (Scenario 1) and the lacto-ovo vegetarian diet (Scenario 2) (Ministry of Agriculture 2015). The Scenario 1 diet is based on the diet of the majority of Iran's population (Ministry of Agriculture 2015). The lacto-ovo diet was estimated according to the ratios of the desired products to their energy and nutrition contents (Table 4). Red and white meat were replaced with larger amounts of other products. In both diets the percentage of energy provided by the three groups of macronutrients (protein, carbohydrates, and fats) is within the desired range according to the recommendation of the World Health Organization. This amounts to 15–35% of the energy provided by fat, followed by 55–75% of carbohydrates, and 10–12% by protein in a desirable diet.

Table 4 Per capita supply of nutrients and energy by basic food products and macronutrients corresponding to scenarios 1 and 2

Food product	Scenario 1					Scenario 2				
	Protein (g)	Fat (g)	Carbohydrates (g)	Energy (kcal)	g/capita/Day	Protein (g)	Fat (g)	Carbohydrates (g)	Energy (kcal)	g/capita/day
Wheat	42.41	11.72	258.15	1306.47	348.81	42.41	11.72	258.15	1306.47	348.81
Rice	6.48	1	86.58	360.1	98	6.48	1	86.58	360.1	98
Beans	6.24	0.75	13.64	83.14	27	18.72	2.25	40.92	249.42	81
Potato	1.37	0.24	12.96	56.35	81	2.329	0.408	22.032	95.795	137.7
Other vegetables	3.36	0.78	14.51	75.86	354	3.696	0.858	15.961	83.446	389.4
Fruit	3.32	8.39	33.81	225.62	332	3.32	8.39	33.81	225.62	332
Red meat	8.32	8.21	0.16	106.13	56	0	0	0	0	0
Chicken	8.04	5.84	0	84.97	65	0	0	0	0	0
Fish	3.97	1.13	0.06	26.44	38	0	0	0	0	0
Egg	4.46	3.86	0	52.48	36	8.028	6.948	0	94.464	64.8
Milk	10.04	11.51	12.1	189.52	258	12.048	13.812	14.52	227.424	309.6
Vegetable oil	0	34.97	0	315	35	0	35.6694	0	321.3	35.7
Sugar	0	0	40	157.6	40	0	0	40	157.6	40

Table 5 Blue and greywater use in vegetable oils production (cubic meters per ton of produce)

Product	Blue water	Greywater
Soy	81	45
Canola	0	48
Cottonseed	1,113	94
Other oilseeds	1,020	2,009

Table 6 Characteristics of food groups of vegetable oil, sugar, fruit, and red meat

Row	Kind	Yield (tons per hectare)	Greywater (m ³ /ton)	Blue water (m ³ /ton)
24	Vegetable oil	0.59	657.41	641.69
25	Sugar	7.27	229.09	1,452.85
26	Fruit	14.42	54.99	449.58
27	Red meat	-	311.23	832.08

All food products, except for sugar and vegetable oils, which are produced from basic agricultural products, are basic agricultural products. The required data for these products were extracted from the agricultural yearbook (Ministry of Agriculture, 2010–2015).

Fruit and red meat are the two main products required basketing the modified diet. The required data on horticultural products, protein-livestock, and poultry products were obtained from the agricultural yearbook (Ministry of Agriculture, 2010–2014). The following sections explain the calculations involved with respect to blue water, greywater, and the areas of cultivated lands to produce sugar, vegetable oils, fruits, and red meat.

According to data for the period 2000–2012, on average, sugar beet accounted for 57% of sugar produced, while sugarcane accounted for 43% of the total sugar production. The average industrial production efficiency of sugar from sugar beets and sugarcane for the study period was estimated at 14.4% and 10.9%, respectively (Najafpur 2013).

Vegetable oil is mainly produced from soybean, rapeseed, cottonseed and other oilseeds, which have shares of 22%, 53%, 13% and 13%, respectively, in Iran. Their industrial production efficiency is estimated to be 18%, 40%, 50% and 50%, respectively (Ministry of Agriculture 2018). Their blue and greywater uses are listed in Table 5.

Oranges and tangerines, apple, grapes, and sour lemons had shares of 32, 35, 28 and 47% of the fruit group, respectively. The share of beef in red meat production was 52%; the mutton (lamb) and goat meat share were 48%. The blue, and greywater footprints of products were estimated by establishing the weighted average of the share in the production of each group. The total production of a product group was divided by the total land under cultivation of that group. The calculated results are listed in Table 6. An average annual 527,700 tons of fish were produced to supply the modified diet. This was used as the average value for computations during the study period (Ministry of Agriculture, 2010–2014).

4 Model Calibration

The SDM AB model of the WFE nexus required calibration based on data concerning water and energy use and food production. The gross agricultural water use was 81.7 billion cubic meters in 2010. The water uses by other products (i.e., those not selected in Scenario 1 diet) was estimated to be 8.39 billion cubic meters in the same year. Greywater-use data were

obtained from Mekonnen and Hoekstra (2010, 2011). These water uses were applied in model calibration, along with energy-use data for the agricultural sector published by the Ministry of Energy (Table 2), which were available for all the study years. Other energy data used in model calibration were from Amidpour (2014). Model calibration was achieved with the dynamic AnyLogic operating system aided by trial-and-error. The results of model calibration are listed in Table 7, where it is seen the model produced accurate predictions after calibration with the software and by trial and error in some instances. The evaluation of goodness-of-fit between observed data and model simulations was conducted using widely used calibration metrics, namely the Nash-Sutcliffe Efficiency (NS), Ratio of Root Mean Square Error to Standard Deviation of observed data (RSR) and R^2 (Moriasi et al. 2007).

5 Results and Discussion

The current imbalance between water resources and water use is pronounced in Iran. The average annual water use in Iran is about 8% higher than the total annual renewable water resources (Mesgaran and Azadi 2018). It is imperative, therefore, to modify water use given the scarcity of water resources. The current Iranian policy is based on increasing the extraction of water resources and expanding agriculture. Further reliance on this policy may lead to water and food shortages. The WFE nexus approach may be applied to search for effective policies by simultaneously examining feedbacks between the agricultural, industrial, and urban sectors (Zarei et al. 2020).

This work proposed Scenario-1 and -2 diets to remedy the depletion of water resources while providing suitable nutrition to Iran's people. Figures 4 and 5 depict the calculated results obtained with SD and AB modeling of the WFE nexus corresponding to the dietary scenarios. There would be lower energy use under Scenarios 1 and 2 because of the reduction in water pumping. Energy use would also be reduced because of lower product consumption due to the removal of some products from the national level program of agricultural production. On the one hand, under both scenarios, the export of agricultural products has been eliminated, but there is no need to import agricultural products to ensure food security. On the other hand, in the current situation, food waste is more than the normally accepted and overeating is common among some people. Therefore, considering the desired food basket for preparing the agricultural production plan under both scenarios seems a sound agricultural production policy for the purpose of achieving food, water, and energy security in the country. Further reduction in energy use under Scenario 2 is mainly related to the absence of chicken meat. The poultry sub-sector has a high share of energy usage in the agricultural sector in the current situation. Under Scenario 1 energy intake would be an average 3,040 kcal of energy per person per day, and the shares of protein, fat and carbohydrate to this energy provision equal 13%, 26%, and 61%, respectively. The balance of surface water resources both cumulatively over the entire study period and in each year would be positive. However, this would not be the case with the cumulative and individual year balances of

Table 7 The values of statistical indicators calculated to measure the model efficiency according to the calculated and observational values of changes in surface water and groundwater storage

Indicator	NS	R^2	RSR
Error criteria for surface water volume changes	0.99	0.99	0.03
Error criteria for ground water volume changes	0.99	0.99	0.02

Fig. 4 Energy saving under dietary Scenarios 1 (S1) and 2 (S2)

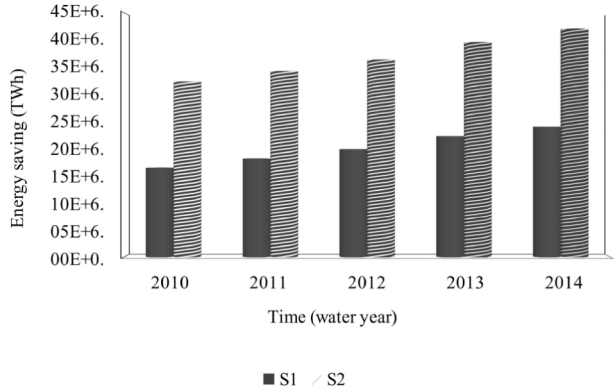
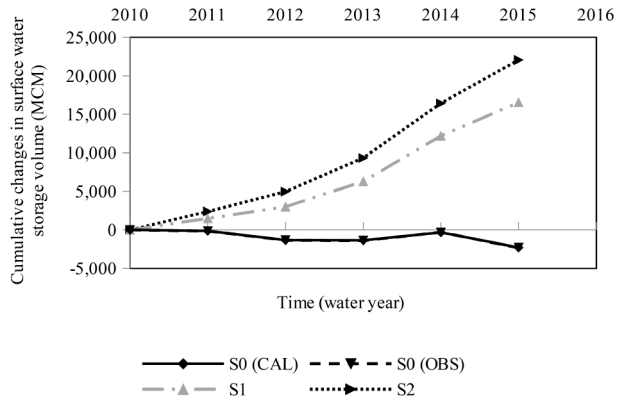
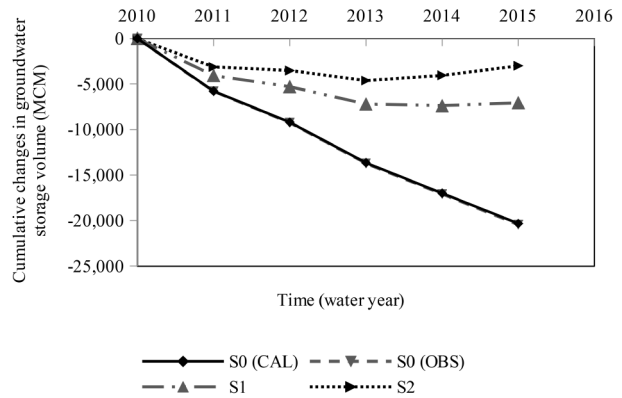


Fig. 5 Cumulative changes in the volume of water resources (MCM = 10^6 m^3): (a) surface and (b) groundwater in the current situation (S0) (observational (OBS) and computational (CAL)), Scenario 1 (S1) and Scenario 2 (S2)



(a)



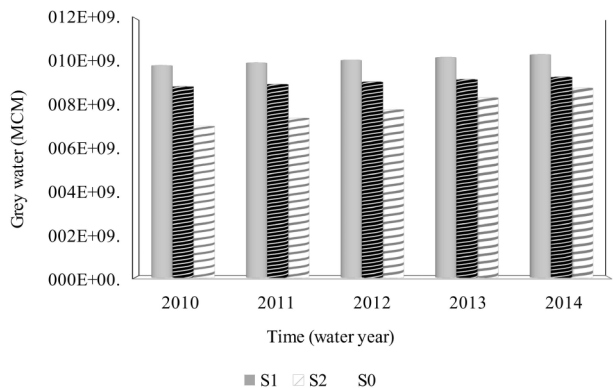
(b)

groundwater resources, with the latter becoming positive only in the last year of the study period. Implementation of Scenario 1 over the five-year period would reduce surface water and groundwater use by $18.9 \times 10^9 \text{ m}^3$ and $13.4 \times 10^9 \text{ m}^3$, respectively, in comparison to water use in the current situation. The energy intake would be an average 3,084 kcal per person per day under Scenario 2, and the shares of protein, fat, and carbohydrate to this energy provision would be 12%, 22% and 66%, respectively. The cumulative balance of groundwater resources would be negative, and only the last two years would be positive. Surface water and groundwater use would be reduced by $24.4 \times 10^9 \text{ m}^3$ and $17.4 \times 10^9 \text{ m}^3$, respectively, under Scenario 2 in comparison to water use in the current situation. The different water uses under Scenarios 1 and 2 stems from the elimination of meat in the Scenario-2 diet. Animal products generally have larger water footprints than crops per unit mass of product. The same holds true for the water footprint of caloric content of food. The average water footprint per calorie from beef is twenty times larger than for cereals (Hoekstra 2012).

The calculated reduction in water use in Iran under Scenarios 1 and 2 is less than expected based on studies of water conservation from dietary shifts (Vidal 2004; Hoekstra 2012; Vanham et al. 2016). This is explained by considering that about 48% of the red meat consumed in Iran is mutton and goat. The shares of green (precipitation), blue (surface water and groundwater), and greywaters (non-fecally contaminated sewage) used to raise mutton and goat are 63%, 4%, and 1%, respectively. The large share of green water (precipitation) in meeting the water needs of mutton and goat means lower dependence on blue and greywaters. In addition, a significant amount of fish is from sea fisheries (about 67% in the study period), which further reduces the use of water by aquaculture.

Figure 6 compares greywater use under the current diet and Scenarios 1 and 2, where it is seen that greywater use would be larger under Scenarios 1 and 2 than in the current situation. It is imperative to note that the quantity of water saved under the scenarios would be sufficient to offset the relatively minor increase in the generation of grey water. This means that this practice would not harm the environment, has and it would also has the potential to improve environmental conditions. A portion of the water saved could be blended with polluted water (to resolve gray water issues), thus enhancing its quality. In addition, a significant proportion of the water saved could be re-purposed to meet the quantity demands of the environment, ultimately leading to an improvement in environmental conditions as a whole. This underscores the importance of implementing water conservation measures as they have the potential to address quantity-related issues and improve water quality in the environment (Kheirinejad et al. 2022). Scenario 2 would generate less greywater than

Fig. 6 Greywater use (MCM = 10^6 m^3) in the current situation (S0), Scenarios 1 (S1) and 2 (S2)



Scenario 1 because the largest share of the water footprint of animal products is devoted to producing animal feed.

This works projects how the desired food baskets are provided through domestic or internal agriculture. All the diet scenarios demonstrate a reduction in water and energy consumption when production is domestic. Larger water and energy savings would occur if some of the products were imported. One possible risk of food importation, however, is interruptions of the supply chain by natural or human-induced factors (Aljerf and Aljerf., 2023). The critical water conditions indicated that the production of agricultural products for export to other countries would be a counterproductive policy under the scenarios considered in this article, in which the focus of agriculture would be ensuring the country's food security.

6 Concluding Remarks

This paper introduces a comprehensive model designed to encapsulate the intricacies of the WFE nexus. By integrating system dynamics with agent-based modeling, we have developed and calibrated a model reflective of the current situation to assess the feedback mechanisms within the nexus. Our research pioneers the investigation of how dietary changes at a national level influence the WFE nexus, paying close attention to the implications for both renewable and nonrenewable resources. This work proposes two dietary scenarios to explore their potential impacts on the WFE nexus. It is evident from the results that scenarios 1 and 2 achieve a better cumulative balance of surface water resources. It is anticipated that Scenarios 1 and 2 would reduce the groundwater deficit during the study period but would leave the cumulative balance negative. Under both scenarios, energy savings would be significant, with Scenario 2 achieving greater energy savings as meat is removed from the diet. Scenarios 1 and 2 would result in more greywater use. Nationally, scenario 2 may be difficult to implement since it would require a cultural shift. The recognition of the close interactions between human systems and water, the social and cultural attitudes towards water use, and the manner in which these interactions are understood through hydro-social studies could facilitate the implementation of the proposed dietary changes (Bozorg-Haddad et al. 2021). The dietary changes herein considered may appeal to policy makers because of its potential health benefits (reduction in obesity, heart disease, high blood pressure, diabetes 2, and certain types of cancer) as well as its possible positive impact on resource conservation. The approach developed in this study for modeling the WFE nexus is of a general nature. With proper adjustments to account for inter-country differences, it can also be applied to other regions besides Iran. The following research areas will be explored in the future:

1. Assessing possible impacts of changes in the WFE nexus on socio-economic factors. In the agricultural sector, for example, changes are likely to have a significant impact on farmers' livelihoods.
2. Analyzing all aspects of the WFE nexus from an economic standpoint, including costs and revenues generated by agricultural and industrial products, costs associated with technologies involved in the WFE nexus, water and energy extraction costs and revenues, and considering the role of virtual water embedded in the export and import of agricultural and industrial goods.

3. Exploring the impact of fat modification in animal products on nutritional quality, as well as its potential to reduce water and energy consumption in food production systems.
4. Investigating the energy consumed by the transportation sector and the processing of agricultural products, and taking this information into account when assembling the WFE nexus. A better understanding of the interactions between agriculture, water, and energy would be possible using this approach.

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Data Availability The data that support the findings of this study are available from the corresponding author upon reasonable request.

Declarations

Ethics Approval All authors accept all ethical approvals.

Consent to Participate All authors consent to participate.

Consent for Publish All authors consent to publish.

Competing Interests There is no conflict of interest.

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