CIRCULAR ECONOMY APPLICATION IN DESIGNING SUSTAINABLE MEDICAL WASTE MANAGEMENT SYSTEMS



# A review on water simulation models for the WEF Nexus: development perspective

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## Abstract

The primary impediment to adopting the Water, Energy, and Food (WEF) Nexus is a lack of a comprehensive and userfriendly simulation model. According to our search on Google Scholar and the Scopus databank, WEF Nexus studies can be divided into three broad categories: (1) studies about the nexus concept, (2) studies related to nexus modeling and software development, and (3) case studies. Given that the present study's objective is to review various solutions for WEF Nexus modeling and also to prepare a checklist of available models to find a better model for nexus simulation, we excluded papers and studies which were related to the nexus concept. After that, we split up other papers that talked about nexus and software development into (1) integrated and (2) compiled approaches. Then, it was attempted to identify the shortcomings in each approach. It was shown that the existing integrated WEF Nexus models (such as MUSIASEM, NexSym, CLEW, and ANEMI) had some significant drawbacks compared to compiled alternatives. Several of the major shortcomings of existing integrated models include the following: (1) They did not cover all spatial scales; (2) they included only a limited number of interactions across WEF subsystems; and (3) some of these models were unavailable. Therefore, as a general result of the current study, it was shown that compiled approach is generally preferable compared to available integrated models. In this regard, we tried to find the best water simulation models to implement in the nexus concept. We searched for papers about water simulation models and defined water subsystem requirements in the nexus concept. So, we evaluated each water simulation model based on its ability to cover water subsystem requirements. This work illustrates the capability of a suitable water simulation model to be utilized in the nexus concept and provides a holistic checklist to choose the preferred water simulation model based on the needs of each issue.

 $\label{eq:constraint} \begin{array}{l} \mbox{Keywords} \ \mbox{Water-Food-Energy Nexus} \cdot \mbox{Sustainable development} \cdot \mbox{Integrated simulation} \cdot \mbox{Compiled simulation} \cdot \mbox{Water simulation} \ \mbox{model} \end{array}$ 

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## Introduction

Despite the progress made in recent decades, the development of human society has some restrictions, such that one-seventh of the world's population does not have food security and has limited access to treated water, new energy resources, and health (Mohtar and Daher 2016). From a global perspective, food crises, water scarcity, and limited energy are considered primary and fundamental hazards for the world. On the other hand, the increased population growth rate signifies more need for vital resources such as water, food, and energy.

Many efforts have been advocated to sustain human demands and resource potential (Liu and Chen 2020; Cansino-Loeza and Ponce-Ortega 2021; Hua et al. 2021).

As an illustration, Integrated Water Resources Management (IWRM) and Twin Track are two approaches for water management and food subsystem, respectively (Gain et al. 2013). It is worth noting that these one-dimensional models, which concentrate only on one subsystem, cannot consider the interactions between resources (Cansino-Loeza and Ponce-Ortega 2021), while water, food, and energy resources are inextricably connected (Leck et al. 2015). More precisely, actions taken in one sector have effects in other sectors (Ghodsvali et al. 2019; Molajou et al. 2021a). Many researchers believe that these one-dimensional approaches lost their capability to manage resources that have complex interconnections with each other (Hoff 2011; Hagemann and Kirschke 2017; Ravar et al. 2020; Ma et al. 2021). For example, IWRM is a water-centric strategy that focuses on water sustainability above food and energy sustainability. More specifically, when some policies and decisions are attended to one subsystem to attain sustainability and security, it is possible to overlook the sustainability of other subsystems.

Water-food-energy nexus (WEF Nexus) is a new paradigm to cope with the aforementioned problems (Daohan et al. 2019; Purwanto et al. 2021; Molajou et al., 2021b). Nexus expression indicates the existence of interdependent interactions between subsystems. Prior to the definition of the nexus framework, a number of its basic concepts had been employed in some studies. It should be mentioned that the nexus concept was first coined in 1970. Water-stressed South Africa identified the interaction of urban, energy, and industrial water needs as its critical focus (South Africa Commission of Enquiry into Water Matters 1970). Following that, in the 1980s, the United Nations project on energy-food interactions addressed the significance of the nexus concept, and then, the Second International Symposium on the Link between Food, Energy, and Ecosystems was held in India (Sachs & Silk, 1990). Also, it should be noted that according to research, studies of the nexus in the western USA in the mid-1980s had been focused on the connection between water and electricity (Scott 2011). By the early 1990s, these views had been formalized into IWRM as a step in the progression of the "development versus environment" debate. At the 1992 Dublin Conference, it was confirmed that codifying IWRM through a set of universal principles that prioritize water as a finite resource could increase stakeholder participation and treat water as a valuable economic good (Suhardiman et al., 2012).

From the mid-1990s to the early 2000s, the link between India's water, energy, and agriculture was studied by the Columbia Water Center at Columbia University (Scott 2011). The nexus framework was further developed with virtual water and water footprint concepts. Allan (1998) introduced the concept of "virtual water" as the water content embedded in food products and presented the "water footprint" to make the concept operational. After introducing virtual water and water footprint concepts, the nexus concept reemerged in the context of water and food to explain how regional water scarcity can be addressed by trade in food (Pandey and Shrestha 2017).

Eventually, a comprehensive definition for nexus was introduced at Bonn International Conferences in 2011. In this conference, nexus was defined as an approach to aggregate different administrative sectors to reach a green economy. This comprehensive approach can consider all three water, energy, and food (WEF) subsystems holistically and equally, which is called a multi-centered approach. In a multi-centered approach, the effects of action in one of the WEF resources can be evaluated on the other two resources (Molajou et al. 2021a). Also, it can diminish the repercussions of inappropriate policies by taking into account diverse interactions between subsystems on spatiotemporal scales (Hoff 2011).

Prior to the nexus approach, many managers prioritized their own benefits over those of other subsystems. For example, the primary and most important goal of the food subsystem was to increase crop production regardless of available water. It is obvious that this strategy results in severe problems in other subsystems. The nexus approach requires all managers in each subsystem to consider both their own benefits and those of other subsystems. The nexus approach seeks to accomplish each subsystem's objectives without jeopardizing the stability of the other subsystems.

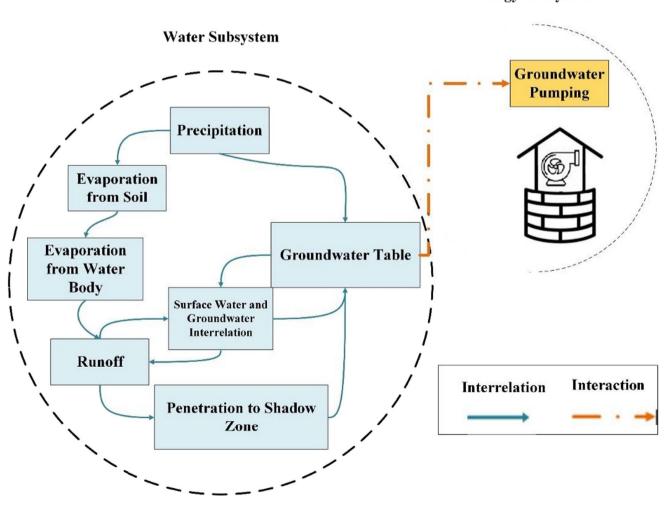
In light of the nexus's complex and dynamic nature, policymakers need mathematical models to measure different scenarios and assess the impact of changes on different components. Modeling provides a way of predicting the behavior or performance of proposed system infrastructure designs or management policies. Modeling also helps to better understand the behavior of one system over time and can assist in better managing vital resources (Loucks and Beek 2017). So, better modelling assists more accurate prediction of any possible scenarios in each subsystem and finally finds the best way to attain sustainability in all subsystems.

Numerous studies have attempted to implement nexus models (Smajgl et al. 2016; Wichelns 2017). However, researchers think there is a severe limitation that prevents the implementation of nexus models (Middleton et al. 2015). These limitations are largely reflected by considerable data and knowledge gaps and a lack of systematic analytical tools to apply nexus thinking effectively (Liu et al. 2017). We guess that the predominant problem in applying nexus modeling is the absence of a holistic and user-friendly model to assess the consequences of different strategies and scenarios.

A holistic nexus model should simulate interrelations within each subsystem as well as interactions between subsystems. Interrelations refer to the relationships that exist within each subsystem's boundary, while interactions refer to the mutual effects of one subsystem on another. It is critical to remember that interrelations and interactions have an effect on one another (Afshar et al. 2021). Both interrelations and interactions are critical components of nexus modeling, and ignoring them creates severe problems in implementing the nexus concept. For instance, it is necessary to simulate the most critical interrelations in the water subsystem to determine the groundwater table. More specifically, the groundwater table will fluctuate through the hydrological water cycle. When rain falls, it follows various paths like evaporation, runoff, penetration into the shadow zone, recharging rivers, and percolation into the groundwater. In the same vein, surface water and groundwater have interrelations with each other. The surface water and groundwater interrelation will be changed due to water cycle variation during different seasons. Sometimes, rivers recharge groundwater and vice versa. It is known that the groundwater table is an important element of the water subsystem for the energy subsystem, such that it determines the amount of energy demand for pumping (see Fig. 1).

As illustrated in Fig. 1, the interrelations in the water subsystem can change the groundwater table. So, if the groundwater table changes, the energy demand for pumping will be varied. It means that one interrelation in the water subsystem can change the interaction between water and energy subsystems. The pumping station is mentioned as one component of the energy subsystem in this example. It is obvious that the energy subsystem contains numerous other elements that must be considered in the nexus concept.

After introducing the nexus concept at the Bonn conference, many researchers have tried to develop some nexus models (Wang et al. 2018; Zisopoulou et al. 2018; Huang et al. 2020). These models include all subsystems on a single platform, and the main disadvantage is that they ignore most of the interrelations within each subsystem and only consider limited interactions with other subsystems. However, combining different water, food, and energy simulation models has played an important role in the fulfillment of the nexus concept (Yates et al. 2013; Siad et al. 2019; McCallum



**Energy Subsystem** 

Fig. 1 An example of the mutual effect of water subsystem interrelations and interaction with energy subsystem

et al. 2020). When different models are combined, interrelations in each subsystem are considered regarding involved stakeholders, and also the required interactions are remarked with other subsystems.

Therefore, it is obvious that using this new approach can help better estimate Nexus behavior and improve the management of vital and demanded resources.

To link models, it is crucial to find the best models in water, food, and energy subsystems to satisfy the nexus requirements and achieve its goal. In this study, we tried to introduce many frequently used water simulation models and then evaluate them to determine whether they are suitable to link with food and energy models in the nexus concept or not.

# Method

Figure 2 shows the current study's schematic flowchart. As illustrated in Fig. 2, in the first step, IWRM as a one-dimensional approach is compared with nexus. Step one emphasizes that regardless of whether IWRM is water-centric, it

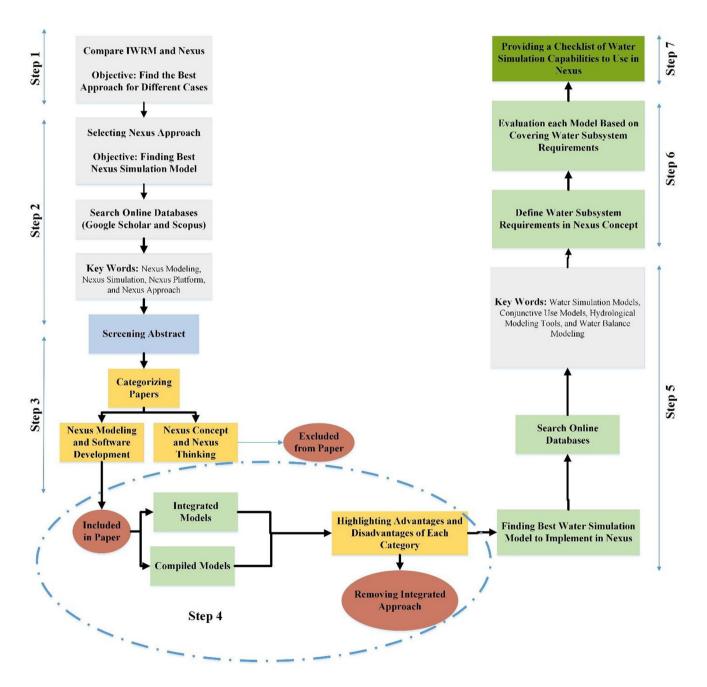


Fig. 2 Schematic flowchart of paper

may be the more appropriate approach in some cases due to their spatial scales or other factors. In this paper, we have tried to determine IWRM and Nexus differences such that decision-makers can find the best approach between them for specific cases. We also believe that it is necessary to clarify IWRM and Nexus differences to select the best nexus models. When IWRM is compared with nexus, some of its deficits are highlighted, which helps decision-makers select nexus models that do not have IWRM limitations.

The current study's primary goal is to review various solutions for WEF Nexus modeling and identify the best nexus simulation model based on the study target and desired scale. To achieve the current paper's objective, in step 2, we searched different keywords such as Nexus Modeling, Nexus Simulation, Nexus analysis, Nexus Platform, Nexus tool, and Nexus Approach in Google Scholar and Scopus databases. In step 3, we found that some papers are related to the nexus concept or nexus thinking, which are not suitable for helping to find the appropriate nexus model. So, we omitted them from our selection. After that, we categorized the remaining papers, which are related to nexus modeling and software development, into two classes: (1) integrated models and (2) compiled models. In an integrated approach, one model or framework is used to simulate the nexus concept, and interactions between subsystems are considered in each time step. However, in compiled approach, some models will be linked to each other to simulate all subsystems. For example, WEAP-LEAP (Water Evaluation and Planning-Long-range Energy Alternatives Planning) models are linked to assess both water and energy subsystems. So, we have to use some different water, food, and energy simulation models to use the compiled approach. The current study examines many frequently used water simulation models to implement the nexus concept.

The primary reason for categorizing the nexus model into integrated and compiled models is to make model evaluation easier. Because these two categories have inherent differences, such as their run time, the method considers the interactions between subsystems or the interrelation in each subsystem. For example, Nexus Tool 2 belongs to the integrated approach, while the combination of WEAP and LEAP models belongs to the compiled approach. Nexus Tool 2 cannot simulate each subsystem's interrelations and stimulate limited interactions between subsystems in each time step. In contrast, in 14-LEAP models, more interrelations are simulated and, as a result, the interactions with food and energy subsystems will be determined more accurately.

After investigating each category and their models' flaws, we think that integrated models are not suitable for the simulation of the nexus concept comprehensively. The main drawbacks of integrated models are as follows: (1) they do not cover all spatial scales, (2) they consider only limited interactions between subsystems, and (3) some of these

models are not available. Thus, the authors believe that using compiled approach is a more intellectual way to simulate both interrelations and interactions in the nexus system. In this regard, we continue our research to find the best water simulation model to implement in nexus.

In step 5, we explored keywords like "Water Simulation Models," "Conjunctive Use Models," "Hydrological Modeling Tools", and "Water Balance Modeling" in the database to select the most frequent water simulation models and their capabilities. Following that, it was attempted to evaluate the most frequently used water simulation models in related papers. Then, in step 6, we defined the most critical water subsystem requirements for incorporation into the nexus concept and evaluated water simulation models with these requirements included.

We can say that the current paper offers a perspective for decision-makers wishing to choose the water simulation model for use in the nexus concept. We believe that the final checklist can help decision-makers find the best water simulation model based on different scales, goals, and different components of each case to implement in the nexus. Also, decision-makers can get a better idea of the weaknesses of each model to use on the nexus and develop and fix them if needed.

It is essential to mention that investigating the capabilities of food and energy simulation models is beyond the scope of this study. In the following, both the nexus modeling approach are scrutinized, and their flaws in implementation in the nexus are highlighted. Finally, the best water simulation model is remarked.

## **Nexus following IWRM**

As mentioned earlier, there are some one-dimensional approaches to manage each subsystem. About the water resources subsystem, IWRM was a predominant approach for many years (Biswas 2008; Grigg 2008; Bielsa and Cazcarro 2015). IWRM approach was introduced at Mar del Plata Water Conference (Biswas 2008). Some scholars assert that IWRM was unsuccessful in fulfilling its intended goals (de Loë and Patterson 2017). One of the momentous criticisms about IWRM is the lack of consideration of government policy which has a notable effect on projects (Kurian et al. 2016). So, the nexus approach is suggested to resolve IWRM deficiencies (Abdullaev and Rakhmatullaev 2016). Both approaches consider interdisciplinary attitudes to tackle complex issues as their primary goal, and both are emanated from system thinking (Grigg 2019). Meanwhile, the two approaches have some differences. Regarding many papers on the IWRM and nexus approach, we found four criteria that signify the differences between IWRM and nexus: (1) priority for subsystems, (2) involved decision-maker, (3) spatial scale, and (4) attitude to sustainability (Hagemann and Kirschke 2017; Benson et al. 2015; Grigg 2019; Ibisch et al. 2016).

First, IWRM focuses on water management, and its main objective is to make water use more efficient for conflicting purposes, with the main focus on the water subsystem (Jeffrey and Gearey 2006). Not only does the nexus approach identify interactions, synergies, and conflict between subsystems, but also it considers the same priority for all subsystems (Kaufmann et al. 2010; Abdullaev and Rakhmatullaev 2016; Owen et al. 2018). The nexus concept is a well-known method for bringing together experts in different fields to solve cross-border and environmental issues, including scientists, researchers, physicians, decision-makers, and civil society (van Gevelt 2020). Second, decision-makers in IWRM encompass water managers, whereas in nexus, determining decision-makers due to nexus complex nature is not as easy as IWRM (Grigg 2019). Therefore, regarding spatial scale, various decisionmakers can participate in the nexus concept. Third, IWRM is suitable for watershed scale. In contrast, nexus can extend spatial scale even on the international and global scale (Gain et al. 2013). Finally, in IWRM, all decisions should be made based on efficient allocation and equitable access, but in nexus, decisions must satisfy economic facets (Benson et al. 2015). In Table 1, all differences are summarized.

Regarding Table 1, it can be concluded that the chief goal of IWRM is creating a linkage between upstream and downstream of the watershed. It means IWRM just considers water sustainability (Bielsa and Cazcarro 2015), while the nexus approach considers exogenous interactions between subsystems so that the nexus concept can fulfill sustainability in both water and food subsystems as well as energy subsystems. On the other hand, IWRM considers water subsystem interrelations and limited one-way interactions with two other subsystems. However, the nexus approach considers both interrelations in each subsystem and twoway interactions between subsystems. By providing Table 1, we want to put paramount importance on both IWRM and nexus approaches. In fact, there is no emphasis that nexus is a much better solution in all cases. More specifically, in small watersheds with few stakeholders and interactions

between water, food, and energy, the IWRM approach is an intellectual selection.

# Nexus modelling approaches

Based on the literature review, different nexus approaches can be classified into (1) integrated Models and (2) compiled models. Integrated models mainly simulate water-food and energy simultaneously, while compiled models incorporate different models to comprehensively evaluate WEF Nexus. There are some frequently used models for each approach, which are analyzed in the following sections.

#### Integrated approaches

Many computer models such as the Water-Energy-Food Nexus Simulation Model (WEFSIM), The Climate, Land, Energy and Water Systems (CLEW), Multi-Scale Integrated Analysis of Societal and Ecosystem Model (MUSIASEM), Water-Energy-Food Nexus Tool2, A New Model for Integrated Assessment (ANEMI), and Nexus Simulation System (NexSym) exist for an integrated approach. These models help decision-makers to evaluate different scenarios and find the best management scenario. The strength of these models is their simplicity. To be more precise, there is no need to have a strong programming language to use the integrated models. However, they have some severe flaws, which are explored in the following sections.

#### WEFSIM framework

WEFSIM framework assesses interactions between waterfood-energy resources based on input parameters. Analyzing interactions is based on the concepts of "actual availability" and "indirect demand." The modeling process is (i) gathering data, (ii) calculating demand, (iii) calculating potential resources availability, (iv) allocating resources, and (5) Calculating reliability index (Wicaksono et al. 2019, 2020). In the WEFSIM model, the interactions between WEF Nexus are considered, and the interrelations of each subsystem are neglected, so as far as we are concerned, the interrelations of each subsystem have severe effects on the interactions

Criteria	IWRM	Nexus
Priority	Water centric	Equal for WEF resources
Decision-makers	Water managers (due to limited spatial scale)	Dependent to spatial scale
Spatial scale	Watershed	Local to international
Attitude to sustainability	Efficient allocation Equitable access	Rational economic efficiency

Table 1Comparison betweenIWRM and nexus approaches

between them. This is known as the main flaw of the WEF-SIM framework.

## **CLEW framework**

CLEW framework is one of the most popular approaches, incorporating many models in different areas such as water resources, land use, energy, and weather (Hermann et al. 2012). CLEW is a bottom-up approach, and it can utilize diverse models like WEAP, MESSAGE, OseMosys, and AEZ (Ramos et al. 2020). As the WEAP model simulates the water subsystem in the lumped method, it is difficult to determine many interrelations in the water subsystem. Also, the MESSAGE model is an optimization model for energy, so there is a lack of simulation tools for energy in the CLEW framework. Therefore, the CLEW framework is not the best method for implementing nexus (Saif and Almansoori 2017; Engström et al. 2018; Almulla et al. 2018; Sridharan et al. 2020; Schlör et al. 2021).

#### **MUSIASEM framework**

MUSIASEM is a new tool that consists of economic systems theories and complex systems. This framework describes economic, social, and ecological systems. With the help of this framework, diverse scenarios can develop and evaluate to assist decision-makers (Giampietro et al. 2009, 2013). The main drawback of MUSIASEM is the absence of time series variables. MUSIASEM cannot consider the changes of different variables over time (Tabatabaie and Murthy 2021), and the user has to enter any constant variables which are required. So, MUSIASEM approach is not proper to plan for future events because it cannot predict any future events (Wang et al. 2017; Pérez-Sánchez et al. 2019; Rodríguez-Huerta et al. 2019; Cadillo-Benalcazar et al. 2020; Rosales-Asensio et al. 2020; Velasco-Fernández et al. 2020; Chen et al.2021; Manfroni et al. 2021).

#### WEF Nexus Tool 2

WEF Nexus Tool 2 can consider water, energy, land, local carbon footprint, and financial issues. It is a scenario-based model; somehow, each user can develop a new scenario by defining water, land, and energy elements. All scenarios will be compared with others based on sustainability indicators. The sustainability index is an indicator that identifies if a proposed scenario is suitable for adoption in the study area. This sustainability index is calculated based on resource requirements for a scenario (water, land, energy, finances, carbon) and importance factors for each subsystem defined by stakeholders (Mohtar and Daher 2016). WEF Nexus Tool 2 model is ideally assigned to Qatar country. On the other hand, all parameters are related to Qatar country, so

the WEF Nexus Tool 2 model cannot be used in other countries (Daher and Mohtar 2015). Apart from that, WEF Nexus Tool 2 considers limited interactions between resources.

#### **ANEMI** model

ANEMI first generation was an integrated tool for simulation of whole elements of nexus like water and weather cycle, carbon cycle, economic, land use, population, hydrological cycle, water demand, and water quality. After that, ANEMI 2 was developed to eliminate ANEMI drawbacks. So, ANEMI 2 added both food and diverse energy resources and used a dynamic system approach for simulation (Davies and Simonovic 2010). Lately, ANEMI 3 was introduced. The significant structural modifications of the ANEMI 3 include (i) implementation of the energy-economy system based on the principles of system dynamics simulation, (ii) incorporation of water supply as an additional sector in the global economy that parallels the production of energy, (iii) inclusion of climate change effects on land yield and potentially arable land for food production, and (iv) addition of nitrogen and phosphorus-based nutrient cycles as indicators of global water quality, which affect the development of surface water supplies (Breach and Simonovic 2021). The predominant flaw of the ANEMI 3 model is dismissing many interrelations in each of the subsystems. Actually, this flaw emanates from the system dynamic approach, which simulates many subsystems in the lumped method.

#### NexSym

The development of NexSym is supported by adapting a generic framework for modelling local production subsystems (Martinez-Hernandez et al. 2017). NexSym is envisioned as a tool for simulating processes and their interactions in local production subsystems. The modeling scope includes energy, water, food production, waste treatment, and interacting components important for the WEF Nexus, such as ecosystems, consumption, and other local system components (Martinez-Hernandez et al. 2017). The software platform is based on an Excel spreadsheet and Visual Basic for Applications (VBA). One main limitation of the NexSym model is its spatial scale which is just assigned to the local scale.

The nexus approach is a comprehensive concept that comprises many different aspects of sustainability, such as food, land, and climate sustainability. So, it is crucial to find the essential criteria to compare nexus models with each other to find the best model regarding decision-makers' purpose. Several studies have shown that most nexus research focuses on some fundamental elements, which are shown in Table 2 (Ringleret al. 2013; Simpson and Jewitt 2019). In the authors' opinion, these are the most important

Table 2 Capabilities of integrated nexus models	f integrated n	exus models	S							
	Criteria									
Name	Water	Food	Energy	Climate	Climate Land use Economic	Economic	Time vari- Scale ation	Scale	Simulation method	Accessibility
WEFSIM	x	×	X	1	I	I	I	National	System dynamic	I
CLEW	Х		Х	x	x	I	I	National-international	Mass balance	X
MUSIASEM	Х	Х	x		X	Х	I	Local-international	Flow fund	I
WEF Nexus Tool 2	Х	X	Х	X	x	X	I	National	Mass balance	Х
ANEMI	Х	Х	x	X	x	х	I	Global	System dynamic	I
NexSym	Х	Х	X	X	I	I	Х	Local	Dynamic model	Х

comparison criteria covering different aspects of the nexus, such as water, food, energy, and additional elements like land, climate, and economics.

To figure out if each of these models fulfills these criteria, we examined many papers that used these models to extract their capabilities. Also, in some cases that the aforementioned models have available web programs such as WEF Nexus Tool 2, we searched about the ability of models by investigating their sites.

In conclusion, the main problems of models which belonged to the Integrated category are (i) inadequacy for all spatial scales, (ii) dismissing all interactions between subsystems and just considering some of them, and (iii) Unavailability of these models or just covering some locations. For instance, WEF Nexus Tool 2 is suitable only for Qatar country. To address these deficits, we need to find a better solution. Compiling models is an alternative approach that aims to be more valuable and holistic.

## **Compiled approaches**

Another approach is used to consider all interrelations of each subsystem and most of the interactions between subsystems, which combines some models of different areas. In this approach, water, food, and energy models are simulated individually, and the result of one model is used as input for other models. A few recent studies are shown in Table 3, whose results are incorporated into the nexus framework. Although the main objective of the publications mentioned in Table 3 may not consider nexus interactions, one of the purposes of presenting these studies is to show that it is possible to link between these models and use them to implement nexus.

As shown in Table 3, it is crucial to simulate each subsystem individually then combine their results. In the current study, specifically, the ability of water subsystem models was investigated. The primary purpose of this study is to find the best water subsystem model to utilize in compiled approach.

## Water subsystem simulation models for WEF Nexus

In the last decades, water simulation models have been categorized differently (Jajarmizadeh et al. 2012). One of the most useful of these classifications divides water simulation models into (i) lumped, (ii)s emi distributed, and (iii) distributed categories. In the lumped approach, the whole watershed is considered a unique part. On the other hand, spatial parameters are constant for the entire watershed. Semi-distributed approach can be known as two types, the

	Nexus subsystems					
Compiled model	Water	Food	Energy	Publication		
WEAP-LEAP	Х	Х	X	(Yates et al. 2013; Dale et al. 2013, 2015; Lin et al. 2019; Fard and Sarjoughian 2020; Endo et al. 2020; Liu et al. 2021, Nasrollahi et al. 2021)		
WEAP-AquaCrop	Х	Х	-	(Dale et al. 2017; Kirshanth and Sivakumar 2018)		
SWAT-MODFLOW	Х	Х	-	(Libera et al. 2019)		
HYDRUS 2D/3D—AquaCrop	Х	Х	-	(Kanda 2019; Kanda et al. 2021)		
WEAP-LEAP-AEZ	Х	Х	Х	(Agrawal et al. 2018)		
SAWT-WOFOST-TerrSysMP	Х	Х	Х	(McCallum et al. 2020)		
WRFV.3.3-CLM4- AgroIBIS	Х	Х	-	(Siad et al. 2019)		
EPIC-SWAT	Х	Х	_	(Siad et al. 2019)		

Table 3 Compiled models for nexus framework

first models, which simulate some parts of the watershed as a lumped model, and the rest of the basin as a distributed model or models which divide the watershed into some smaller units and in each unit consider constant parameters. Finally, distributed models via division watershed to many cells consider spatial variation more. These cells can vary in size from 1 km<sup>2</sup> to the desired size. The primary goal of this approach is to simulate the water subsystem in a way that is more realistic. Hence, it is anticipated the lumped approach declines many important interrelations that can affect interactions and cannot be an appropriate approach for the water subsystem model, which is suitable for use in the nexus concept. In the following, this claim is more expanded.

The water subsystem has comprised a multitude of interlocked elements. Some of them have an interrelation with others, and some of them interact with food and energy subsystems. A proper water subsystem model to use in nexus should consider both important interrelations and interactions. For instance, evaporation or surface water interrelation with groundwater has a considerable impact on the quality and quantity of water resources. So, the suitable water subsystem model should be able to simulate evaporation, reservoir operation rules, water demand sites, and their withdrawal and return flows, the interrelation between surface water and groundwater, and qualitative simulation of water or at least simulate total dissolve solid, which is crucial for interactions with the food subsystem. Table 4 shows the most important interrelations in the water subsystem and their reasons to be selected.

As Table 4 shows, a proper water simulation model should simulate these important interrelations. Based on the author's research, these interrelations have significant impacts on the water subsystem and also can affect interactions with two other subsystems. Through the simulation of these interrelations, the interactions with other subsystems can be determined more precisely. For instance, when the reservoir operation rule is changed, the accessible water will be changed for irrigation sites, which is known as an interaction between the water and food subsystem. Another important interrelation in the water subsystem is the salinity which is important for the food subsystem, specifically for irrigation sites. So, all mentioned interrelations in Table 4 can change the quality or quantity of water and, as a result, change the water subsystem interactions with food and energy subsystems. In addition to these mentioned interrelations, there are fundamental interactions between WEF subsystems, which have been studied in many papers. Figure 3 shows significant interactions between WEF subsystems.

Researchers have shown that a comprehensive nexus simulation tool should simulate both interactions and

Table 4	Selected water
subsyste	em components

Water subsystem components	Reasons to be selected
Evaporation	Change the quantity and quality of water resources
Surface water routing	Change water level, consider return flow effects, consider reservoir operation effects
Groundwater simulation	Change groundwater head
Surface water and groundwater interrelation	Change amount of water level and groundwater head
Reservoir operation rule	Change the accessible water in demand sites
Water withdrawal	Change the quantity of surface water and groundwater
Quality simulation (salinity)	Determine desirable salinity for irrigation sites

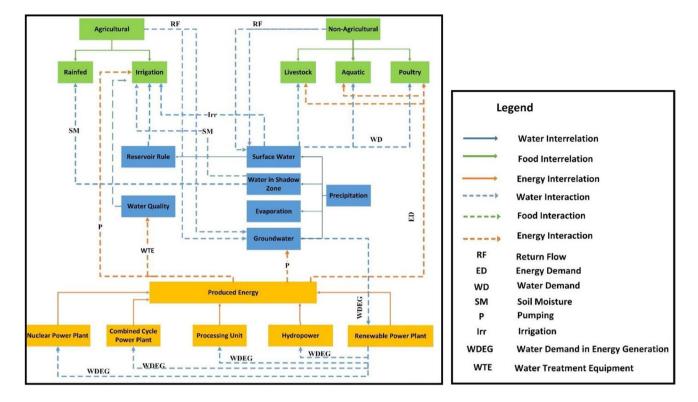


Fig. 3 Water-Food-Energy Nexus interactions adapted from Molajou et al. (2021a)

interrelations (Molajou et al. 2021a). In this regard, an appropriate water simulation model for use in the nexus concept would be able to take into account both the interrelations outlined above as well as the interactions presented in Fig. 3. In this study, some of the most well-known water models are presented, and their sufficiency for nexus is checked based on covering requirements of a proper water simulation model, which is mentioned in the "13" section. On the other hand, a suitable water subsystem model would simulate the mentioned interrelations in Table 4 as well as simulate the interactions with two other subsystems. So, in the following, some frequent-used water simulation models are evaluated regarding the interrelations and interactions they can simulate.

There are many different models to simulate the water subsystem. Based on the basic requirements of the water subsystem model in the WEF Nexus simulator, a good water simulator should simulate both surface water and groundwater. So, in the current study, we have tried to select water simulation models which are able to simulate both surface water and groundwater simultaneously or are able to link with other water simulations to consider both surface water and groundwater. Based on our research, Water Evaluation and Planning System (WEAP), Soil & Water Assessment Tool (SWAT), Precipitation Runoff Modeling System (PRMS), MODFLOW, MIKE SHE, HYDROGESPHERE, Groundwater and Surface Water Flow Model (GSFLOW), Parallel, Integrated Hydrology Model (PARFLOW), C2VSIM, Australian Water Resources Assessment (AWRA), and Community Water Model (CWatM) are the most useful models in recent years (Sulis and Sechi 2013; Soleimani et al. 2021), and we selected them to investigate. In the following, the advantages and disadvantages of these models will be discussed.

#### WEAP

WEAP software is a scenario-based simulation tool that can assess water subsystems through different developed scenarios. Stockholm Environmental Institute introduced this software in 1998 for the first time. WEAP can simulate water demand and supply, runoff, evapotranspiration, infiltration, irrigation demand, ecosystem services, water storage in groundwater and surface water, and operation rule for reservoirs (Tian et al. 2015; Kaddoura and el Khatib 2017). WEAP is an object-oriented model which is used in agricultural and rural systems in a basin or multireservoir systems (Ashrafi and Mahmoudi 2019). WEAP model belongs to the semi-distributed approach because it simulates groundwater as one uniform storage. WEAP cannot simulate surface water and groundwater interrelation, which is known as a severe problem of this model (Ahmadi et al. 2019).

#### SWAT

The SWAT model is a soil and water accounting tool that can simulate the quality and quantity of surface and groundwater. Also, SWAT predicts environmental impacts of land use, land management strategies, and climate change (Douglas-Mankin et al. 2010). It was first introduced in 1998 (Arnold et al. 1998) and developed by the United States Department of Agriculture. SWAT can simulate water and weather, surface runoff, return flow, infiltration, evapotranspiration, reservoir storage, crop growth and irrigation, shallow groundwater flow, sediment erosion, and transfer of pesticides (Douglas-Mankin et al. 2010). Surface water simulation is based on Hydrograph Response Unit (HRU). Each HRU has specific land use, management strategy, slope, and homogenous soil attributes (Guzman et al. 2015). So, SWAT is a semi-distributed model capable of simulating groundwater head in each HRU (Melaku and Wang 2019) or linking with a distributed groundwater model (Liu et al. 2019). The lack of simulation of reservoir operation rule limits the use of SWAT models in the nexus concept. Since the reservoir operation rule has an immense effect on the amount of water available downstream, ignoring it is a fundamental issue in the water simulation model.

#### MODFLOW

MODFLOW was introduced in 1984 by the United States Geological Survey. It simulates the quantity and quality of groundwater and considers surface water-groundwater interrelation. MODFLOW is a physic-based and fully distributed model. Because MODFLOW can simulate groundwater, it needs to be linked with other surface water models to be eligible for use in the nexus approach (Ahmadi et al. 2019).

#### Mike SHE

Mike SHE was introduced by System Hydrologic European in 1997 (Abbott et al. 1986). Despite many models, Mike SHE simulates all processes of the hydrologic cycle. This model encompasses two modules. First, the motion module considers evapotranspiration, water movement in the soil, surface water, and groundwater. Second, the water quality module simulates sedimentation, nutrients, and toxins (Golmohammadi et al. 2014). Mike SHE belongs to distributed models' category and needs huge data that, most of the time, are unavailable, so concerning immense required data and high model run time, Mike SHE cannot consider a suitable model for simulating water in the nexus.

#### HydroGeoSphere

The original name of this model is FRAC3DV which was created by René Therrien in 1992 (Therrien and Sudicky 1996) and then developed by the University of Waterloo and Laval University. Finally, in 2002, it was introduced as HydroGeoSphere. HydroGeoSphere simulates all processes of the hydrological cycle (Talebmorad et al. 2018). As a distributed model, HydroGeoSphere needs a vast amount of data. So, similar to Mike SHE, it is not a proper model for using in nexus (Brunner and Simmons 2012).

#### PRMS

PRMS is a semi-distributed rainfall-runoff model used for the evaluation of surface water. It simulates evapotranspiration, runoff, infiltration, and melting snow. This is an included model in 20 for simulation of surface water (Leavesley et al. 1983).

## **GSFLOW**

GSFLOW is a combined model for simulation of both surface water and groundwater presented in 2008 by The United States Geological Survey (Cundy and Tento 1985). In the GSFLOW model, both PRMS and MODFLOW are combined. As mentioned in the "19" section, PRMS is responsible for all processes on the surface, and MODFLOW simulates non-saturated and saturated zones (Markstrom et al. 2008). GSFLOW has five main parts: (1) simulation of evapotranspiration; (2) segmentation of rainfall to surface infiltration, surface flow, and shallow penetration; (3) routing surface water; (4) calculation of vertical flow in the non-saturated zone; and (5) simulation of groundwater in saturated zone (Markstrom et al. 2008). The most important flaw of GSFLOW to use in nexus are the absence of simulating operation reservoir rule and water withdrawal and return flow of demand sites.

#### PARFLOW

The development of PARFLOW was started by the Center for Applied Scientific Computing (CASC) in 1990 (Kuffour et al. 2020). PARFLOW simulates both surface water and groundwater as well as root zone. Also, it is possible to simulate water quality (Kollet and Maxwell 2006). PAR-FLOW can link with other models to simulate different processes on the land surface, underground and earth surface, and atmosphere (Kuffour et al. 2020). PARFLOW belongs to distributed model approach. The absence of simulation reservoir operation rules, groundwater pumping, and irrigation zone are the limitations of the PARFLOW model to use in the nexus concept (Maxwell et al. 2015).

## C2Vsim

C2VSim is emanated from California Central Valley Groundwater-Surface Water Simulation Model (CVGSM). It was introduced in 1990 for the first time, and then, it was developed and changed to C2Vsim (Brush et al. 2013). C2VSim simulates rainfall-runoff, deep percolation, water division system, groundwater pumping, and return flow. C2VSim is a distributed model and requires many data, so its application is limited. Besides, it is not able to simulate water quality (MacEwan et al. 2017). Since water quality can alter by water-food and energy interactions, it is crucial to be considered. Therefore, C2Vsim is not capable of implementing in nexus.

#### AWRA

Critorio

AWRA was presented by both the Commonwealth Scientific and Industrial Research Organization and Bureau of Meteorology in 2016. It encompasses AWRA-L for processes between atmosphere and land surface and AWRE-R for simulation surface water, groundwater, and subsurface flow (Hafeez et al. 2021). AWRA-L part is a semi-distributed model, which simulates evapotranspiration, runoff, soil moisture, groundwater recharge, infiltration, and drainage. AWRA-R is used for routing flow, flood modelling, irrigation modelling, surface water and groundwater modelling, storage routing, and simulating water use in urban consumption. AWRA is a semi-distributed model that is not apt to simulate water quality and reservoir operation rules. Besides

Table 5 Capabilities of water simulation model to implement in nexus

these flaws, AWRA uses satellite images as its input data. So, the accuracy of satellite images can affect the accuracy of model results.

## CWatM

CWatM was developed by the International Institute for Applied Systems Analysis (IISAS). CWatM simulates surface water, groundwater, reservoir operation rule, groundwater pumping, irrigation, return flow, snow melting, lake flow, evapotranspiration, and capillary rise. CWatM simulates groundwater with the linear reservoir method. On the other hand, it cannot simulate the water table and offers to link with some groundwater models like MODFLOW. Also, water quality simulation is not possible in the CWatM model (Burek et al. 2020).

Table 4 shows a summary of the capabilities of the different water simulation models to implement in the nexus concept. It is noteworthy to mention that the proper water simulation model should link with food and energy subsystems. So, in Table 5, in the last column, the publications which used these models in the nexus concept are mentioned.

As Table 5 shows, the WEAP model is rejected due to the absence of simulation surface water and groundwater interrelation and groundwater simulation. The SWAT model cannot consider reservoir operation rule and return flow, so it is not suitable to use in the nexus approach. In the MODFLOW model, there is a lack of surface water simulation. All models, like GSFLOW, PARFLOW, C2Vsim, and AWRA, are eliminated from the proper choices due to some reasons such

Criteria								
Publication	SW and GW interrelation	Qualitative simulation	Return flow	Reservoir operation	Evaporation	Groundwater	Surface water	Name
(Momblanch et al. 2019; Lin et al. 2019; Fard and Sarjoughian 2020; Guan et al. 2020; Liu et al. 2021)	_	Х	Х	Х	Х	-	Х	WEAP
(Karabulut et al. 2016; Schull et al. 2020; Corona-López et al. 2021; Shrestha et al. 2021; Zhang and Ren 2021)	Х	Х	-	-	Х	Х	Х	SWAT
(Nazari et al. 2015)	Х	Х	_	_	_	Х	_	MODFLOW
(Sishodia et al. 2018)	Х	Х	Х	Х	Х	Х	Х	Mike She
-	-	Х	Х	Х	Х	Х	Х	HydroGeoSphere
(Sun et al. 2018)	Х	Х	-	-	Х	Х	Х	GSFLOW
-	Х	Х	-	-	-	Х	Х	PARFLOW
(Alam et al. 2019)	Х	-	Х	-	Х	Х	Х	C2Vsim
-	Х	_	Х	_	Х	Х	Х	AWRA
(Burek et al. 2020)	Х	-	Х	Х	Х	Х	Х	CWatM

as the absence of simulation reservoir operation rule or massive required data. Therefore, among water simulation models investigated in the current study, HydroGeoSphere and CWatM are more capable of simulating all interrelations and interactions of the nexus system. However, HydroGeoSphere is not as suitable as CWatM because HydroGeoSphere cannot simulate surface water and groundwater interrelation. It is essential to mention that Table 5 shows which water simulation models have been used in the nexus approach, and if some models do not have any references, it means that based on our research, they have not been used in the nexus concept up to now.

## Conclusion

Water resources issues can be addressed in a variety of ways. Some of these approaches are known as the one-dimensional approach, which considers water the main component, and researchers call them water-centric approaches. IWRM is one of the most well-known one-dimensional approaches. In contrast, multi-centric approaches consider more than one subsystem and consider the same priority for all subsystems. The nexus approach is known as a multi-centric approach. The nexus approach is reliable to attaining sustainability among demand and supply of WEF resources. Both approaches are rational, and decision-makers must decide which is best for their problem in terms of scale, components, and other considerations. In this regard, a holistic comparison between IWRM and nexus is mentioned to help decision-makers find the best approach for their problems.

The concept of nexus as a solution to the existing water, food, and energy crises has received more attention. The lack of a comprehensive tool that can simulate both interrelations and interactions of nexus and also be able to implement in different spatial scales has been known as a severe problem. In the current study, we searched different keywords about nexus. Then, nexus models were categorized into two main approaches-first, integrated models, and second compiled approach. This classification aims to facilitate the comparison of different models so that we may find the best model to simulate nexus. As mentioned before, integrated models cannot simulate all interrelations of each subsystem, and most of them are usable for specific spatial scales and cannot cover local to an international scale. So, a combination of diverse models, called a compiled model, is a better way to investigate more interrelations in each subsystem. Here, in 12 specifically was discussed water models, proper water simulation model should be able to simulate the necessary interrelations of the water subsystem and interactions with two other subsystems simultaneously. We searched the water simulation models in Google Scholar and Scopus databank and selected their repeated and most frequently used of them to investigate.

In the "13" section, we introduced water subsystem requirements in the nexus concept. According to our research and knowledge, these requirements represent the most significant interrelations in the water subsystem, which affect interactions with other subsystems. Hence, in determining the best water simulation model to use in the nexus concept, the model should include all these interrelations.

The selected water simulation models are evaluated based on covering water subsystem requirements. Finally, we provide a checklist to compare different water simulation models. Using this checklist, we believe decision-makers can find the best water simulation models regarding their preferences and specific goals. Based on our research, GSFLOW, PARFLOW, C2Vsim, and AWRA models are rejected due to some reasons, such as the absence of simulation reservoir operation rule and massive required data. The SWAT model cannot consider reservoir operation rule and return flow. The WEAP model is rejected due to the absence of simulation surface water-groundwater interrelation and groundwater simulation. MODFLOW cannot simulate surface water. Therefore, among water simulation models investigated in the current study, HydroGeoSphere and CWatM are more capable of simulating all interrelations and interactions of the nexus system. However, HydroGeoSphere is not as suitable as CWatM because HydroGeoSphere cannot simulate surface water and groundwater interrelation. To our knowledge, this is the first attempt at classifying nexus approaches and analyzing each one.

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**Data availability** The authors declare that the data are not available and can be presented upon the request of the readers.

#### Declarations

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