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Water-energy-food-health solutions & innovations for low-carbon, climate-resilient drylands

Edited by
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Water-energy-food-health solutions & innovations for low-carbon, climate-resilient drylands

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Editorial: Water-Energy-Food-Health Solutions and innovations for low-carbon, climate-resilient drylands

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Editorial on the Research Topic
Water-Energy-Food-Health Solutions and innovations for low-carbon, climate-resilient drylands

We live in a world of complex and tightly interconnected grand challenges that threaten the sustainability of our societies. Examples of such challenges are summed up in the United Nations Sustainable Development Goals (UN-SDGs), which include specific goals to address water, energy, and food insecurities. Our ability to address these challenges depends on our readiness to collaborate across disciplines and sectors to reimagine thriving, healthy, resilient societies that respect the boundaries and health of our planet. As nations work toward implementing the UN- SDGs, we need to support decision makers, create synergies, and avoid unintended competition between societal goals. Thus, the urgent need for innovative simulation and assessment tools and governance models to represent these complex systems in an accessible manner.

Drylands face important resource gaps including access to water, food, energy, nutrition, and healthcare. These gaps are expected to increase with demographic conflicts and climate change. The highly interlinked primary resources carry high risks and vulnerabilities. Understanding these interlinkages and associated risks and vulnerabilities to better comprehend the complex system of systems they represent is crucial and requires multi-disciplinary work that encompasses technologies, science, policies, health, communication, and socioeconomics at both local process and system-level scales.

In 2018, the American University of Beirut (AUB) launched WEFRAH: the Water-Energy-Food- Health Nexus of Renewable Resources initiative. WEFRAH comprises one of the largest research communities in the Middle Eastern North Africa (MENA) region. It is a university-wide initiative led by the Faculty of Agricultural and Food Sciences. WEFRAH includes a critical mass of faculty from disciplines across the University whose focus is collaboration to achieve security of primary resources. Its core conviction is achieving water, energy, and food security, improving health, harmonizing humans with nature, and implementing integrated solutions that require holistic, system-level thinking.

This Research Topic presents some of the collaborative research outcomes from the WEFRAH community. It also honors Professor Rabi H. Mohtar, Department of Biological and Agricultural Engineering, Texas A&M University. Mohtar's leadership of multiple initiatives during his interdisciplinary career has resulted in seminal contributions to the development of Water-Energy- Food nexus research, education, and engagement globally.

The 2021 annual symposium of the American Chemical Society (ACS), Toward Creating a Water- Energy-Food Nexus Community of Practice - A Symposium in Honor of Professor Rabi H. Mohtar, included invited and contributed oral and poster sessions, with multi-stakeholders from academia, private, civil society, and public sectors. The symposium focused on the various thematic areas related to operationalizing WEF nexus research and development, and highlighted lessons learned from cross-disciplinary collaborations using national and global case studies in this research space. The symposium focused on the opportunities that lie in creating a cross-cutting and inclusive WEF nexus Community of Practice and the role of existing disciplinary societies in that Community.

Research Topic of the WEFRAH Initiative and of the ACS symposium included.

- *Water-Energy-Food-Health nexus and the Sustainable Development Goals*
- *Sustainable food production systems*
- *Renewable energy and sustainable agri-food systems*
- *Building systems thinking and leadership capacity*
- *Behavioral changes towards sustainability in the Water–Energy–Food Nexus*
- *Governance of the Water–Energy–Food Nexus*
- Introductory perspective to the Nexus in drylands
- *Approaches to integrate the WEFH nexus in drylands*
- Health as a resource and its contribution to the Nexus
- *Circular and Sustainable food production systems*
- *Antibiotics and other contaminants fate in the environment (soils, water, and plants) and technologies for their removal*
- *Food or water waste management*
- *Building climate resilience in drylands*
- *Climate smart agriculture in drylands*

This Research Topic represents these contributions, and a synthesis is offered below.

Nuwayhid and Mohtar highlight the ways in which health is included in the nexus literature and argue for its inclusion in the WEF nexus conceptualization and definition. They note that, despite the relatively short history of the WEF Nexus as a discipline, it has been adopted by many international agencies. Including health as part of the resource nexus is timely.

Ramos et al. present the SIM4NEXUS approach to address a gap in the Nexus research and introduce comprehensive, transferable, accessible methodologies with operational potential. SIM4NEXUS, a project funded by the European Commission under the Horizon 2020 programme, investigated the Water-Energy-Food-Land and Climate (WEFLC) Nexus. SIM4Nexus was operationalized in twelve Case Studies of differing spatial scope, socioeconomic, and biophysical contexts, and thus, differing Nexus challenges. They found that trans-disciplinarity and integration of qualitative and quantitative methodologies are vital elements for policy support in Nexus assessments. They propose steps to advance Nexus assessments that include integration of the policy cycle in research, multidisciplinary collaboration, and inclusion of ecosystems.

Jalloul et al. present a review of the contamination of irrigation water with tetracycline (TC), its impact on edible crops, and associated health risks. They propose a solar-mediated photocatalytic degradation using a Titania-based photocatalyst to remove the antibiotic from irrigation water and highlight the methods as efficient, cost effective, and ecofriendly photocatalysts for degrading TC in irrigation water.

Ioannou and Laspidou study the impact of climate change on water–energy–food security. They present a resilience policy analysis framework for a water–energy–food nexus system under climate change in Greece. They performed parametric sensitivity analysis for socioecological systems in a case study based on the structure of a system dynamics model. The model maps sector-specific data from major national and international databases using engineering and ecological resilience metrics, then quantifies system resilience and identifies policies that increase system resilience.

Mohtar presents an historical background of the Nexus journey, beginning in a Purdue University classroom, continuing to the World Economic Forum and promoting the concept among decision makers and industry leaders. He describes how the Nexus emerged into the discipline that it is today, offers definitions, success stories from around the world, and reflections on the future of the Nexus.

Jalloul et al. investigate photocatalytic degradation as a potential treatment of tetracycline (TC) antibiotic-contaminated water using a TiO_2 semiconductor sensitized with Fe ions and immobilized beta (BEA) zeolite support. They showed improved TC adsorption resulting from the expanded surface area due to the immobilization of the TiO_2 on the BEA zeolite. They also showed that the presence of Fe3+ ions reduces the band gap energy of the TiO_2, leading to a red shift in its absorption spectrum to the visible light region, minimizing the extent of recombination of the charge carriers.

Mohtar et al. present key messages and conclusions from the ACS Environmental Chemistry Symposium honoring his contribution to the field. It includes anticipated challenges and opportunities as we move toward establishing a resource-nexus community of science and practice and outlines the roles of chemistry and chemical processes in understanding the interlinkages of nexus systems. The paper proposes including the resource of health, highlighting major challenges and opportunities in the Water-Energy-Food-Health-Ecosystems (WEFH) Nexus, and highlights future steps for fostering dialogue among this broad, multidisciplinary, multi-stakeholder community as it moves toward establishing an inclusive community of science and practice.

Mohtar and Fares present a new, more sustainable approach to water-for-food reduction and identify inter-dependencies between food and fresh water by exploring new and alternative sources of water, including improved efficiencies of green and recycled water.

Karam et al. create a novel image generation tool, made publicly available, to detect pests on plant leaves. Early and accurate detection of plant pests will allow both small and large-scale farmers to treat the plants in a timely manner, thus improving crop yield. In addition, the work proposes the use of a novel Generative Adversarial Networks (GANs)-based pseudo-automated pipeline for data augmentation, thereby leveraging synthetic data generation to increase dataset sizes, decrease data Research Topic, and improve performance of lightweight Convolutional Neural Networks (CNNs) for detecting and counting large numbers of small pests on plant leaves.

Muell et al. develop and evaluate a Water-Energy-Food-Waste nexus-based analysis and resource allocation tool to evaluate the economic, environmental, and social feasibility of the Closed-loop dairy system. The study shows that the closed-loop dairy system can be profitable for dairy farms of 200 cows or more.

Daher et al examine the resilience of resource systems in Lebanon and show how the Water-Energy-Food (WEF) Nexus can help us understand the dynamics of the interactions of this system. The paper explores some of the underlying political and economic challenges and the impact of climate and socioeconomic shocks and triggering events on the interconnected resource systems. The paper identifies emergent themes, including decentralization and systems thinking and their roles as catalysts toward more resilient resource systems. It also highlights the opportunities that lie in creating platforms for integrative resource planning and decision making, as well as empowering decentralized initiatives at the local level to build resilient, bottom-up solutions to WEF challenges.

Antukh et al (2022) present a review of currently available biogas upgrading technologies for anaerobic digestion (AD) of waste biomass. They highlight biological technologies, especially a hydrogenotrophs-based one, that would be more cost-effective and sustainable in upgrading biogas produced by an AD system.

Author contributions

RHM, MA, BD, CL, HK, and VS all made substantial contributions to the conception and design of the work and to drafting and revising it for important intellectual content.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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Antibiotics Contaminated Irrigation Water: An Overview on Its Impact on Edible Crops and Visible Light Active Titania as Potential Photocatalysts for Irrigation Water Treatment

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Sub-therapeutic levels of antibiotics (ABs) are given to animals and poultry to promote growth and reduce disease. In agricultural environments, ABs reach croplands *via* animal manure used as fertilizer and/or ABs-contaminated water used for irrigation. The continuous discharge of ABs into the ecosystem raises growing concerns on the ABs contamination of edible crops. Tetracyclines (TCs) are among the most widely used ABs around the world. In this review, we discuss the contamination of irrigation water with TCs, its impact on edible crops, and the potential risks of crop contamination with TCs on human health. We propose solar-mediated photocatalytic degradation using Titania (TiO_2) photocatalyst as a promising method to remove TCs from irrigation water. The photocatalytic activity of TiO_2 can be enhanced by chemical modification to expand its activity under visible light irradiation. Herein, we aim for providing literature-based guidance on developing a visible light–active TiO_2-based system to degrade TCs and other ABs in water streams. We include a summary of recent advances on this topic based on three main modification methods of Titania: metal/non-metal/mixed doping, composite formation, and heterojunction construction. Among the investigated photocatalysts, Fe_2O_3-TiO_2/Fe-zeolite and the N-doped TiO_2/rGO immobilized composite catalysts were found to be very efficient in the degradation of TCs under visible light irradiation (i.e., 98% degradation within 60 min). Most immobilized TiO_2 based composite systems exhibited improved performances and hence we highlight these as efficient, cost effective and ecofriendly photocatalysts for the degradation of TCs in irrigation water.

Keywords: antibiotics, crops, photocatalysis, TiO_2, irrigation water

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1 INTRODUCTION

Fresh water scarcity is an urgent global issue. Only (4%) of water on earth is fresh, and increasing global population, climate change, urbanization, and over exploitation continue to contaminate this scarce resource (Gothwal and Shashidhar, 2015). Pharmaceutical and organic chemical contamination of water is a critical threat to the natural ecosystem and public health (Zeghioud et al., 2016). Amongst these pharmaceuticals, antibiotics (ABs) are a major concern (Anjali and Shanthakumar, 2019). ABs are natural or synthetic antimicrobial compounds used to treat bacterial infections in humans, animals, and plants by inhibiting or killing bacterial growth (Daghrir and Drogui, 2013; Anjali and Shanthakumar, 2019; Danner et al., 2019). ABs have efficacious applications in human and veterinary medicine; however, sub-therapeutic AB levels are routinely given to animals and poultry to promote growth (Gothwal and Shashidhar, 2015). In agricultural environments, these ABs reach croplands *via* animal manure used as fertilizer and/or the use of AB-contaminated irrigation water (Anjali and Shanthakumar, 2019; You et al., 2019).

The escalating use of ABs and their continuous discharge into the environment results in frequent detection of ABs in different environments, with concentrations of ng/L–mg/L in wastewater (Pan and Chu, 2017). Wastewater is commonly used for irrigating agricultural lands due to the scarcity of fresh water. There is evidence from greenhouse and field experiments that irrigating crops with ABs-contaminated water leads to crop contamination; studies performed on different edible crops (lettuce, cucumber, spinach, and pepper) using different groups of ABs detected these ABs in plant leaves and roots (Pan and Chu, 2017).

Bioaccumulation of ABs in edible crops and in water environments lead to potential risks to human health. The proliferation of ABs in the environment led to the emergence of antibiotic resistant bacteria and antibiotic resistance genes (Singh et al., 2019). Antibiotic resistance is defined as the ability of the target microbe to resist the action of the antibiotic drug that previously caused cell death. In human health, antibiotic resistant bacteria cause untreatable infections and increased mortality (Chen M. et al., 2019; Singh et al., 2019). Human consumption of ABs-contaminated edible crops and drinking water poses major health risks due to the potential antibiotic resistance transfer to human pathogens (Sponza and Koyuncuoglu, 2019). Current reports indicate that antibiotic resistance is an urgent health-threatening issue, causing 0.7 million deaths/year and estimated to grow to 10 million deaths by 2050 (Singh et al., 2019).

There are currently 250 different antibiotics classified in seven groups (Anjali and Shanthakumar, 2019). Tetracyclines are reported as the second most widely used AB group worldwide (Xu L. et al., 2021). Tetracyclines are a group of ABs that include chlortetracycline, oxytetracycline, tetracycline hydrochloride, and tetracycline (Daghrir and Drogui, 2013). Tetracyclines have gained specific attention due to their wide use in medical, agricultural, and poultry sectors, and due to their poor adsorption in humans and animals and high stability in soil and wastewater (Saadati et al., 2016a). For example (50–80%), of the tetracycline consumed by humans/animals is excreted through urine and feces, and they are stable in wastewater for 34–329 h due to their low volatility and high hydrophobicity (Daghrir and Drogui, 2013; Xu L. et al., 2021). Sources for tetracyclines discharge include pharmaceutical industries, farms, homes, and hospitals. Hence, the occurrence of these ABs in the environment is proportional to the economic status of the country and the size of the livestock and the pharmaceutical industries. On the other hand, TCs discharge into the environment is also a consequence of the inefficiency of the current water treatment technologies used in removing these ABs (Christou et al., 2017; Pan and Chu, 2017). Particularly, tetracyclines are detected in the low (μg/L) level in municipal wastewater, in the high (μg/L) level in hospital wastewater, and in the (ng/L) level in underground, surface, and sea water (Homem and Santos, 2011). Although these concentrations appear low, they still impose risks to human health and the ecosystem *via* the potential development of antibacterial resistance (Danner et al., 2019).

Numerous studies have worked to develop efficient methods for removing ABs and specifically tetracyclines from water streams to eliminate potential threats to the ecosystem and humans (Saadati et al., 2016a; Minale et al., 2020). Removal technologies include adsorption, conventional technologies (biological processes, coagulation, flocculation, sedimentation, and filtration), membrane processes, chlorination, and advanced oxidation methods such as photolysis, electrochemistry, and photocatalysis (Homem and Santos, 2011; Wei et al., 2020). However, most of the conventional technologies such as the biological methods, filtration, coagulation/flocculation/sedimentation, and membrane processes suffer from the drawbacks of low efficiency, low degradation rate, incomplete mineralization, and high toxicity (Homem and Santos, 2011; Anjali and Shanthakumar, 2019). Solar light–activated photocatalytic degradation of ABs is an efficient, safe, residue-free, economical, and ecofriendly method to remove tetracyclines from wastewater, especially under visible light and ambient conditions (Homem and Santos, 2011; Wei et al., 2020). Various semiconductors and photocatalysts have been investigated for the photocatalytic degradation of tetracyclines including ZnO, TiO_2, WO_3, CdS, Fe_3O_4, g-C_3N_4, ZnS, and Bi_2O_3 (Niu et al., 2013; Zhu et al., 2013; Zhang et al., 2014; Li et al., 2015; Vázquez et al., 2016; Wang T. et al., 2017; Yan et al., 2020). Semiconductors based on Titania (TiO_2) are the most widely studied catalysts due to their low cost, high stability, low toxicity, good activity, and ease of modification (Teoh et al., 2012; Ibhadon and Fitzpatrick, 2013; Koe et al., 2019; You et al., 2019; Zhang et al., 2019). However, the photocatalytic activity and application of TiO_2 is limited to the UV region of the light spectrum (200–400 nm), and further modifications are needed to expand its activity into the visible light region (400–700 nm). Recently, immense efforts have been dedicated for TiO_2 modification to expand its activity to the visible light region, and several modification methods and approaches have been reported (Basavarajappa et al., 2020).

This review discusses the escalating use of ABs; their continuous discharge into the agroecosystems contaminating both the soil and water; and the risks associated with using wastewater for crop irrigation. We present a summary of the latest literature studying the impact of ABs-contaminated irrigation water on the quality of edible crops and potential consequences for human health. Current research indicates that the use of ABs-contaminated irrigation water has potential risks to humans and ecosystems, and highlights an urgent need to develop efficient irrigation water treatment technologies. Here, we focus on tetracyclines degradation under visible light using TiO_2-based photocatalysts, and present a detailed summary of the latest advances in Titania modification to enhance its visible light activity for the photocatalytic degradation of tetracyclines in water. We identify the most efficient catalysts and discuss their advantages and disadvantages. For literature collection, we focused on studies investigating modified Titania-based catalysts for the photocatalytic degradation of tetracyclines under visible light irradiation between 2011 and 2021. We chose to discuss the three most reported modification methods; metal-nonmetal, mixed metal-nonmetal doping, TiO_2-based composite formation, and TiO_2-based heterojunction construction. For TCs presence in the environment, we adopted numerical data from recent studies which assessed the occurrence of TCs in various water media and their bioaccumulation in edible crops.

2 IMPACT OF ABs-CONTAMINATED IRRIGATION WATER ON EDIBLE CROPS AND POTENTIAL RISKS FOR HUMAN HEALTH

Fresh water scarcity has led to the reuse of wastewater for crop irrigation. Approximately 20×10^{10} m^2 of global agricultural land is irrigated with treated wastewater (Raschid-Sally and Jayakody, 2008). Countries that extensively use reclaimed water for irrigation include Australia, Columbia, United States, and China (Gudda et al., 2020). Conventional water treatment methods (coagulation, flocculation, sedimentation, and filtration) and biological treatment methods are only moderately effective in removing low concentrations of persistent organic contaminants such as antibiotics. Generally, these methods have very low efficiency in removing ABs from wastewater, and the efficiency depends on the physiochemical properties of the AB to be removed and the operating conditions of the treatment system (Pan et al., 2014; Christou et al., 2017). The use of reclaimed wastewater for crop irrigation introduces these organic contaminants into the soil and ultimately to crops.

Antibiotics have been detected in diverse edible crops. For example, in Minnesota, United States, sulfamethoxazole was detected in *Lactuca sativa* (lettuce) at concentrations of 100–1,200 μg/kg tissue (Christou et al., 2017). In Tianjin, China, tetracycline and sulfamethoxazole were detected in spinach and radish at concentrations of 6.3–330 μg/kg tissue (Hu et al., 2010). In the Pearl River delta, China, tetracyclines were detected in cabbage and *Ipomoea aquatica* (water spinach) at concentrations of 6.6 and 7.4 μg/kg tissue, respectively (Pan et al., 2014).

Several studies investigated the impact of ABs-contaminated irrigation water on the uptake of the crops of these contaminants. Both greenhouse (pot) and field experiments were reported. Herein, we present results of some of these experiments. In the summer of 2020, we conducted pot experiments to evaluate the accumulation of gentamicin and oxytetracycline in three crops that are consumed fresh, including radish, lettuce, and cucumber (Imad Keniar et al., 2021). The crops were irrigated with 20 mg/L of each of the studied ABs. After harvesting, these ABs were detected in crop extracts using ELISA. The results detected gentamicin accumulation up to 13, 16, and 18 ng/g in cucumber, lettuce, and radish, respectively, whereas oxytetracycline accumulation was less than 3.0 ng/g in all three crops. Azanu et al. (Azanu et al., 2016) evaluated the accumulation of tetracycline and amoxicillin in potted lettuce and carrot irrigated with water containing known concentrations of 0.1–15 mg/L of tetracycline and amoxicillin. ABs were extracted from lettuce leaves and carrot tubers using accelerated solvent extraction, and then analyzed using liquid chromatography-tandem mass spectrometry. Tetracycline was detected in concentrations ranging between 4.4 and 28.3 ng/g in lettuce, and 12–36.8 ng/g in carrots. Whereas, amoxicillin was detected in concentrations ranging between 13.7 and 45.2 ng/g in both crops, which indicated that the amoxicillin uptake by lettuce and carrot was significantly higher than that of tetracycline. Hussein et al. (Hussain et al., 2016) conducted a field study in Lahore, Pakistan, which irrigated wheat, spinach, and carrot using pharmaceutical wastewater. The results showed that each of these crops accumulated 0–1 ng/g tissue of ciprofloxacin, ofloxacin, levofloxacin, oxytetracycline, and doxycycline.

Current data provide clear evidence that the use of ABs-contaminated irrigation wastewater can contaminate the soil and ultimately lead to ABs accumulation in edible crops. The extent of plant uptake of ABs from contaminated water depend on the type and concentration of the AB, its water solubility, sorption potential, and lipophilicity (Azanu et al., 2016). A clear understanding of AB bioaccumulation in crops and their ecotoxicological effects requires greater knowledge of the physiochemical properties of ABs in the soil and the mechanism of their translocation and bioaccumulation in plants (Pan and Chu, 2017). Field studies are necessary to accurately assess ABs uptake by various crops under different environmental conditions, and determine the impact of ABs accumulation in these crops (Pan and Chu, 2017).

Excessive use of treated wastewater in agriculture is increasing the risk of transmitting AB resistant pathogens/genes to the crops, which could potentially be transferred to the human microbiome through the food chain (Gudda et al., 2020). The level of this risk on human health will depend on the level of exposure to these contaminated crops through consumption. Pan et al. (Pan and Chu, 2017) proposed that human exposure to ABs through annual consumption of edible crops grown in manure-amended or wastewater-irrigated soil is likely to be low. For example, assessments of annual human exposure to different ABs through consumption of various crops in China indicated that consumption of corn and rice led to the highest AB exposure. The daily human exposure to tetracyclines, quinolones, and chloramphenicol was assessed as (0.34–2.77 μg) and (11.0–21.8 μg) *via* consumption of corn and rice, respectively. These values remained lower than the recommended acceptable daily intake (20–200 mg/day) of these ABs. However, a comprehensive analysis of the impact of AB-contaminated edible crops on human health is lacking. This would require

TABLE 1 | Maximum detected tetracyclines concentrations in different environments and different countries (Pan and Chu, 2017).

Antibiotic	Wastewater (μg/L)	Soil (μg/g)	Manure (μg/g)	Biosolid (μg/g)	Plants (μg/g)
Tetracycline	254.820	0.178	43.500	0.513	0.0101
Country	Korean	Korean	China	Canada	China
Oxytetracycline	1.236	2.683	183.500	0.7436	0.330
Country	South Korean	China	China	United States	China
Chlortetracycline	444.20	107.9	268.00	0.3466	0.532
Country	Korean	China	China	United States	China

well-defined dietary studies to develop human exposure models and further integrate those models with disease outbreak analysis and clinical data. This will help estimate the relationship between the ingestion of AB resistant pathogens and their impact on human defense mechanisms and health (Pan and Chu, 2017; Sanganyado and Gwenzi, 2019).

3 TETRACYCLINES OCCURRENCE IN WATER ENVIRONMENTS

This review focuses on the tetracyclines group as model ABs. Tetracyclines are one of the most prescribed ABs in human and animal infectious therapies due to their wide antimicrobial spectrum and low cost (Minale et al., 2020; Xu L. et al., 2021). Tetracyclines are extensively utilized as fertilizers and growth promoters in animal husbandry and agricultural industries (Daghrir and Drogui, 2013). Approximately (70%) of locally produced antibiotics are used for non-medical applications in the United States, and 4,200 tons of tetracyclines are utilized only in the agricultural industry (Xu L. et al., 2021). Tetracyclines have poor adsorption in humans/animals and high stability in soil and wastewater (Saadati et al., 2016a). For example (50–80%), of tetracyclines consumed by humans/animals are excreted through urine and feces, and after discharge into aquatic media, they are stable for 34–329 h due to their low volatility and high hydrophobicity (Daghrir and Drogui, 2013; Xu L. et al., 2021). AB contaminants are also persistent in soil and slowly degrade; for example, it took 90 days to degrade (44–75%) of the initial tetracycline concentration in a sterilized soil (Pan and Chu, 2017). Tetracyclines are released into the environment through animal manure, biosolids, sewage discharge, pharmaceutical wastewater, and the use of ABs-contaminated wastewater for irrigation (Pan and Chu, 2017). The AB concentration in each medium is directly related to the pollution source(s) and their distance from the medium. Tetracyclines are detected at low μg/L concentrations in municipal wastewater, at high μg/L concentrations in hospital wastewater, and at ng/L concentrations in underground, surface, and sea water (Homem and Santos, 2011). Although these concentrations seem rather low, they still carry risks for human health and the ecosystem through the development of antibiotic resistant bacteria and antibiotic resistance genes (Danner et al., 2019).

Table 1 presents the maximum detected concentration ranges of tetracycline, oxytetracycline, and chlortetracycline in wastewater, soil, manure, biosolids, and plants in different countries. The highest concentrations of tetracycline and chlortetracycline were detected in wastewater, whereas the highest concentration of oxytetracycline was in manure. The highest tetracycline concentrations detected in wastewater were tetracycline 254.820 μg/L in Korea, chlortetracycline 44.420 μg/L in Korea, and oxytetracycline 1.236 μg/L in South Korea. The highest tetracyclines concentrations detected in soil, manure, and biosolids were 2.683, 183.500, and 0.7436 μg/g of oxytetracycline, in China and United States. The highest tetracycline concentration detected in plant contamination was 0.532 μg/g of chlortetracycline in China.

Several studies have investigated ABs contamination of surface water. **Table 2** presents the concentrations of tetracyclines in surface water streams in different countries. The predominant tetracycline detected in Ghana (Africa) was chlortetracycline, at concentrations of 0.044 μg/L. In the Wangyang River in China, tetracycline was detected at 25.5 μg/L. In Europe, the highest tetracycline concentration in surface water was detected in the United Kingdom, at a concentration of 1 μg/L. In the United States, the highest concentration of tetracycline 102.7 μg/L was detected in the Poudre River, Colorado. In Australia, the tetracycline concentration in surface water was minimal 0.008 μg/L.

The varying levels of tetracycline contaminants in different countries reflect the scale of production and usage of tetracyclines in each country. This in turn is directly correlated to the economic development and industrial scale of the country. The highest concentrations of tetracyclines were detected in China, which is the biggest producer and consumer of ABs in the world. In 2013, China produced (248,000 tons) of ABs and consumed approximately (162,000 tons) (Zhang et al., 2015). China was the highest consumer of veterinary ABs in the livestock industry, reaching approximately (15,000 tons) in 2010 (Robles Jimenez et al., 2019). China will double its AB consumption in the livestock industry by 2030, when it will reach up to (35,000 tons) (Robles Jimenez et al., 2019). Tetracyclines were not detected in surface water in Lebanon (Mokh et al., 2017), likely due to the low scale of livestock activity. However, the latest Lebanese Ministry of Agriculture survey in 2009 reports rapid growth in livestock productivity (Mokh et al., 2020). Farmers use different groups of ABs to promote growth in cattle and poultry. Studies evaluating the presence of AB residues in cattle and poultry in different regions in Lebanon documented AB bioaccumulation in these animals. For example, a 2008 survey investigated the most widely used ABs in dairy cows from 26 random farms (more than 50% of them were small-scale farms with less than 1,000 cattle), and found wide use of streptomycin, gentamicin, penicillin, kanamycin, and oxytetracycline (Abi

TABLE 2 | Maximum tetracyclines concentrations in different surface water streams in different countries (Danner et al., 2019; Singh et al., 2019).

Continent	Country	Antibiotic	Concentration (µg/L)
Africa	Ghana (rivers)	Tetracycline	0.03
	Ghana	Oxytetracycline	0.026
	Ghana	Chlortetracycline	0.044
Asia	Hong Kong	Tetracycline	0.0315
	China (Wangyang River)	Tetracycline	25.5
	China (Huangpu River)	Oxytetracycline	0.0845
	China	Chlortetracycline	0.017
Europe	Luxembourg (Alzette River)	Tetracycline	0.008
	United Kingdom	Tetracycline	1
	Spain	Tetracycline	0.228
	France	Tetracycline	0.007
	Poland (Drweca River)	Tetracycline	0.034
	Croatia	Chlortetracycline	0.43
	France	Chlortetracycline	0.68
	Luxembourg	Chlortetracycline	0.007
	Spain	Chlortetracycline	0.059
America	Cuba	Tetracycline	0.155
	United States (Poudre River)	Tetracycline	102.7
	Canada	Tetracycline	0.035
	Brazil	Tetracycline	0.011
	United States	Oxytetracycline	1.34
Australia	Australia (rivers)	Tetracycline	0.08

Khalil, 2008). Jammoul et al. (Jammoul and El Darra, 2019) evaluated ABs in 80 chicken muscle samples from different regions of Lebanon, and detected contaminating AB residues in (77.5%) of these samples. Ciprofloxacin (quinolones) represented the highest occurrence percentage (32.5%), followed by amoxicillin (lactams) (22.5%) and then tetracyclines (17.5%). The tetracyclines detected in these samples were below the maximum residue limit (MRL) values of 200 µg/kg set by the Food and Agriculture Organization (FAO, 2018). There are no recent studies on AB bioaccumulation in edible crops and water environments in Lebanon.

4 PHOTOCATALYTIC DEGRADATION AS A POTENTIAL TREATMENT FOR CONTAMINATED IRRIGATION WATER

4.1 Photocatalysis

Antibiotics are stable in natural environments and persist in aquatic media because they are only partly biodegradable and are not completely removed by traditional wastewater treatment methods (only 24–36% removal efficiency) (Zeghioud et al., 2016; Pan and Chu, 2017). Hence, there is an urgent need to develop new technologies to detoxify wastewater streams by degrading these pharmaceuticals (Zeghioud et al., 2016). There are two main technologies to remove ABs from the environment: destructive and non-destructive methods.

Non-destructive methods include adsorption, liquid extraction, and membrane separation. Adsorption relies on solid and liquid phases, and the ability of the pollutant to move from the liquid phase to attach onto the solid adsorbent (Anjali and Shanthakumar, 2019). The adsorption efficiency depends on the properties of the adsorbent, including its surface area, porosity, and pore diameter (Homem and Santos, 2011). Conventional treatments refer to methods that are utilized in water treatment plants, and include biological methods, filtration and coagulation/flocculation/sedimentation. In the biological systems, the organic compound degradation occurs in activated sludge tanks with the absence or presence of oxygen gas (O_2) by monitoring the temperature and chemical oxygen demand. Filtration is the elimination of suspended solids in the feed by passing it over a granular solid medium, like sand, activated carbon, or coal. Coagulation/flocculation/sedimentation use particular chemicals like iron salts, polymers, lime, and alum to facilitate pollutant precipitation, particle sedimentation, and colloid generation to further collect them. (Homem and Santos, 2011). Membrane separation methods include reverse osmosis, nanofiltration, ultrafiltration, and ion exchange. These techniques do not degrade or remove contaminants, but entrap organic pollutants on filters (membranes) that require regeneration or disposal. The organic compounds and salts in contaminated wastewater affect the system performance and cause fouling of the membrane, leading to flux deterioration (Homem and Santos, 2011; Anjali and Shanthakumar, 2019). Ion exchange is based on anion and cation exchange between liquid and solid phases (sorbent/membrane), and is primarily used to improve water quality. It is rarely used to remove ABs from wastewater because this method requires ABs molecules to have ionizable groups (Homem and Santos, 2011).

Destructive methods include biodegradation and chemical oxidation processes (Calvete et al., 2019). Chemical oxidation processes include chlorination and advanced oxidation

TABLE 3 | Summary of methods for antibiotics removal from wastewater (Homem and Santos, 2011; Anjali and Shanthakumar, 2019).

Process	Advantages	Disadvantages	Examples of antibiotic
Adsorption	Can be applied to feeds with high concentrations of organic compounds and antibiotics	It only concentrates pollutants in the adsorbent medium that need to be treated or disposed of later. It is not widely used to remove tetracyclines from water	Oxytetracycline and Tetracycline Choi et al. (2008) Chlortetracycline Chen and Huang, (2010) Sulfamerazine Koyuncu et al. (2008)
Conventional	It can be applied to effluents with high flow rates	It has low removal efficiency and complex removal of coagulated pollutants. It is not applied to fluid streams with high pollutant concentrations due to its toxicity	Trimethoprim Kim et al. (2010) Sulfamethazine and Sulfadimethoxine Göbel et al. (2007)
Membrane technology (reverse osmosis, nano-filtration, and ultrafiltration)	Efficiently reduce high levels of dissolved salts. They do not require thermal energy	These methods are slow and inefficient when treating organic compounds such as pharmaceuticals. They are vulnerable to membrane fouling that reduces the efficiency	Sulfamethoxazole Radjenović et al. (2008) Sulfamerazine Adams et al. (2002) Oxytetracycline Kosutic et al. (2007)
Ion exchange	Reversible method that allows the resin or membrane to be reused after regeneration	Susceptible to fouling and requires backwashing. Rarely used for antibiotic removal	Sulfamethoxazole Tetracyclines Chlortetracycline Oxytetracycline Choi et al. (2007) Trimethoprim Adams et al. (2002)
Chlorination	Efficiently removes antibiotics from water containing low percentages of organic compounds	Its efficiency is function of the system pH. It can generate halogenated compounds, which are potentially carcinogenic	Amoxicillin and Erythromycin Navalon et al. (2008) Sulfamethoxazole Stackelberg et al. (2007) Sulfamerazine (Adams et al., 2002)
Photocatalysis	Can be applied under ambient conditions. Can save energy by utilizing solar light	Has not been industrialized due to the low light penetration in large-scale applications in slurry reactors. Difficult to remove and regenerate the catalyst	Amoxicillin Klauson et al. (2010) Lincomycin (Addamo et al., 2005) Tetracycline Zhu et al. (2013)
Electrochemical oxidation	Clean, easy, and effective method to remove high concentrations of antibiotics and toxic organic matter	Limited to small flow rates. Has high capital and operating costs	Lincomycin Carlesi Jara et al. (2007) Anthracyclines Hirose et al. (2005) Enrofloxacin Guinea et al. (2009)
Photolysis	Can be applied to wastewater containing photosensitive compounds and low chemical oxygen demand (COD) percentages	It is less effective than other techniques that use UV light along with catalysts or other additives. It is ineffective in treating wastewater contaminated with antibiotics	Penicillin Arslan-Alaton and Dogruel, (2004) Ciprofloxacin Vieno et al. (2007) Oxytetracycline Jiao et al. (2008)
Fenton and photofenton	These methods have good degradation percentages. They can be applied to wastewater with low COD concentrations	Photofenton cannot be applied to streams with high organic (pharmaceutical) contents due to water turbidity, which blocks light irradiation needed for catalyst activation. Sludge formation as function of the system pH remains challenging in these systems	Amoxicillin Zhang et al. (2006) Penicillin Arslan-Alaton and Dogruel, (2004) Lincomycin Bautitz and Nogueira, (2010)
Ozonation	It has acceptable pollutant degradation efficiency. It is suitable for the treatment of feeds with variable compositions	Expensive. Low mineralization percentage. High toxicity. High capital, operating, and maintenance costs	Amoxicillin Andreozzi et al. (2005) Sulfamethoxazole (Huber et al., 2003) Oxytetracycline Li et al. (2008)

processes. Chlorination oxidizes organic pollutants into less toxic and biodegradable compounds. This method uses low-cost gases such as chlorine and hypochlorite, and it is routinely used as a pretreatment for wastewater streams polluted with pharmaceutical contaminants that are to be treated in biological systems (Homem and Santos, 2011). Advanced oxidation processes oxidize organic pollutants using intermediate radicals such as hydroxyl radicals to transform them into less toxic and more biodegradable species. The intermediate radicals are very reactive, have lower selectivity than other oxidants, and are generated in the presence of ozone, hydrogen peroxide, ultraviolet radiation, or semiconductor photocatalyst (Homem and Santos, 2011). Examples of advanced oxidation processes include ozonation, fenton, and photofenton oxidation, photolysis, electrochemical technologies, and photocatalysis.

The most studied AB removal technologies include ozonation, fenton/photofenton oxidation, photolysis, photocatalysis, electrochemical oxidation, chlorination, ion exchange, membrane technologies, and adsorption (Anjali and Shanthakumar, 2019; Homem and Santos, 2011). **Table 3** presents the advantages and disadvantages of each method. Photocatalysis is considered an environmentally friendly and low cost detoxification technique due to its utilization of solar light and complete mineralization of organic pollutants without generating residual waste or sludge (Sundar and Kanmani, 2020). Complete mineralization of the pollutant converts it into harmless species such as water, carbon dioxide, nitrogen, and other by-products, which in most cases are nontoxic (Zeghioud et al., 2016). The potential toxicity of products generated by photocatalytic degradation can be minimized by achieving high photocatalytic-induced mineralization (>99%) (Libralato et al., 2020). Bouafia-Chergui et al. (Bouafıa-Chergui et al., 2016) studied the toxicity of products generated by photocatalytic degradation

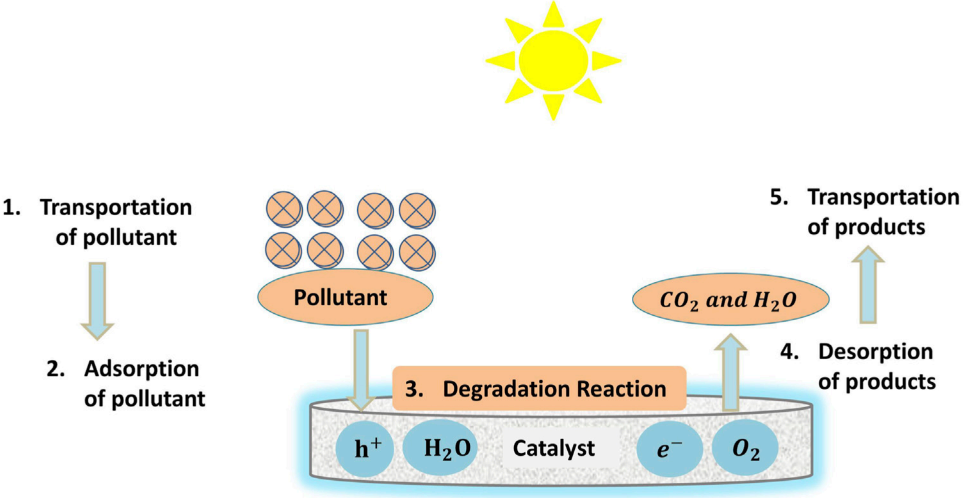

FIGURE 1 | A schematic of photocatalytic reaction steps.

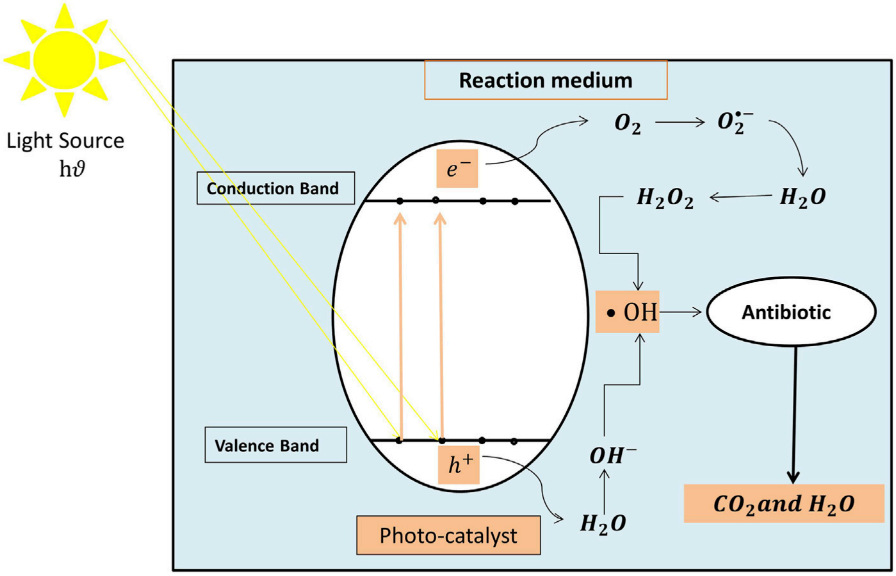

FIGURE 2 | Illustration of photocatalytic degradation mechanism.

of tetracycline by TiO_2 under UV light. The toxicity was evaluated by observing variations in the natural luminescent emissions of *Vibrio fischeri*. The results showed that the photoproduct toxicity increased after 240 min (from 60 to 84% inhibition of luminescence), then decreased to the minimum value after 360 min (35% inhibition of luminescence). This result indicated that total mineralization of tetracycline produced photoproducts with lower toxicity than tetracycline (Bouafia-Chergui et al., 2016).

The main components of photocatalysis systems are the light source, the photocatalyst, and the polluted water (Sundar and Kanmani, 2020). AB degradation *via* photocatalysis follows five steps, as depicted in **Figure 1**: 1) diffusion of the organic pollutant from the bulk of the solution to the surface of the catalyst, 2) adsorption of the organic pollutant onto the surface of the catalyst, 3) degradation of the contaminants on the surface of the catalyst, 4) desorption of the resultant products from the surface of the photocatalyst, and 5) diffusion of the products from the surface of the semiconductor toward the bulk of the solution (Ibhadon and Fitzpatrick, 2013). After illumination by UV/visible light, the semiconductor (e.g., TiO_2) molecules form unlinked pairs of electrons (e^-)/holes (h^+) due to the excitation of the electrons from the valence band (VB) to the conduction band (CB). These charge carriers may either return to the initial state in the semiconductor, or move to the surface of the catalyst to undergo various redox reactions with water molecules, hydroxide ions, and the pollutant. **Figure 2** illustrates the mechanism of photocatalysis, and **Eqs 1–6** define the chemical reactions. In these Equations, TiO_2 represents the catalyst, (e^-) represents the conduction band electron, and (h^+) represents the valence band hole (Zeghioud et al., 2016).

$$\mathrm{TiO_2} \rightarrow^{h\vartheta} e^- + h^+ \quad (\lambda \leq 380\ \mathrm{nm}) \tag{1}$$

The positive hole (h^+) can produce hydroxyl radicals *via* two paths. The first path is hole transfer to the water molecule; the second path is hole transfer to a hydroxyl ion (**Eqs 2**, **3**, respectively) (Zeghioud et al., 2016).

$$h^+ + \mathrm{H_2O} \rightarrow \bullet\mathrm{OH} + \mathrm{H^+} \tag{2}$$

$$h^+ + \mathrm{OH^-} \rightarrow \bullet\mathrm{OH} \tag{3}$$

The positive hole (h^+) can also oxidize the antibiotic pollutants (P) in water (**Eq. 4**), followed by the formation of intermediates produced from reactions with the hydroxyl radicals (**Eq. 5**) (Zeghioud et al., 2016).

$$h^+ + P_{ads} \rightarrow P_{ads}\cdot \tag{4}$$

$$\bullet\mathrm{OH} + \mathrm{P_{ads}}\cdot \rightarrow \text{intermediates/degradation products} \tag{5}$$

•OH radicals also can react with water pollutants to cause mineralization into water and carbon dioxide (**Eq. 6**) (Zeghioud et al., 2016).

$$\bullet\mathrm{OH} + \mathrm{P} \rightarrow \mathrm{H_2O} + \mathrm{CO_2} + \text{inorganic acids} \tag{6}$$

In the presence of molecular oxygen, the excited electrons interact with the adsorbed oxygen on the catalyst surface (**Eq. 7**) and produce superoxide radicals ($O_2^{\bullet -}$). These radicals are capable of preventing the recombination of the electrons with the positive holes (Zeghioud et al., 2016; Ibhadon and Fitzpatrick, 2013) and are converted to hydrogen peroxide and then to hydroxyl radicals as shown in the (**Eqs 8–10**) (Homem and Santos, 2011). Hydroxyl radicals play a significant role in the degradation of the organic pollutant.

$$\mathrm{O_2} + e^- \rightarrow \mathrm{O_2^{\bullet -}} \tag{7}$$

$$\mathrm{O_2^{\bullet -}} + \mathrm{H_2O} \rightarrow \mathrm{HO_2^{\bullet}} + \mathrm{OH^-} \tag{8}$$

$$2\mathrm{HO_2^{\bullet}} \rightarrow \mathrm{H_2O_2} + \mathrm{O_2} \tag{9}$$

$$\mathrm{H_2O_2} + e^- \rightarrow \mathrm{OH^-} + \bullet\mathrm{OH} \tag{10}$$

Many factors influence the efficiency of the photocatalytic degradation of various organic pollutants in water, including the concentrations of the contaminant and the catalyst, the light source and its intensity, the solution pH, the solution turbidity, the presence of other contaminants, and the type of photo-reactor employed (Saadati et al., 2016a). Increasing the initial AB or catalyst concentration increases the rate of degradation until reaching an optimal value, after which the degradation rate decreases (Saadati et al., 2016a). A suitable light source with an appropriate intensity and wavelength is essential to ensure optimum catalyst activation (Liu et al., 2013; Saadati et al., 2016a; Zhang et al., 2019). The effect of pH is a function of the operating conditions and the chemical nature of pollutants and catalyst. The capacity of the catalyst itself to harvest light photons and efficiently utilize the excited electrons in degrading the pollutant is a critical factor that affects system performance (Saadati et al., 2016a). The water turbidity also affects photocatalysis efficiency. For example, high water turbidity in the treated stream can reduce light transmission through the water into the catalyst's surface, thereby reducing light absorption by the catalyst and subsequent electron activation (Teoh et al., 2012; Divakaran et al., 2021). The presence of salts and other organic pollutants in the water may affect AB adsorption onto the catalyst surface, and can increase water turbidity. Ghoreishian et al. (Ghoreishian et al., 2021) compared the performance of Fe and Sn co-doped-TiO_2 nanofibers for tetracycline degradation in synthetic, river, and tap water samples. The results showed that the highest efficiency was obtained for synthetic pure water (96.96%), followed by tap water (81.85%), and then river water (60.59%). This result clearly indicates that photocatalyst performance can be overestimated by experiments that use pure water in laboratory settings.

The choice of photocatalytic reactor is a function of the reaction system, including the chemical structure and concentrations of pollutants and catalyst, the operating flowrate, temperature, and pressure (Ibhadon and Fitzpatrick, 2013). Slurry reactors are conventional reactors that suspend the heterogeneous photocatalysts in a liquid phase in the reactor. Heterogeneous photocatalysts are preferred over homogeneous photocatalysts in slurry reactors because they offer easier catalyst recovery and high efficiency. Accordingly, catalyst immobilization on solid substrates such as polymers, glass, sand, or reactor walls has been receiving great attention recently to achieve efficient catalyst recovery and sustainable system operation (Ibhadon and Fitzpatrick, 2013; Zeghioud et al., 2016).

4.2 Photocatalytic Degradation of Tetracyclines

Tetracyclines contamination of surface and ground water, hence eventually irrigation water, is due to the inefficient removal capacity of current conventional wastewater plants, leading to residual tetracycline concentrations of up to 2.37 μg/L in the final effluent stream released into the environment (Daghrir and Drogui, 2013). Photocatalytic degradation of tetracyclines using UV, visible, and solar light has been explored for complete tetracycline demineralization (Bouafia-Chergui et al., 2016; Chen et al., 2016; Farhadian et al., 2019). Three primary photocatalytic systems have been extensively studied: semiconductor systems such as TiO_2 (Zhu et al., 2013; Niu et al., 2014; Safari et al., 2014) and ZnO (Farhadian et al., 2019); binary composite systems such as Ag-Bi_2WO_6, Ag-$BiVO_4$-Cu_2O, and AgBr-Ag_3PO_4 (Deng et al., 2017; Shen et al., 2018; Yan et al., 2018; Rasheed et al., 2019); and heterojunctions such as AgI/WO_3, CQDs/Bi_2WO_6, C_3N_4/Bi_2WO_6, and CQDS/ZnO (Di et al., 2015; Wang et al., 2016; Chen et al., 2017; Li J. et al., 2019).

Other common examples on materials used for tetracyclines photocatalytic degradation under both UV and visible light

TABLE 4 | Previous work on tetracycline removal by TiO_2 catalyst under UV light.

#	Catalyst	TC initial concentration (mg/L)	Catalyst concentration (g/L)	UV light source	pH	Removal efficiency	Year and ref
1	TiO_2 P25 (Degussa) 20–30 nm	40	1	UV: 300 W ($290 < \lambda < 365$) mercury lamp	4.2	95% after 60 min	2013 Zhu et al. (2013)
2	Commercially available TiO_2 (BIOCHEM ChemoPharma)	5	2	UV: 12 W halogen lamp[a]	Free	100% after 210 min	2016 Bouafıa-Chergui et al. (2016)
3	TiO_2 (US-Research Nanomaterials) 10–25 nm	15	2	UV: 15 W[a]	5	100% after 45 min	2018 Fazilati et al. (2018)

[a] *Light wavelength was not specified in the original paper.*
Free pH: medium pH was not controlled.

include the application and modification of titania (TiO_2) semiconductors. In these studies, both high performance liquid chromatography (Wang et al., 2011; Cao et al., 2016) or UV–VIS spectrophotometer (Yu et al., 2014; Oseghe and Ofomaja, 2018a; Lyu et al., 2019; Ghoreishian et al., 2020) were used for the analysis of the water samples and for the evaluation of the degradation efficiency of the TCs over the investigated photocatalysts. Photocatalytic tetracycline degradation mediated by TiO_2 is expected to proceed *via* the formation of intermediates, which eventually completely degrade into CO_2, H_2O, and NH_4^+. Zhu et al. (Zhu et al., 2013) proposed that TiO_2-mediated tetracycline degradation involved electron transfer, hydroxylation, open-ring reactions, and cleavage of the central carbon.

4.3 TiO_2-Based Photocatalysts for Tetracyclines Degradation

TiO_2 is the most studied and used heterogeneous photocatalyst semiconductor due to its super quantum yield (ratio of emitted photons to absorbed photons), low cost, non-toxicity, hydrophilicity, high photoactivity, interesting charge transport properties, and good chemical and photostability (Ibhadon and Fitzpatrick, 2013; Sommer et al., 2015; Koe et al., 2019; You et al., 2019; Zhang et al., 2019). TiO_2 exists in three polymorphs/crystal forms: anatase, rutile, and brookite. Anatase and rutile forms of TiO_2 are utilized as photocatalysts; however, anatase is preferred due to its superior quantum yield (Koe et al., 2019). A hybrid form of TiO_2 called Degussa (Evonik-Degussa) P-25 consists of a phase-junction mixture of (25%) rutile and (75%) anatase. TiO_2-P25 is widely investigated for photodegradation of organic pollutants due to its availability, stability, reusability, and high oxidation activity compared to other crystal forms of TiO_2 (Ibhadon and Fitzpatrick, 2013; Koe et al., 2019).

TiO_2 has a band gap (E_g) of approximately 3–3.2 eV, which limits its photoactivity to ultraviolet light with a wavelength less than 387 nm (Koe et al., 2019). **Table 4** summarizes some applications of Titania for photodegradation of tetracyclines under UV light. In general, Titania achieves very high degradation efficiencies of (95–100%) in relatively short periods of time (45–60 min).

Despite its promising photocatalytic activities, Titania has some shortcomings that limit its wide application in photocatalysis. For example, due to its wide band gap energy (3.2 eV) TiO_2 can only be activated under UV light which only accounts for (5%) of the solar spectrum. The recombination rate of the charge carriers is significantly high in TiO_2, and this suppresses its AB degradation efficiency. TiO_2 also undergoes agglomeration and aggregation which complicates its recovery and reuse in large-scale applications. Moreover, TiO_2 has low adsorption capacity of nonpolar contaminants due to its polar nonporous surface (Bahadar Khan and Kalsoom, 2019; Li R. et al., 2020).

Further modification of Titania is urgently needed to achieve practical, visible light–induced photocatalytic applications. Many studies have been reported in the literature to enhance Titania properties through modification and/or combination with organic and/or inorganic counterparts (Wang et al., 2011; Chen et al., 2016; Pouretedal and Afshari, 2016; Zhang S. et al., 2017; Zhang F. J. et al., 2017; Chen and Liu, 2017; Jin et al., 2017; Duan et al., 2018; He et al., 2018; Tang et al., 2018; Zheng et al., 2018; Liu M. et al., 2019; Chen Y. et al., 2019; Farhadian et al., 2019; Galedari et al., 2019; Sun et al., 2019; Akel et al., 2020; Zhang T. et al., 2020; Ghoreishian et al., 2020; Liu et al., 2020; Divakaran et al., 2021; Ghoreishian et al., 2021). The following section presents a detailed summary of various methods reported in the literature to achieve visible light sensitization of Titania and its applications for tetracyclines photodegradation.

5 MODIFICATION OF TiO_2 FOR ENHANCED VISIBLE LIGHT ACTIVITY

Researchers have studied TiO_2 modification for more than 30 years to enhance its visible light photocatalytic properties, stability, and reusability using three primary modification methods: 1) hinder the recombination of excited electrons and positive holes; 2) expand titania activity from the UV light spectrum to include visible light (accounts for approximately (43%) of the solar light spectrum) and ultimately solar light; and 3) enhance TiO_2 morphology, surface area, and ease of recovery (Teoh et al., 2012). Recent advances in titania modification include doping with metals and nonmetals, developing hybrid composite systems, and constructing heterojunction photocatalysts (Li and Shi, 2016). Each of

TABLE 5 | Previous studies investigating tetracyclines removal by metal, nonmetal, and mixed metal-nonmetal doped TiO_2 catalysts.

#	Modified titania	TC initial concentration (mg/L)	Catalyst concentration	Light source	pH	Results with doped TiO_2	Results with pure TiO_2	Year and ref
1	Co-doped TiO_2	30 Oxy-(TCH)	0.5 g/L	UV/vis illumination[a]	5	98% after 60 min	97% after 60 min	2020 Akel et al. (2020)
2	Zr/Sn co-doped TiO_2	20 (TC)	0.8 g/L	36 W mercury low pressure lamp[a]	3	100% after 180 min	79% after 180 min	2015 Pouretedal and Afshari, (2016)
3	Fe/Sn co-doped TiO_2	30 (TC)	0.3 g/L	300 W Xenon (Xe) arc lamp (λ > 420 nm)	6	96.96% after 60 min	5% after 60 min	2021 Ghoreishian et al. (2021)
4	H_2O_2 modified Zn-doped TiO_2	80 (TC)	1 g/L	500 W Xe lamp[a]	7	88.14% after 360 min	70% after 360 min	2016 Pang et al. (2016)
5	Y^{3+}/TiO_2 Hal-PMPD	50 (TC)	2 g/L	500 W Xe lamp (λ > 380 nm)	1	78.8% after 50 min	–	2014 Yu et al. (2014)
6	Phosphorous-doped anatase TiO_2	60 (TCH)	0.5 g/L	500 W halogen-tungsten lamp[a]	7	93% after 120 min	62% after 120 min (anatase)	2014 Niu et al. (2014)
7	C-N-S tri-doped TiO_2	5 (TC)	0.5 g/L	6 W (F6T5/D) cold white visible lamp (λ > 420 nm)	9	95% after 180 min	25% after 180 min	2011 Wang et al. (2011)
8	TiO_2 doped with acetylene black	10 (TCH)	0.5 g/L	30 W LED lamp (400 < λ < 780 nm)	4.1	93.3% after 120 min	20% after 120 min	2020 Zhang T. et al. (2020)
9	N-doped TiO_2	10 (TC)	0.2 g/L	Visible light (λ = 420 nm)	7	90% after 120 min	73% after 120 min	2020 Wu et al. (2020)
10	Porous N, S co-doped TiO_2	20 (TC)	0.4 g/L	300 W Xe lamp (λ > 420 nm)	Free	84.9% after 60 min	Comparable results as modified	2020 Ouyang and Ji, (2020)
11	(Sn, Zn) and N co-doped TiO_2	35 (TC)	0.5 g/L	Simulated solar irradiation[a]	7	33% after 120 min	22% after 120 min	2018 Rimoldi et al. (2018)

[a] *Light wavelength was not specified in the original paper.*

Free pH: medium pH was not controlled.

Abbreviations: TC, tetracycline; TCH, tetracycline hydrochloride.

these Titania modification methods is discussed in the following sections.

5.1 Metal and Nonmetal Doping of TiO_2

Doping is the introduction of a metallic and/or nonmetallic element (dopant) into the bulk of a semiconductor without modifying its structure or altering its crystallographic form (Teoh et al., 2012; Ibhadon and Fitzpatrick, 2013). The presence of the dopant results in a large dipole moment that can alter the kinetics of the electron transfer process. It lowers the band gap energy and widens the light absorption spectrum by increasing the number of migrating electrons from the valence band to the conduction band of the main semiconductor (Koe et al., 2019). Consequently, optimal doping conditions enable photocatalyst activation under UV and visible light (380 nm < λ < 500 nm) (Ibhadon and Fitzpatrick, 2013). Studies have investigated various dopants for the visible light sensitization of titania, including metal, nonmetal, or mixed metal-nonmetal doping (Li and Shi, 2016). The development of optimum doping conditions must consider the preparation method, the dopant concentration, and the type of dopant to ensure enhanced photocatalytic performance (Marschall and Wang, 2014). **Table 5** presents examples of the best performing metal, nonmetal, and mixed metal-nonmetal doping of TiO_2 photocatalysts and their performance in tetracyclines photodegradation under visible light.

5.1.1 Metal Ion Doping of TiO_2

Metal ion dopants of Titania include transition, rare earth, and precious metal ions. Metal doping of Titania is achieved by firing at high temperature or auxiliary deposition techniques (Zhang et al., 2019). **Figure 3** illustrates the mechanisms of tetracyclines degradation by metal-doped TiO_2 photocatalysts. Under visible light, electrons in the band gap energy of the doping metal are excited into the metal conduction band, and then move into the conduction band of the bulk catalyst. Simultaneously, Titania electrons are excited by the UV light of the solar light spectrum (**Eq. 1**). Consequently, these electron/hole pairs lead to a series of oxidation-reduction reactions that produce oxygen and hydroxyl radicals (**Eqs 2**, **3**, **7**, **8**, **9**, **10**) which in turn degrade the AB molecules (**Eqs 4**, **5**, **6**). An example of an efficient transition metal–doped Titania is cobalt (Co)-doped TiO_2, which has been used with and without immobilization on reduced graphene oxide surfaces for tetracycline and oxytetracycline removal, respectively (Jamali Alyani et al., 2019; Akel et al., 2020). Cobalt-doped Titania was prepared using the reflux method (Co-TiO_2-R) by Akel et al. (Akel et al., 2020), and resulted in (98%) degradation of oxytetracycline hydrochloride (Oxy-TCH) under UV-visible light illumination. The authors attributed the high initial rate of Co-TiO_2-R to its high surface area and enhanced charge transfer and separation properties imposed by impurity levels in the band gap energy; the Co particles entrapped some of the generated (h^+), thereby minimizing the possibility of electron/hole recombination.

Metal co-doping was recently used to enhance visible light harvesting in TiO_2 catalysts. Co-doping resulted in higher visible light activity than that resulting from single-doping due to a

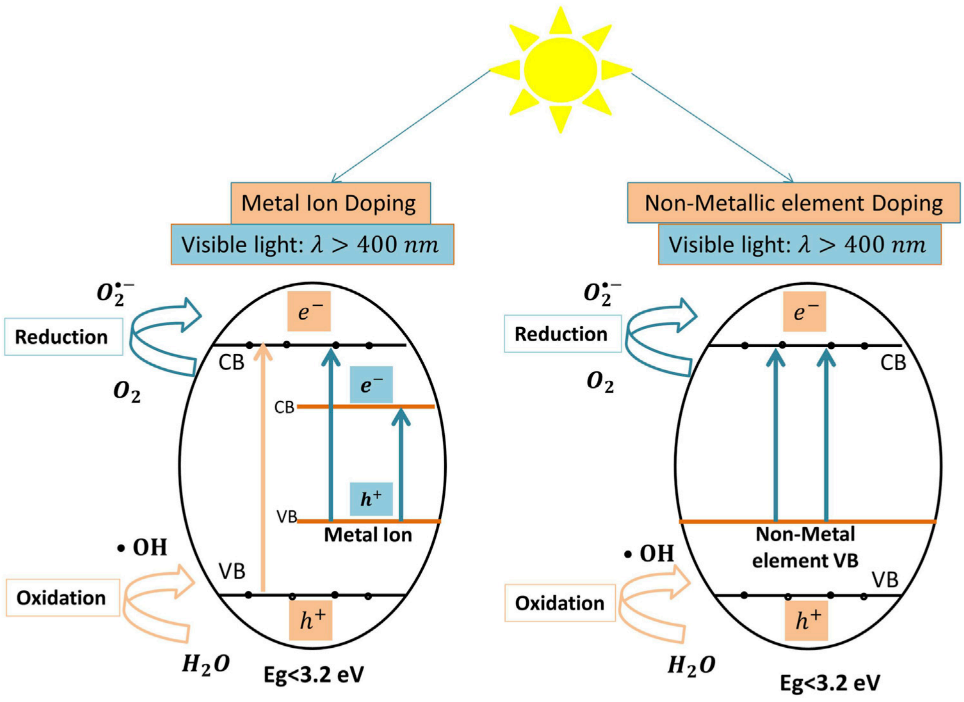

FIGURE 3 | The proposed photocatalytic degradation mechanisms of tetracycline both by metal-doped and non-metal doped TiO_2 systems under visible light.

synergistic effect between the two dopants (You et al., 2019). Recent studies investigated bimetallic doping of TiO_2 for tetracyclines degradation using zirconium (Zr) and tin (Sn) (Pouretedal and Afshari, 2016), and iron (Fe) and tin (Sn) (Ghoreishian et al., 2021). Ghoreishian et al. (Ghoreishian et al., 2021) developed highly efficient Fe-Sn co-doped TiO_2 nanofibers (Fe/Sn-TiO_2 NFs). Fe/Sn-TiO_2 NFs were produced using the electrospinning method, and then used for tetracycline degradation under 300 W xenon (Xe) lamp as the visible light source (Ghoreishian et al., 2021). This co-doped TiO_2 catalyst displayed a very high photocatalytic degradation efficiency (96.96%), which was 1.86, 1.8, and 1.56 times higher than the efficiencies of unmodified TiO_2, Fe-doped TiO_2, and Sn-doped TiO_2, respectively. The authors attributed the enhanced performance of the co-doped catalyst to its small crystal size, tunable and low band gap energy, higher adsorption capability, better visible light absorption, enhanced charge carrier separation, and suppressed charge carrier recombination. This co-doped catalyst also displayed high stability and maintained (92%) degradation efficiency after five cycles of use. Total organic carbon (TOC) analysis was used to assess the extent of AB mineralization achieved by the catalyst. The Fe/Sn-TiO_2 NFs achieved (98%) tetracycline mineralization, compared to only (56%) tetracycline mineralization by the unmodified TiO_2 catalyst.

5.1.2 Nonmetal Doping of TiO_2

Nonmetal doping has been investigated for the visible light activation of TiO_2 (Farhadian et al., 2019; Niu et al., 2014; Oseghe and Ofomaja, 2018a; Tang et al., 2018; Chen and Liu, 2016; Wu et al., 2020; Fang et al., 2019; Oseghe and Ofomaja, 2018b). Nonmetal-doped photocatalysts display higher stability and better photoactivity than metal-doped photocatalysts because metal-doping of TiO_2 can, for example in some applications, lower the doped catalyst stability, reduce its activity, and decrease its photo-quantum efficiency due to rapid recombination of the electrons and the holes (Teoh et al., 2012). Nonmetal dopants of TiO_2 include nitrogen (N) (Farhadian et al., 2019; Wang et al., 2011; Tang et al., 2018; Chen and Liu, 2016; Wu et al., 2020), sulfur (S) (Wang et al., 2011), carbon (C) (Zhang T. et al., 2020), and phosphorous (P) (Niu et al., 2014). Nonmetal doping is performed by creating mid-gap energy levels between the valence and conduction bands of the parent catalyst (Zhang et al., 2019; Ibhadon and Fitzpatrick, 2013; Radwan et al., 2018). The nonmetal dopant can enhance the visible light–induced photocatalytic activity of the catalyst because electrons in the newly created energy level can be excited by visible light into the conduction band of the bulk catalyst (**Eq. 1**). Eventually, these excited electrons settle on the surface of the doped catalyst and generate active radicals *via* redox reactions (**Eqs 2**, **3**, **7**, **8**, **9**, **10**), which consequently attack and mineralize the AB molecules (**Eqs 4**, **5**, **6**) (Ibhadon and Fitzpatrick, 2013; Radwan et al., 2018). Importantly, the nonmetal dopant inhibits the recombination of the charge carriers, due to electron entrapment by the oxygen vacancies created in the catalyst (Feng et al., 2018; Basavarajappa et al., 2020). **Figure 3** illustrates the mechanism of tetracyclines degradation by nonmetal-doped TiO_2 systems.

Nitrogen is the most-studied nonmetal dopant for enhancing the visible light activity of TiO_2 (Marschall and Wang, 2014).

There are several methods to produce N-doped TiO_2, including hydrothermal, microemulsion, chemical vapor deposition, solvothermal, sol-gel, electrospinning, anodic oxidation, sputtering, ball milling, atomic layer deposition, and microwave (Basavarajappa et al., 2020). Several studies have produced N-doped TiO_2 for tetracyclines degradation under visible light (Wang et al., 2011; Chen and Liu, 2016; Tang et al., 2018; Farhadian et al., 2019; Wu et al., 2020). Wu et al. prepared N-doped TiO_2-P25 by treating TiO_2-P25 with NH_3 gas flow at 500°C, and applied the catalyst for tetracycline degradation under visible light (λ = 420). This N-doped TiO_2-P25 displayed higher visible light sensitivity and enhanced photocatalytic performance due to the increased numbers of excited reactive electrons and holes. The authors confirmed that the presence of N in TiO_2 created oxygen vacancies that entrapped the photoexcited electrons, thereby minimizing their recombination effect. The N-doped TiO_2-P25 tetracycline degradation performance (90%) was higher than that of the unmodified TiO_2 (73%), and the doped photocatalyst maintained its stability and degradation efficiency for four consecutive cycles (Wu et al., 2020).

Carbon doping of Titania extends its light absorption into the visible region by acting as a sensitizer or by creating interstitial gap states in the catalyst structure (Palanivelu et al., 2007; Wu et al., 2013). Carbon doping also increases the number of photogenerated charge carriers that degrade organic pollutants in water (Palanivelu et al., 2007). Acetylene black–doped (AcB) and persulfate (PS)-employed TiO_2 (TiO_2/AcB/PS was prepared using the sol-gel method (Zhang T. et al., 2020). Acetylene black lowered the band gap energy of TiO_2 from 3.17 to 2.78 eV, thereby enabling it to be activated under visible light, efficiently minimizing charge carrier recombination, and promoting charge carrier separation. The TiO_2/AcB/PS photocatalyst displayed (93%) tetracycline hydrochloride degradation efficiency, which was higher than that of unmodified TiO_2 (20%), and maintained high degradation efficiency (85%) after five uses (Zhang T. et al., 2020).

Phosphorus (P) doping of TiO_2 enhances the catalytic photoactivity by effectively suppressing charge carrier recombination due to electron entrapment by the oxygen vacancies created in the catalyst (Feng et al., 2018). The presence of a P dopant on TiO_2 decreased its band gap energy and significantly enhanced its visible light–induced photocatalytic degradation of organic pollutants (Gopal et al., 2012). Niu et al. (Niu et al., 2014) used the rapid microwave hydrothermal method to prepare P-doped anatase TiO_2 for tetracycline hydrochloride degradation under 500 W halogen-tungsten lamp. This P-doped TiO_2 displayed (93%) tetracycline degradation efficiency, which was much higher than that of commercial TiO_2-P25 (62%).

Nonmetal element co-doping of TiO_2 has gained enormous interest lately because of its potential to alter the photocatalytic characteristics of the catalyst, such as reducing the band gap energy and enhancing visible light absorption as compared to that of the single-element–doped catalyst (Chen et al., 2007). Co-doping and tri-doping were applied to TiO_2 for enhanced tetracycline degradation. Wang et al. (Wang et al., 2011) used the sol-gel method to prepare C-N-S tri-doped TiO_2 for tetracycline degradation under 6 W white visible light lamp. The C-N-S tri-doped TiO_2 exhibited enhanced degradation performance (95%) compared to that of unmodified TiO_2 (25%). The authors ascribed this improvement to the high surface area of the modified catalyst, the formation of a well-defined TiO_2 anatase phase, the red shift of the light absorption spectrum of TiO_2, the enhanced visible light sensitivity because of the narrowed band gap energy of TiO_2, and the existence of carbon behaving as photosensitizer of TiO_2, which led to synergistic enhancement of tetracycline adsorption.

5.1.3 Mixed Metal-Nonmetal Doping of TiO_2

Mixed metal-nonmetal doping enables optimization of the advantages and minimization of the disadvantages of each doping method. This hybrid method specifically enhances the catalyst photo-efficiency by broadening the photo-activated spectrum toward the visible range. The N-TiO_2 catalyst is most commonly used for tetracyclines degradation under visible light, along with other nonmetal-doped TiO_2 in mixed doping systems (Huo et al., 2016; Chen and Liu, 2017; Rimoldi et al., 2018; Chen Y. et al., 2019; Ghoreishian et al., 2020). Rimoldi et al. (Rimoldi et al., 2018) used the sol-gel method to prepare Sn-, Zn-, and N-doped TiO_2 for tetracycline degradation under simulated solar irradiation. The authors reported that metal co-doping of N-doped TiO_2 induced a further red-shift in the light spectrum (400–600 nm). They attributed this improvement to the generation of intra-gap states in the TiO_2 structure by the introduction of some defects caused by Sn-doping. TiO_2-N was reported to have quasi-spherical crystallites of high crystallinity and corresponding inter-planar distances of anatase TiO_2. For TiO_2-N-Sn crystalline particles (3–6 nm) were detected along with the corresponding inter-planar distances of anatase and brookite TiO_2 and small content of SnO_2 cassiterite. In the TiO_2-NZn, the presence of Zn resulted in the formation of a guest phase of ZnO wurtzite. Particularly, Zn doping resulted in better photocatalytic performance due to its low crystallinity, unique amorphous structure, and high surface area as compared to the Sn-doping alone. The mixed metal-nonmetal Zn/Sn/N-doped TiO_2 exhibited (33%) tetracycline degradation efficiency compared to (22%) tetracycline degradation efficiency of the unmodified TiO_2. This significant increase was attributed to the synergistic effect of the dopants, their ability to widen the light absorption spectrum, and the higher surface area of the catalyst. Although (33%) tetracycline degradation efficiency is relatively low, the selected metal-nonmetal pairs and their concentrations can be optimized to improve photocatalyst performance.

In general, co- or tri-doping of TiO_2 can overcome some of the drawbacks of single doping, and enhance catalyst performance and stability in tetracyclines degradation due to the synergistic effect among the dopants. The choice of the dopant should consider its cost, toxicity, doping conditions, and preparation method. The dopant concentration also needs to be optimized to ensure enhanced performance of the final catalyst (Marschall and Wang, 2014).

TABLE 6 | Examples of titania-based composites and their tetracyclines degradation efficiencies.

#	Modified titania	Tetracycline initial concentration (mg/L)	Catalyst concentration	Light source	pH	Removal % by TiO_2-Based composite catalysts	Removal % by unmodified TiO2	Year and ref
A. Immobilized titania composites								
1	Chitosan modified N-, S-doped TiO_2	10 (TC)	0.6 g/L	Visible light[a]	8.2	92% after 50 min	–	2019 Farhadian et al. (2019)
2	2D sandwich-like TiO_2-rGO composite	20 (TCH)	0.4 g/L	Xenon (Xe) lamp[a]	5.2	96% after 120 min	28% after 120 min	2017 Zhang S. et al. (2017)
3	Fe_2O_3-TiO_2–modified zeolite composites	20 Oxy-(TC)	1 g/L	200 W λ = 455 nm LED light	Free	98% after 60 min	–	2019 Liu M. et al. (2019)
4	N-doped TiO_2/rGO	10 (TCH)	1 g/L	300 W Xe lamp (λ > 400 nm)	7	98% after 60 min	10% after 60 min	2018 Tang et al. (2018)
5	Ce/N co-doped TiO_2/$NiFe_2O_4$/diatomite	20 (TC)	0.5 g/L	150 W Xe lamp (λ > 400 nm)	7	100% after 180 min	–	2017 Chen and Liu, (2017)
6	Floating Fe/N co-doped TiO_2/diatomite	10 (TC)	5 g/L	150 W Xe lamp (filter to isolate UV light)[a]	Free	96.5% after 150 min	–	2019 Chen Y. et al. (2019)
7	Zn-doped TiO_2 nanoparticles/GO	40 (TC)	1 g/L	500 W Xe lamp[a]	Free	98.5% after 120 min	20% after 120 min	2017 Zhang F. J. et al. (2017)
8	Cobalt-doped TiO_2 nanosheets/rGO	20 Oxy-(TCH)	1 g/L	500 W halogen lamp (350<λ < 800 nm)	Free	68% after 180 min	–	2019 Jamali Alyani et al. (2019)
9	N-doped TiO_2/diatomite	20 (TCH)	5 g/L	Xe lamp[a]	6	93% after 300 min	–	2016 Chen and Liu, (2016)
10	Black TiO_2 nanoparticle/porous carbon	50 (TC)	0.6 g/L	Xe lamp (λ > 420 nm)	5	90% after 160 min	–	2019 Fang et al. (2019)
11	Fe_3O_4/rGO/TiO_2 nanocomposites	20 (TCH)	0.4 g/L	150 W Xe lamp[a]	3	92.6% after 330 min in the presence of H2O2	–	2017 Wang W. et al. (2017)
12	Silver/TiO_2 nanosheets/rGO	30 (TC)	0.75 g/L	Halogen 500 W lamp (350 <λ < 800 nm)	7	52.56% after 180 min	–	2020 Tabatabai-Yazdi et al. (2020)
13	Ce-doped TiO_2-MGO hybrid photocatalyst	25 (TC)	0.5 g/L	300 W Xe lamp[a]	Free	82.92% after 60 min	10.9% after 60 min	2016 Cao et al. (2016)
14	TiO_2/Semnan natural zeolite	8 (TC)	0.8 g/L	60 W visible lamp[a]	6	87% after 90 min	10% after 90 min	2016 Saadati et al. (2016b)
15	Ce-doped TiO_2/halloysite nanotubes	20 (TC)	0.5 g/L	300 W Xe lamp (λ > 420 nm)	7	78% after 60 min	8% after 60 min	2019 Wang et al. (2019)
16	Au-TiO_2/polydopamine (pDA)-coated PVDF	10 (TC)	–	300 W Xe lamp (λ > 420 nm)	7	92% after 120 min	–	2017 Wang C. et al. (2017)
17	Bimetallic Au- and Ag-doped TiO_2 nanorods/cellulose acetate	5 (TC)	Fixed on a membrane	Xe lamp (λ > 420 nm)	Free	90% after 120 min	–	2019 Li W. et al. (2019)
18	C-doped titania-polymethylsilsesquioxane aerogels	10 (TCH)	10 g/L	Visible light (λ > 420 nm)	7	98% after 180 min	–	2021 Xu H. et al. (2021)
B. Nanostructured Titania Composites								
19	TiO_2 nanobelts modified by Au and CuS nanoparticles	5 Oxy-(TC)	4 cm^2	Simulated solar light, a 35 W Xe lamp[a]	7	96% after 60 min	48% after 60 min by TiO_2 nanobelts	2016 Chen et al. (2016)
20	TiO_2 doped with acetylene black	10 (TCH)	0.5 g/L	30 W LED lamp (λ 400–780 nm)	4.1	93.3% after 120 min	20% after 120 min	2020 Zhang T. et al. (2020)
21	(1D) MIL-100(Fe)/TiO_2 nanoarrays	100 (TC)	Film sample	450 W Xe lamp[a]	Free	90.79% after 60 min	35.22% after 60 min	2018 He et al. (2018)
22	Ag/AgBr- modified TiO_2	10 (TC)	1.2 g/L	5W LED white lamp[a]	4.5	95.3% after 60 min	20% after 60 min	2019 Sun et al. (2019)
23	TiO_2-Fe_2O_3	15 (TC)	0.75 g/L	60 W lamp[a]	4.7	93% after 90 min	–	2019 Galedari et al. (2019)
24	Carbon-modified TiO_2	5 (TCH)	0.3 g/L	White LED (λ = 450 nm)	7	73.53% after 120 min	40% after 120 min	2018 Oseghe and Ofomaja, (2018b)

(Continued on following page)

TABLE 6 | (*Continued*) Examples of titania-based composites and their tetracyclines degradation efficiencies.

#	Modified titania	Tetracycline initial concentration (mg/L)	Catalyst concentration	Light source	pH	Removal % by TiO_2-Based composite catalysts	Removal % by unmodified TiO2	Year and ref
25	Pine cone–derived C-doped TiO_2	5 (TCH)	0.3 g/L	25 W white vis-LED strip^a	7	83% after 120 min	–	2018 Oseghe and Ofomaja, (2018a)
26	Bismuth-titanate nanoparticles	50 (TC)	1 g/L	360 W halogen lamp (λ > 400 nm)	7	65% after 180 min	–	2017 Khodadoost et al. (2017)
27	C-TiO_2 nanocomposites	10 (TC)	0.2 g/L	–*	7	90% after 160 min	30% after 160 min	2019 Ma et al. (2019)
28	CdS-TiO_2 heterostructure composite	50 (TCH)	1 g/L	500 W Xe lamp (λ > 400 nm)	7	87.06% after 480 min	7.68% after 480 min	2018 Li et al. (2018)
29	$SrTiO_3/Fe_2O_3$ nanowires	10 (TC)	1 g/L	250 W Xe lamp (λ > 420 nm)	Free	82% after 140 min	–	2016 Liu et al. (2016)
30	$Bi_4Ti_3O_{12}$/BiOCl composite	20 (TCH)	0.66 g/L	300W Xe lamp*	Free	83.7% after 150 min	–	2018 Liu et al. (2018)
31	Perovskite-type W-doped $BaTiO_3$	5 (TC)	0.8 g/L	Visible metal halide light*	5.6	93% after 180 min	–	2019 Demircivi and Simsek, (2019)
32	Platinum-doped amorphous TiO_2-filled mesoporous TiO2	50 (TCH)	0.5 g/L	500 W Xe lamp *	7	100% after 300 min	–	2019 Lyu et al. (2019)
33	Mn-doped $SrTiO_3$ nanocubes	10 (TC)	1 g/L	250 W Xe lamp (λ > 420 nm)	7	66.7% after 60 min	–	2015 Wu et al. (2015)
34	Cu-doped TiO_2 micro/ nanostructures	20 (TCH)	20 mg/L	1000 W Xe (λ > 420 nm)	7	90% after 240 min by calcined Cu-doped TiO2	50% after 240 min	2018 Cao et al. (2018)
35	Carbon-doped TiO_2 ultrathin nanosheets	20 (TC)	0.5 g/L	300 W Xe lamp (λ > 420 nm)	Free	89.1% after 120 min	50% after 120 min	2021 Bao et al. (2021)
36	rGO coordinated titania nanoplatelet	20 (TCH)	10 mg/L	500 W Xe lamp (350<λ > 1,100 nm)	7	95% after 120 min	70% after 120 min	2020 Li C. et al. (2020)

^{a}Light wavelength was not specified in the original paper.

Free pH: medium pH was not controlled.

Abbreviations: TC, tetracycline; TCH, tetracycline hydrochloride.

5.2 Titania-Based Composites

5.2.1 Immobilized Titania Composites

In addition to enhanced visible light activity, the practical and large scale application of Titania would necessitate catalyst stability and recyclability. Accordingly, many studies have investigated the immobilization of doped-TiO_2 on various polymeric (Chen Y. et al., 2019; Mahdavi et al., 2019), carbonaceous and ceramic supports such as polyphenylenediamine (POPD) (Yu et al., 2014), graphene, reduced graphene oxide (rGO) (Cao et al., 2016; Huo et al., 2016; Wang W. et al., 2017; Zhang F. J. et al., 2017; Tang et al., 2018; Jamali Alyani et al., 2019; Tabatabai-Yazdi et al., 2020), mesoporous carbon (Fang et al., 2019), MOFs (He et al., 2018; Yuan et al., 2021), zeolites (Saadati et al., 2016b; Liu M. et al., 2019), and silica (Yu et al., 2014; Chen and Liu, 2016; Chen and Liu, 2017; Zyoud et al., 2017; Li J. et al., 2019; Chen Y. et al., 2019; Wang et al., 2019). These systems are prepared as composites (Li R. et al., 2020), and the solid support provides three primary advantages: 1) high surface area which increases tetracycline adsorption, 2) enhanced light absorption and electron entrapment which enhances photocatalytic activity, and 3) reduced sintering and aggregation which leads to superior stability. The superior performance of these composite systems is also attributed to the presence of synergistic effects between the dopant and support (Bahadar Khan and Kalsoom, 2019). **Table 6** presents examples of immobilized TiO_2-based composite systems and their efficiencies for tetracycline degradation under visible light spectra.

Graphene is a planar form of carbon atoms with a crystal-like honeycomb structure, high specific surface area, good charge carrier transfer, zero band gap energy, and high interfacial adsorbing properties. Graphene immobilization of TiO_2 can shift the light spectrum absorbance of the photocatalyst toward visible light and minimize recombination of the electron/hole pairs (Koe et al., 2019). Zhang et al. (Zhang S. et al., 2017) prepared a 2D sandwich-like TiO_2-reduced graphene oxide (TiO_2-rGO) composite using the Pickering emulsion approach to investigate tetracycline hydrochloride degradation under xenon lamp as a visible light source. The unique mesoporous structure on both sides of the rGO significantly enhanced the tetracycline hydrochloride degradation by increasing the surface area of the catalyst and adsorption of the contaminant, promoting electron transfer, and minimizing recombination of the $(e^-)/(h^+)$ pairs. TiO_2-rGO degraded (96%) of the initial tetracycline hydrochloride concentration, whereas unmodified TiO_2 only degraded (28%) of the tetracycline hydrochloride. The authors suggested that the large number of mesoporous voids increased the number of exposed active sites of

TiO_2, decreased the transport route length, and accelerated the electron transfer step. The visible light activity of this graphene-immobilized catalyst was attributed to the addition of rGO, which lowered the band gap energy of TiO_2 to 3.05.

Polymeric supports are nontoxic, low cost, widely available, resistant to UV light, durable, mechanically stable, and photostable. The hydrophobic properties of many polymers enables them to promote catalyst adsorption by increasing the pollutant concentration on its outer surface (Arif et al., 2020). Wang et al. (Wang C. et al., 2017) prepared a photocatalytic nanocomposite membrane of Au-doped TiO_2 supported on polydopamine (pDA)-coated polyvinylidene fluoride (PVDF) (Au-TiO_2/pDA/PVDF). The nanocomposite membrane was used to degrade tetracycline under 300 W Xenon lamp as a visible light source. The authors reported that the visible light–induced tetracycline removal efficiency of Au-TiO_2/pDA/PVDF was (51%) higher than that of undoped TiO_2/pDA/PVDF and (26%) higher than that of Au-doped TiO_2. They also reported that pDA acted as a glue to stabilize TiO_2 on the PVDF membrane, and functioned as a photosensitizer to widen the light absorbance spectrum of the catalyst. The authors proposed that the plasmon resonance effect of Au enhanced catalyst activity by accelerating photogenerated electron transfer from Au into the conduction band of the mother catalyst TiO_2.

Ceramics have a large surface area, very good permeability, excellent strength, and high absorptivity (Mohd Adnan et al., 2018). Chen et al. (Chen and Liu, 2017) used the sol-gel method to prepare a magnetically recyclable Ce/N co-doped $TiO_2/NiFe_2O_4$/diatomite ternary hybrid catalyst (CN-TND) for tetracycline degradation under 150 W xenon lamp as a visible light source. Each of the N and Ce dopants improved the photocatalyst surface properties and suppressed the formation of TiO_2 crystals. The authors observed that Ce/N co-doped TiO_2/diatomite exhibited a slight redshift in its light absorption spectrum. CN-TND had slightly better tetracycline degradation efficiency (98%) than the N-doped $TiO_2/NiFe_2O_4$/diatomite (95%) degradation efficiency due to the addition of Ce. The presence of ferrite ($NiFe_2O_4$) enhanced electron transfer and reduced charge carrier recombination. The improved performance of CN-TND was ascribed to the synergistic effect of the Ce and N dopants, which effectively widened the visible light absorption by the catalyst. CN-TND had ferromagnetism properties, was easily recovered from the reaction medium, and was reused five times with minimal loss in activity (0.5%). CN-TND achieved nearly complete tetracycline mineralization with (100%) TOC removal compared to only (52%) removal by the Ce/N co-doped TiO_2.

Microporous structured supports such as zeolites were investigated for TiO_2 modification. Liu et al. (Liu M. et al., 2019) used the hydrothermal method to synthesize a Fe_2O_3-TiO_2/Fe-Zeolite immobilized composite (Fe_2O_3-TiO_2/FeZ). The composite catalyst was tested for oxytetracycline degradation using a 200 W 455 nm LED lamp as a visible light source. The Fe_2O_3-TiO_2/FeZ composite exhibited a higher surface area (1,445 m^2/g) than that of zeolite (844 m^2/g), and had outstanding adsorption of oxytetracycline (94%) and improved activity under visible light. The visible light photocatalytic degradation efficiency of Fe_2O_3-TiO_2/FeZ was (98%), indicating its improved visible light absorption (400–600 nm), high adsorption of oxytetracycline, and enhanced rate of photogenerated charge carriers. Fe_2O_3-TiO_2/FeZ had good stability after the fourth use and maintained (80%) efficiency.

In addition to zeolites, metal-organic frameworks (MOFs) have been investigated for the immobilization of TiO_2. MOFs are hybrid organic-inorganic, low cost, and environmentally friendly micro-porous materials with unique morphological properties and superior surface areas (Gautam et al., 2020). When combined with semiconductors such as TiO_2, MOFs form hierarchical nanostructures with enhanced photocatalytic properties (He et al., 2018). He et al. (He et al., 2018) applied one-dimensional MOF [Materials Institute Lavoisier 1D (MIL)-100(Fe)] over TiO_2 nanoarrays [1D MIL-100(Fe)/TiO_2] by insitu growth of MIL-100(Fe) on the TiO_2 nanoarrays. The catalyst was tested for tetracycline degradation using a 450 W Xe lamp as a visible light source (He et al., 2018). The growth of 1D MIL-100(Fe) over TiO_2 nanoarrays increased the surface roughness of these nanoarrays, enhanced the visible light absorption of the composite catalyst (<600 nm), and improved the electron/hole separation and the accessibility of active sites. The composite 1D MIL-100(Fe)/TiO_2 photocatalyst achieved (90.79%) tetracycline degradation efficiency compared to only (35.22%) degradation efficiency achieved by unmodified TiO_2 nanoarrays. The composite catalyst was easily recovered and maintained good stability (70%) after the fifth use.

The proposed mechanism of tetracycline degradation by 1D MIL-100(Fe)/TiO_2 is presented in **Figure 4**. Upon irradiation, electrons in the VB of TiO_2 are excited into its CB (**Eq. 1**), while MIL-100(Fe) is activated *via* the direct excitation of FeO as well as ligand-to-metal charge transfer. The electrons and holes react with water and oxygen molecules to produce (•OH) and ($O_2^{\bullet -}$) radicals (**Eqs 2**, **3**, **7**, **8**, **9**, **10**). In the presence of H_2O_2, Fe(III) in MIL-100(Fe) undergoes Fenton-like reactions and reacts with H_2O_2 to further boost the formation of (•OH) radicals as shown in (**Figure 4**). The formed radicals synergistically degrade TC molecules under visible light (**Eqs 4**, **5**, **6**).

5.2.2 Nanostructured Titania Composites

Nanostructured Titania composites enhance the catalyst's surface area and crystal morphology, and they include TiO_2-based nanospheres, nanosheets, nanowires, nanorods, nanotubes, and nanoparticles (Choi et al., 2014; Bahadar Khan and Kalsoom, 2019). Nanostructured Titania composites also enhance chemical, mechanical, electronic, and optical properties of Titania. **Table 6** presents examples of nanostructured TiO_2-based composite systems that have been used for tetracyclines degradation under visible light.

Chen et al. (Chen et al., 2016) used the electrochemical anodic oxidation method to modify immobilized TiO_2 nanobelts (NBs) with Au and CuS nanoparticles, and tested the composite catalyst for oxytetracycline removal using simulated solar light irradiation (35 W Xe lamp). Au-CuS/TiO_2 NBs exhibited enhanced visible light (solar) absorption due the lowest band gap energy (2.65 eV) and the highest visible light absorption intensity (520–620 nm) compared to Au-TiO_2 NBs, CuS-TiO_2 NBs, and TiO_2 NBs. The oxytetracycline degradation efficiency of Au-CuS/TiO_2 NBs after

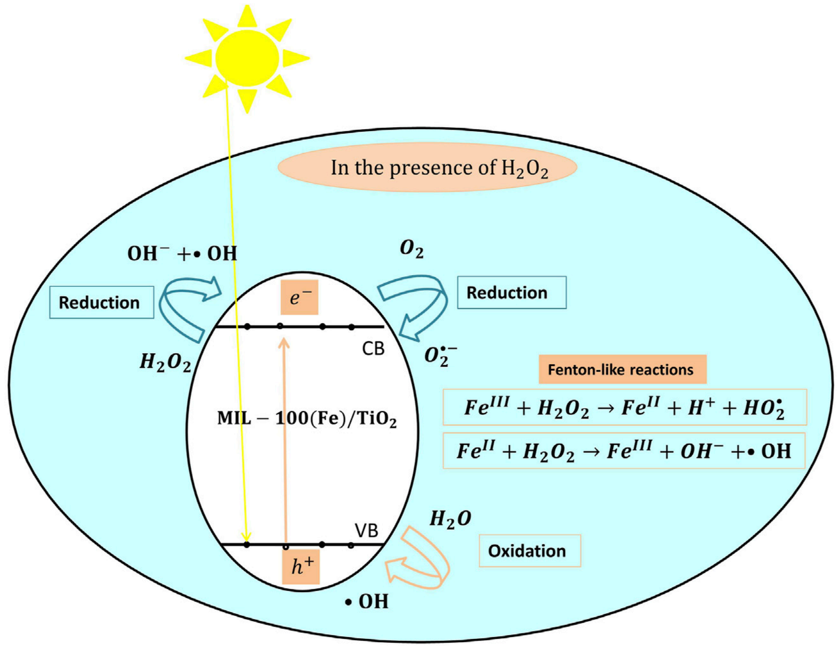

FIGURE 4 | The proposed photocatalytic degradation mechanism of tetracycline by 1D MIL-100(Fe)/TiO_2 catalyst under visible light.

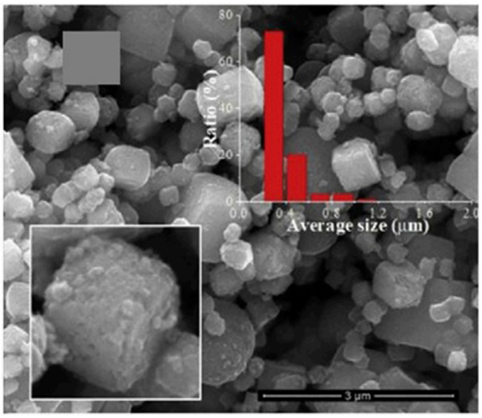

FIGURE 5 | SEM image of the core-shell structured platinum (Pt)-enhanced amorphous (Am) TiO_2-filled mesoporous TiO_2 crystals (MCs) (MCs@Pt@Am) photocatalyst, reprinted with permission from Elsevier (Lyu et al., 2019).

1 h was as high as (96%), whereas the oxytetracycline degradation efficiencies of Au-TiO_2 NBs, CuS-TiO_2 NBs, and TiO_2 NBs were (85%), (76%), and (66%), respectively. The authors ascribed the improved degradation efficiency of this catalyst to its ability to hinder recombination of photogenerated electron-hole pairs as a result of efficient interfacial charge transfer, and to the increased number of charge carriers participating in photocatalysis. The authors also concluded that visible light absorption was promoted by the plasmon resonance effect of Au, whereas CuS-TiO_2 NBs promoted light absorption in the near-infrared region. Additionally, the authors attributed the improved performance of Au–CuS/TiO_2 to the ideal dispersion of both the Au and CuS on the smooth surface of TiO_2 NBs that formed a uniform surface composite structure. The total organic carbon (TOC) removal efficiency achieved by Au-CuS/TiO_2 NBs was (68%), whereas that of TiO_2 NBs was only (40%).

Lyu et al. (Lyu et al., 2019) used the hydrothermal method coupled with chemical reduction to prepare platinum (Pt)-enhanced amorphous (Am) TiO_2-filled mesoporous TiO_2 crystals (MCs) (MCs@Pt@Am). This catalyst was tested for tetracycline hydrochloride degradation using a 500 W xenon lamp as a visible light source (Lyu et al., 2019). The authors created a new hierarchical porous core-shell structure by filling amorphous TiO_2 in the pores of Pt-doped mesoporous TiO_2 crystals, and reported that the core-shell structured catalyst (**Figure 5**) exhibited a larger surface area and particle size, higher tetracycline hydrochloride adsorption capacity, and reduced shell thickness as compared to TiO_2 crystals. These properties inhibited recombination of the electron/hole pairs and facilitated the migration of the positive hole into the catalyst surface while Pt-doping reduced the band gap energy of the catalyst and enhanced its visible light absorption. The photocatalytic degradation efficiency of tetracycline hydrochloride by MCs@Pt@Am was (100%), whereas that of amorphous TiO_2-coated mesoporous TiO_2 crystals was (89%), and that of mesoporous TiO_2 crystals was (60%). MCs@Pt@Am degraded (77%) of the initial TOC content, whereas amorphous TiO_2-coated mesoporous TiO_2 crystals degraded only (60%) of the initial TOC concentration.

TABLE 7 | Examples of titania-based heterojunction photocatalysts.

#	Modified titania	TCs initial concentration (mg/L)	Catalyst concentration	Light source	pH	Removal % by TiO_2-Based heterojunction photocatalysts	Removal % by titania	Year and ref
A. Titania-Based heterojunctions: Binary heterojunctions								
1	TiO_2@ sulfur- doped carbon nitride nanocomposite	10 (TC)	0.1 g/L	300 W xenon (xe) lamp (λ > 420 nm)	4.5	98.1% after 60 min	35.1% after 60 min	2021 Divakaran et al. (2021)
2	N-doped TiO_2@ $Bi_2W_xMo_{1-x}O_6$ core-shell nanofibers	40 (TC)	0.3 g/L	300 W Xe lamp (λ > 400 nm)	6	100% after 90 min	20% after 90 min	2020 Ghoreishian et al. (2020)
3	TiO_2 nanoparticle/ $SnNb_2O_6$ nanosheet	35 (TCH)	1 g/L	500 W Tungsten lamp[a]	Free	75.5% after 240 min	63.8% after 240 min	2017 Jin et al. (2017)
4	CuO/Ti-MCM-48	19.24 (TCH)	1 g/L	Solar simulator[a]	Free	93% after 80 min	50% after 80 min	2018 Duan et al. (2018)
5	TiO_2-coated α-Fe_2O_3 core-shell heterojunction	50 (TCH)	0.2 g/L	300 W Xe lamp (λ > 420 nm)	5.5	100% after 120 min	–	2018 Zheng et al. (2018)
6	CeO_x-coupled MIL-125-derived C-TiO_2	40 (TC)	1 g/L	500 W Xe lamp (λ > 400 nm)	Free	83.5% after 180 min	30.3% after 180 min	2021 Yuan et al. (2021)
7	Ultrafine TiO_2 nanoparticle-modified g-C_3N_4 heterojunction	20 (TCH)	0.25 g/L	150 W Xe lamp[a]	7	99.4% after 120 min	95.81% after 120 min	2020 Zhang B. et al. (2020)
8	Black-TiO_2/$CoTiO_3$ Z-scheme heterojunction	20 (TC)	1 g/L	50 W LED lamps (450<λ < 650 nm)	Free	82.4% after 30 min	28.3% after 80 min by black-TiO_2	2021 Mousavi and Ghasemi, (2021)
9	TiO_2/high-crystalline g-C_3N_4 composite	10 (TC)	0.2 g/L	300 W Xe lamp (λ > 400 nm)	Free	91% after 120 min	6% after 120 min	2020 Guo et al. (2020)
10	Ag/Ag_3PO_4 nanoparticles/ cobalt- doped TiO_2 nanosheets	20 (TC)	1 g/L	500 W halogen lamp[a]	Free	66.80% after 140 min	—	2021 Mokhtari Nesfchi et al. (2021)
11	TiO_2-coupled $NiTiO_3$ nanocomposites	—	1 g/L	250 W Xe lamp (UV-vis, 300<λ < 800 nm)	Free	58% after 120 min	—	2018 Lakhera et al. (2018)
12	BiOXs/TiO_2	30 (TC)	0.2 g/L	300 W Xe lamp (λ > 400 nm)	Free	90% after 180 min	80% after 180 min	2019 Li L. et al. (2019)
13	$BiFeO_3$/TiO_2 p-n heterojunction	20 (TC)	1 g/L	300 W Xe lamp[a]	5	72.2% after 180 min	38.3% after 180 min	2021 Liao et al. (2021)
14	Co_3O_4-TiO_2/GO	10 Oxy-(TC)	0.25 g/L	300 W Xe solar simulator (λ > 420 nm)	Free	91% after 90 min	30% after 90 min	2017 Jo et al. (2017)
15	Reduced graphene oxide-Ag_2O/TiO_2 nanobelts composites	10 (TC)	0.4 g/L	300 W Xe arc lamp (λ > 420 nm)	Free	18% after 60 min	18% after 60 min	2017 Hu et al. (2017)
16	Z-scheme CdTe/TiO_2 heterostructure	20 (TCH)	0.6 g/L	400 W halogen lamp (λ > 420 nm)	Free	78% after 30 min	62% after 30 min	2018 Gong et al. (2018)
17	Carbon fiber/TiO_2/Bi_2WO_6 heterojunctions	10 (TCH)	Bundles (length ~4 cm, weight 0.15 g)	300 W Xe lamp (λ > 400 nm)	Free	95.1% after 60 min	—	2018 Xu et al. (2018)
18	TiO_2/BiOCl composite	30 (TC)	1 g/L	300 W Xe lamp (λ > 400 nm)	3	90% after 240 min	33% after 240 min	2019 Hu et al. (2019)
19	Mo-C co-doped TiO_2 with fluorine-doped tin- oxide	20 (TC)	—	500 W Xe lamp (λ > 420 nm)	7	90% after 100 min	—	2019 Niu et al. (2019)
20	N-doped TiO_2/calcium ferrite/diatomite	10 (TC)	1 g/L	150 W Xe lamp (λ > 400 nm)	Free	91.7% after 120 min	—	2019 Chen Y. et al. (2019)
21	N-doped TiO_2/strontium ferrite/diatomite	10 (TC)	2 g/L	150 W Xe lamp (λ > 400 nm)	Free	92.2% after 120 min	—	2019 Wu, (2019)
22	g-C_3N_4@Co-TiO_2 membrane	20 (TCH)	5 mg of membranes (2 × 2 cm^2)/10 ml of solution	300 W Xe lamp (λ > 420 nm)	7	90.8% within 60 min	—	2020 Song et al. (2020)
23	CeO_2/TiO_2 composites	40 (TC)	1 g/L	500 W Xe lamp (λ > 420 nm)	Free	99% within 80 min	10% within 80 min	2020 Pudukudy et al. (2020)
24	$MnCo_2O_{4.5}$ Deposited TiO_2 Nanotube Array	10 (TC)	2.25 cm^2	500 W Xe lamp[a]	Free	93.1% within 120 min	—	2020 Bi et al. (2020)

(Continued on following page)

TABLE 7 | (*Continued*) Examples of titania-based heterojunction photocatalysts.

#	Modified titania	TCs initial concentration (mg/L)	Catalyst concentration	Light source	pH	Removal % by TiO_2-Based heterojunction photocatalysts	Removal % by titania	Year and ref
B. Titania-Based Heterojunctions: Ternary Heterojunctions								
25	Carbon plane/g-C_3N_4/TiO_2 nanocomposite	10 (TC)	1 g/L	500 W Xe lamp (λ > 400 nm)	Free	94.0% after 180 min	46% after 180 min	2019 Liu C. et al. (2019)
26	K-doped g-C_3N_4/TiO_2/CdS	20 (TC)	1 g/L	300 W Xe lamp (λ > 420 nm)	Free	94.2% after 30 min	69.47% after 30 min	2021 Liu et al. (2021)
27	g-C_3N_4/Ti_3C_2/TiO_2 nanotube arrays on Ti meshes	10 (TCH)	1.5 × 1.0 cm	300 W Xe lamp (λ > 420 nm)	Free	85.12% after 180 min	—	2020 Diao et al. (2020)
C. Titania-Based Homogeneous Junctions: Facet Junction								
28	{101} and {001} facets co-exposed TiO_2 hollow sphere	10 (TC)	0.2 g/L	300 W Xe lamp (λ > 400 nm)	Free	90.1% after 120 min	—	2020 Zhang S. et al. (2020)

[a] *Light wavelength was not specified in the original paper.*
Free pH: medium pH was not controlled.
Abbreviations: TC, tetracycline; TCH, tetracycline hydrochloride.

All reported composite systems significantly improve TiO_2 catalyst performance for tetracyclines degradation under visible light. These properties arise from the synergistic effects between different moieties of the composite system and from the enhanced surface area and morphology of the photocatalyst. Many studies have successfully constructed and applied immobilized and nanostructured Titania composites for tetracycline degradation under visible light, and we conclude that both approaches are valuable for Titania modification. Although both immobilized and nanostructured Titania composites have high AB degradation efficiency percentages (>90%), immobilized Titania composites are preferred over nanostructured Titania composites due to their ease of recovery and reuse, especially in industrial applications.

5.3 Titania-Based Heterojunctions

Heterojunction construction is another approach for the modification of Titania and the enhancement of its photocatalytic properties (Marcelino and Amorim, 2019; Li R. et al., 2020). Heterojunctions are constructed by forming a direct contact interface between two different semiconductors (Li R. et al., 2020; Yang et al., 2021). The two semiconductors must have different band gaps, a wide band gap (TiO_2) and a narrow band gap, with the minimum band gap energy in the visible light region (Marcelino and Amorim, 2019; Li R. et al., 2020). This condition enhances the visible light absorption and photocatalytic activity of the heterojunction (Li R. et al., 2020). Heterojunctions promote the migration of charge carriers (electrons and holes) from one semiconductor to the other and minimize charge carrier recombination (Marcelino and Amorim, 2019; Li R. et al., 2020). Most TiO_2-based heterojunctions are binary and can be classified based on the mechanism of separation of $(e^-)/(h^+)$ pairs: p-n heterojunctions; type I (straddling gap); type II (staggered gap); type III (broken gap); and direct Z-scheme heterojunctions (Li R. et al., 2020; Yang et al., 2021). **Table 7** summarizes these systems along with their efficiencies for tetracyclines degradation under various visible light irradiations. As shown in **Table 7**, binary heterojunctions are the most widely applied composites compared to ternary heterojunctions and homojunctions. Although ternary heterojunctions have very good tetracyclines removal efficiencies under visible light compared to binary heterojunctions, they require the use of an additional semiconductor, which involves additional costs.

5.3.1 Binary TiO_2-Based Heterojunctions

Binary heterojunctions are composed of two different semiconductors with different band gap energy levels (Marchelek et al., 2016). Conventional binary heterojunctions include type (I), type (II), and type (III) (Low et al., 2017). Nonconventional binary heterojunctions include p-n heterojunctions and Z-scheme heterojunctions (Li R. et al., 2020). The various conduction and valence level arrangements and mechanisms of these heterojunction catalysts are detailed in the following references (Low et al., 2017; Li R. et al., 2020).

Examples of binary TiO_2-based heterojunctions include TiO_2/BiOCl (Hu et al., 2019) and α-Fe_2O_3@TiO_2 (Zheng et al., 2018). The α-Fe_2O_3@TiO_2 is a type (I) heterojunction where the covalent bond (CB) of the first semiconductor (TiO_2) exists at a higher position than the CB of the second semiconductor (Fe_2O_3), but the valence bond (VB) of Fe_2O_3 is above that of TiO_2. In this type, electrons move from the semiconductor with lower CB (α-Fe_2O_3) into the semiconductor with higher CB (TiO_2). The α-Fe_2O_3@TiO_2 catalyst resulted in (100%) tetracycline hydrochloride degradation efficiency and (98%) TOC removal efficiency in

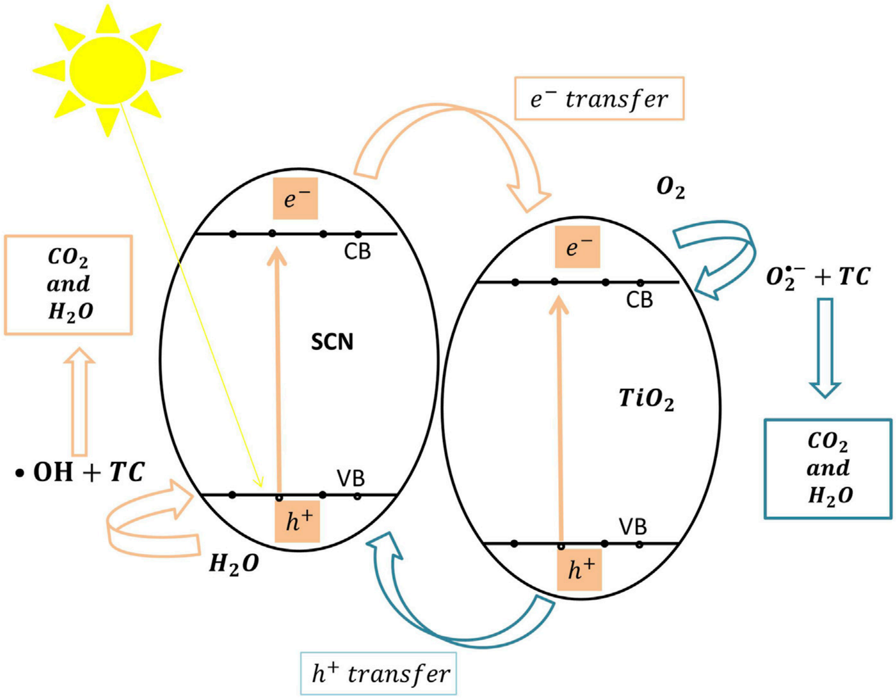

FIGURE 6 | The proposed photocatalytic degradation mechanism of tetracycline by TiO_2@sulfur doped carbon nitride nanocomposite catalyst classified as type (II) heterojunction under visible light.

only 120 min using a 300 W xenon lamp (Zheng et al., 2018). The proposed mechanism for the degradation of tetracycline hydrochloride over the Fe_2O_3@TiO_2 includes reduction/oxidation reactions by electron/hole pairs followed by the formation of the radicals (**Eqs 2**, **3**, **7**, **8**, **9**, **10**) necessary for tetracycline hydrochloride degradation (**Eqs 4**, **5**, **6**).

The TiO_2-coated cubic α-Fe_2O_3 core-shell heterojunction was synthesized using the hydrothermal method. The excellent visible light performance of the catalyst was primarily attributed to the well-matched interface between the cubic α-Fe_2O_3 and TiO_2 shell, the low band gap energy (1.97 eV), and enhanced visible light harvesting. The α-Fe_2O_3@TiO_2 also had enhanced electron transfer through the heterojunction interface, better charge carrier separation, and minimized electron/hole recombination. The α-Fe_2O_3@TiO_2 maintained excellent degradation efficiency (95%) and stability even after the fifth use. The authors reported that the core-shell structure of the TiO_2 shell and the cubic morphology of α-Fe_2O_3 core led to an enhanced electron transfer and minimized electron/hole recombination effect.

Several studies have investigated type (II) TiO_2-based binary heterojunctions. TiO_2@sulfur doped carbon nitride nanocomposite reported by Divakaran et al. (Divakaran et al., 2021) and TiO_2/$SnNb_2O_6$ nanosheet reported by Jin et al. (Jin et al., 2017) are examples of this type of binary heterojunctions. In type (II), the CB and VB of the first semiconductor (sulfur doped carbon nitride: SCN) are higher than the corresponding CB and VB of the second semiconductor (TiO_2) (**Figure 6**). This leads to significant charge carrier separation because excited electrons migrate to the second semiconductor and the positive holes move into the first semiconductor. TiO_2@sulfur doped carbon nitride nanocomposite achieved (98.1%) degradation efficiency of the initial tetracycline concentration in 60 min, and the TiO_2/$SnNb_2O_6$ nanosheet achieved (75.5%) degradation efficiency of tetracycline hydrochloride. Additionally, Gong et al. (Gong et al., 2018) applied Z-scheme CdTe/TiO_2 heterojunction which was able to degrade (78%) of the initial tetracycline hydrochloride concentration after 30 min. A Z-scheme heterojunction has the same CB and VB arrangements of type (II) heterojunction with totally different electron migration route between the first and second semiconductors (Low et al., 2017; Li R. et al., 2020). Upon photo-excitation of electrons, the photo-generated electrons in the second semiconductor combine with the positive holes in the first semiconductor. Consequently, these electron/hole pairs generate the reactive radicals *via* (**Eqs 2**, **3**, **7**, **8**, **9**, **10**) which themselves degrade the TC into CO_2 and H_2O via (**Eqs 4**, **5**, **6**).

Liao et al. (Liao et al., 2021) prepared a binary p-n junction using $BiFeO_3$/TiO_2 catalyst, and reported a (72.2%) tetracycline degradation efficiency after 180 min. This catalyst is composed of p-type and n-type semiconductors separated by a charged space region around the interface known as an internal electric field. This electric field minimizes charge carrier recombination by accelerating migration of the excited electrons and positive holes into the CB of the n-type semiconductor and VB of the p-type semiconductor, respectively (Low et al., 2017). In the mechanism

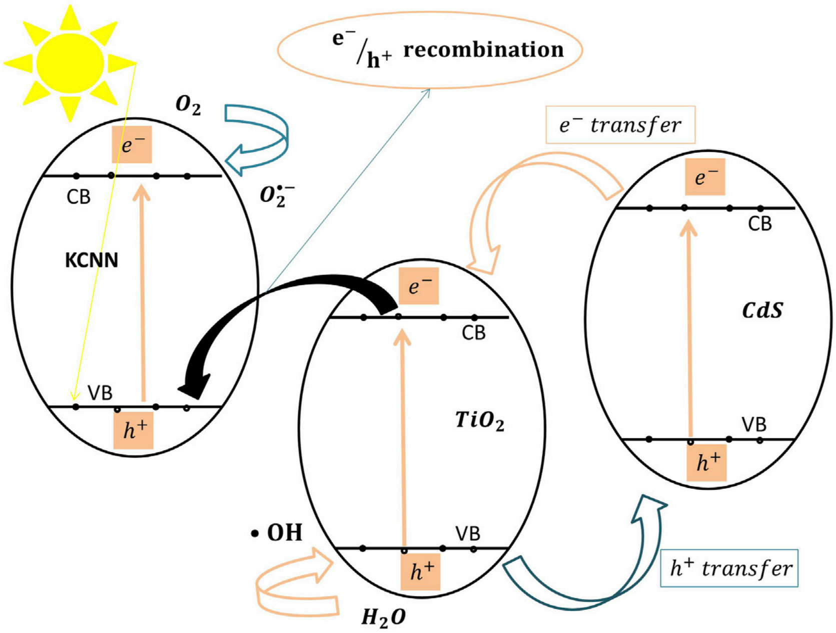

FIGURE 7 | The proposed photocatalytic degradation mechanism of tetracycline by the KCNNT@CdS ternary heterojunction catalyst under visible light.

proposed by Liao et al., excited electrons in the CB of $BiFeO_3$ move into the CB of n-type TiO_2 semiconductor and similarly the positive holes in the VB of $BiFeO_3$ move into VB of n-type TiO_2 ensuring minimized recombination effect of $(h^+)/(e^-)$. The rapid migration of the charge carriers in this catalyst is mainly due to the ferroelectric effect of $BiFeO_3$. While (h^+) oxidizes water molecules into hydroxyl radicals, (e^-) reduces adsorbed oxygen molecules into super oxide radicals (**Eqs 2**, **3**, **7**, **8**, **9**, **10**). Tetracycline molecules are photocatalytically degraded by these radicals under visible light according to (**Eqs 4**, **5**, **6**).

5.3.2 Ternary TiO_2-Based Heterojunctions

Ternary heterojunctions are composed of three coupled semiconductors to form a ternary contact interface, which enhances electron excitation and photo-efficiency (Marchelek et al., 2016). Liu et al. (Liu et al., 2021) used the hydrothermal method to construct a novel ternary composite heterojunction with superior photocatalytic properties, which consisted of a synthesized K-doped g-C_3N_4/TiO_2/CdS (KCNNT@CdS) ternary heterojunction nanocomposite. This nanocomposite photocatalyst was tested for tetracycline degradation efficiency under visible light using a 300 W xenon lamp. This photocatalyst showed excellent visible light–induced tetracycline degradation efficiency (94.2%) as compared to that of unmodified TiO_2 (69.47%). KCNNT@CdS degraded (40.1%) of the initial TOC concentration after 30 min. The authors attributed this performance enhancement to the presence of CdS, which behaved as an electron supplier and promoted charge carrier separation. The presence of TiO_2 itself was crucial to enhance the adsorption of tetracycline molecules on the surface of the composite KCNNT@CdS. The K dopant on the g-C_3N_4 nanosheet enhanced visible light absorption, and the nanostructured morphology of g-C_3N_4 minimized charge carrier recombination and enhanced electron transfer (Liu et al., 2020). KCNNT@CdS maintained excellent stability after four uses. **Figure 7** shows the photocatalytic degradation mechanism of the KCNNT@CdS ternary heterojunction system. In this proposed mechanism, CdS behaves as an electron provider for TiO_2 because all excited electrons of CdS migrate into the CB of TiO_2 and then move into the VB of KCNN to combine with the positive holes. Specifically (•OH), (h^+), and $(O_2^{\bullet-})$, generated according to (**Eqs 2**, **3**, **7**, **8**, **9**, **10**) are critical for tetracycline degradation under visible light irradiation.

Immobilized TiO_2-based heterojunction systems offer easy catalyst recovery. Carbonaceous nanomaterials function as catalyst supports and can form a heterojunction with TiO_2 at the molecular level, thereby generating a ternary heterojunction. The nanocarbon material in the ternary heterojunction participates in the photocatalytic degradation process by controlling the electron transfer mechanism (Scaria et al., 2020). Liu et al. (Liu M. et al., 2019) prepared a ternary carbon plane/g-C_3N_4/TiO_2 nanocomposite heterojunction by anchoring the carbon plane into g-C_3N_4 and then coupling it with TiO_2, and they tested it for tetracycline degradation under visible light using a 500 W xenon lamp. The authors reported that the presence of the carbon plane was necessary to form the required ternary heterojunction contact in the prepared carbon plane/g-C_3N_4/TiO_2 nanostructured catalyst. The carbon plane/g-C_3N_4/TiO_2 photocatalyst degraded (94.0%) of the initial tetracycline concentration, whereas unmodified TiO_2 only degraded (46%) of the tetracycline. This improved visible light activity of the photocatalyst was ascribed to the heterojunction structure with effective ternary contact that enhanced charge carrier separation and transfer, and the inhibited charge carrier recombination.

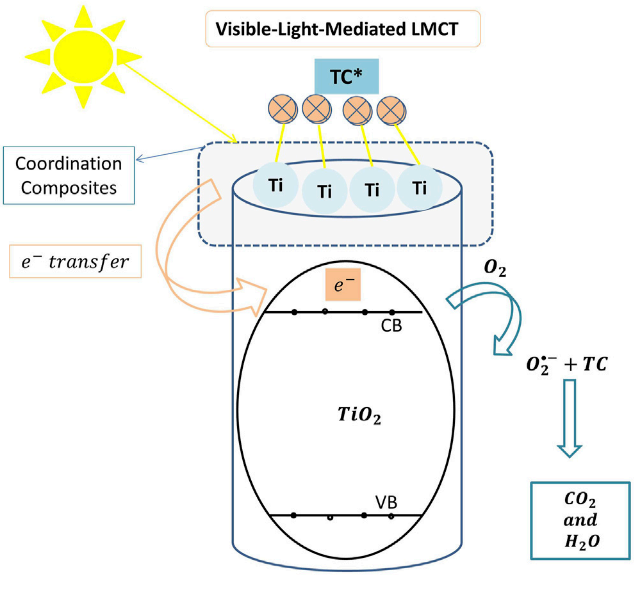

FIGURE 8 | The proposed photocatalytic degradation mechanism of tetracycline by the TiO_2 hollow sphere (001-HT) facet heterojunction catalyst under visible light.

5.3.3 TiO_2-Based Homogenous Facet Junctions

Homogenous facet junctions are composed of different crystal planes of the same semiconductor in the same catalyst particle. The exposed surfaces generate a synergistic effect that enables local redox reactions and enhances charge separation and photoexcitation of the electrons (Yang et al., 2021). Zhang et al. (Zhang S. et al., 2020) prepared a homogeneous facet junction composed of {101} and {001} facets that were co-exposed to a TiO_2 hollow sphere (001-HT) facet heterojunction using a gentle sodium fluoride (NaF) treatment. This catalyst was used for tetracycline degradation under visible light using a 300 W xenon lamp. The reported tetracycline degradation efficiency of the 001-HT facet heterojunction photocatalyst (90.1%) was higher than that of the {101} facet-exposed TiO_2 hollow sphere (HT) that was obtained without NaF treatment (80%). The authors attributed the improved photocatalytic degradation of 001-HT to the formation of a {101}/{001} facet heterojunction, which enhanced visible light absorption, extended the life of excited electrons, increased charge carrier migration, and minimized charge carrier recombination. The enhanced visible light absorption of 001-HT was attributed to ligand-to-metal charge transfer (LMCT) due to the formation of coordination complexes between tetracycline molecules and Ti (IV) ions (**Figure 8**). Higher surface area, larger pore diameter, rougher surface, and bigger crystalline grains were reported for (001-HT) as compared to (HT). The photogenerated electrons in the highest occupied molecular orbital (HOMO) of the tetracycline antibiotic migrate into the CB of TiO_2 hollow sphere while no electron excitation occurs in TiO_2. The transferred electrons reduce the oxygen molecules into super oxide radicals which attack the tetracycline molecules in the aqueous medium and convert them into H_2O and CO_2 (**Eqs 4**, **5**, **6**).

5.4 Recommendations on Most Promising TiO_2 Systems for Tetracyclines Degradation

In summary, all previous studies investigating Titania modifications clearly indicate that a combination of more than one modification method is crucial to achieve superior properties of photoactivity, stability, and ease of recovery for practical applications of the catalyst. For example, metal/nonmetal doping can enhance the visible light absorption of Titania; however, further immobilization of the doped TiO_2 through the formation of composite systems is essential to enhance catalyst morphology, photocatalytic properties, and stability. In metal/nonmetal doping, optimal dopant concentrations are recommended to prevent excess charge carriers, which can promote charge carrier recombination (Sponza and Koyuncuoglu, 2019; Zhang et al., 2019). The construction of heterojunction composites through the formation of a direct interface between Titania and another semiconductor enhances TiO_2 photocatalytic properties by improving the migration rate of charge carriers (i.e., both electron and positive holes) and minimizing their recombination. However, large-scale application of heterojunction photocatalysts is limited due to the complexity of fabrication, high cost, and low recycling efficiency (Li R. et al., 2020; Yang et al., 2021). A conclusion on the optimal modification method requires a complete understanding of the thermodynamics of the surface redox reactions and reaction mechanisms (Basavarajappa et al., 2020).

Based on our literature review, the best performing systems include 1) TiO_2 nanobelts modified with Au and CuS nanoparticles composite (Chen et al., 2016) which degraded (96%) of the initial oxytetracycline concentration in 60 min, indicating excellent degradation efficiency compared to other composites; 2) N-doped TiO_2/rGO composites (Tang et al., 2018) that exhibited superior activity, with (98%) tetracycline hydrochloride degradation efficiency in 60 min due to N-doping and the addition of the rGO support; 3) Fe_2O_3-TiO_2/modified zeolite composite (Liu M. et al., 2019), which also exhibited 98% oxytetracycline degradation in 60 min. We recommend the following TiO_2 modifications to be further considered in future studies for the photocatalytic degradation of TCs and antibiotics in irrigation water:

- Non-metal doping of Titania (C and N) to enhance its activity under visible light, to achieve high stability, and to avoid toxic metal leaching in case of metal doping (**Sections 5.1.2**, **5.2.2**, **5.3.1**) (Palanivelu et al., 2007; Teoh et al., 2012; Wu et al., 2013; Marschall and Wang, 2014; Chen and Liu, 2016; Oseghe and Ofomaja, 2018a; Zhang T. et al., 2020; Li C. et al., 2020; Ghoreishian et al., 2020; Wu et al., 2020).
- Metal doping of Titania or composite formation using non-toxic and ferromagnetic element such as iron to enhance its visible light performance and facilitate its recovery in large-scale applications by external magnets due to the acquired

ferromagnetic property (**Section 5.2.1**) (Cao et al., 2016; Wang W. et al., 2017; Chen and Liu, 2017).

- Immobilization of the doped Titania on non-toxic supports such as carbonaceous materials to minimize recovery and maintenance costs in commercial applications and improve degradation efficiency (**Sections 5.2.1**, **5.3.2**) (Cao et al., 2016; Zhang S. et al., 2017; Zhang F. J. et al., 2017; Tang et al., 2018; Liu C. et al., 2019; Fang et al., 2019; Jamali Alyani et al., 2019; Koe et al., 2019; Scaria et al., 2020).
- Formation of doped-Titania nanostructured composites (nanosheets, nanowires, nanobelts) that enhances the catalyst's surface area and performance and facilitates its recovery and reuse in industrial scale systems (**Section 5.2.2**) (Choi et al., 2014; Chen et al., 2016; Bahadar Khan and Kalsoom, 2019; Lyu et al., 2019; Li C. et al., 2020).
- Optimization of the synthesis procedures and immobilization steps of the TiO_2 to ensure high and stable efficiency upon continuous reuse and to facilitate the recovery of the deactivated catalyst for proper and safe disposal (Sponza and Koyuncuoglu, 2019; Zhang et al., 2019; Scaria et al., 2020).
- Avoid the construction of complex and expensive heterojunction Titania photocatalysts of low recyclability, because this will create additional costs in large-scale systems and thus lower the overall cost efficiency of the proposed system (Li R. et al., 2020; Yang et al., 2021).

6 THE ENVIRONMENTAL IMPACT OF THE TiO_2 MODIFIED SYSTEMS

The environmental impact of the materials used in TiO_2 modification should be considered during the development of visible light–activated TiO_2 based photocatalysts. Safe materials with low toxicity and durable supports should be employed for catalyst immobilization to reduce the release of metals and generating secondary pollutants. These considerations will protect the environment and minimize the costs of system maintenance and catalyst recovery (Marcelino and Amorim, 2019; Li R. et al., 2020). Another important aspect is the leaching of any of these materials, used for TiO_2 modification, into the water medium and eventually into the environment. Usually researchers investigate catalyst recovery and reuse without presenting a study on the possibility of leaching of these materials (Yang et al., 2017). Nevertheless, and specifically in metal doping of TiO_2, some researechers did present leaching studies. For example, Wang et al. studied the leaching of Fe ions from Fe_3O_4/rGO/TiO_2 when used for the degradation of tetracycline hydrochloride. The authors reported only 0.5 mg/L of Fe leaching into the soution, during the first cycle of catalyst use, which they concluded to be negligible. Moreover, after five cylcels of use (Wang W. et al., 2017), the samples were characterized by XRD and FTIR and no structrual changes were detected, confirming the textural and structural stability of the Fe_3O_4/rGO/TiO_2 catalyst. For the CeO_2/TiO_2 binary heterojunction, Pudukudy et al. (Pudukudy et al., 2020) confirmed using FESEM elemental mapping, no Ce leaching after the 7^{th} use of the catalyst. Similarly, Bi et al. reported that the leached percentages of Mn and Co metals from $MnCo_2O_{4.5}$/TiO_2 catalyst were in the range (4–10%). However, it was concluded that leaching reduced the degradation efficiency of TC by only 2.9% after five runs (Bi et al., 2020).

In general, the stability of the catalyst and the leaching probability would very much depend on the water medium and the photocatalytic degradation conditions, such as the pH (Yang et al., 2017). Therefore, in real irrigation water media, it may be expected to have more pronounced leaching of the various used elements compared to laboratory distilled water media. In fact, immobilizing the catalyst on carbonaceous materials like graphene can help minimize metal leaching from titania catalysts (Scaria et al., 2020). Although, as mentioned in the above examples, metal leaching does not seem to be significant in photocatalysis, researchers should study and report the leaching of any of the catalyst's components during a photocatalytic degradation reaction using analytical techniques such as atomic absorbance spectroscopy and/or inductively coupled plasma (Marcelino and Amorim, 2019). In general, catalysts that may lead to leaching and further polluting and toxifying the water streams should be avoided, to prevent the need for a further water purification step (Bhadouria et al., 2020).

7 CONCLUSIONS AND FUTURE RESEARCH

There is clear evidence for antibiotic contamination of global ecosystems, water, and edible crops. The level of antibiotic contamination depends on the regional production and consumption of these pharmaceuticals. The use of wastewater in irrigation, animal manure, and biosolids in agriculture are important routes for the introduction of ABs into the ecosystem and edible crops. Current technologies for removing/degrading these pharmaceuticals from wastewater, such as conventional methods (biological processes, coagulation, flocculation, sedimentation, and filtration) and membrane methods, are incapable of removing these low-level and persistent organic pollutants from water. The development of innovative and efficient removal/degradation methods is urgently needed. Photocatalytic degradation is a promising method for removing organic pollutants from wastewater before using it for crop irrigation. This review summarized the current knowledge of Titania modification for the photocatalytic removal/degradation of tetracyclines from water. Titania is the most promising and studied semiconductor in this technology due to its low cost, high stability, low toxicity, good activity, and ease of modification (Teoh et al., 2012; Ibhadon and Fitzpatrick, 2013; Koe et al., 2019; You et al., 2019; Zhang et al., 2019). We recommend that a combination of methods is essential to achieve superior catalytic properties of photoactivity, stability, and ease of recovery; these methods include metal-nonmetal doping, construction of a heterojunction interface with a second semiconductor, and immobilization on a stable porous support.

The large-scale application of the proposed visible light active Titania for irrigation water is plausible, however, there still remain many challenges to bring this into application. One of the primary challenges is that the efficiency of these photocatalytic systems in large scale applications remains limited due to various reasons. One of these is the low and non-uniform light transmission into the catalyst surface (Tong et al., 2012). This limitation can be overcome by optimizing the various components of the reaction medium including the photocatalyst, the light illumination, and the reactor design to develop a commercial system for irrigation water treatment (Li and Shi, 2016). Moreover, further research is required to enhance the activation of the photocatalyst over a wide range of wavelengths, including the visible light region. It is also necessary to improve the overall mineralization and quantum efficiencies and the ease of recyclability and reusability of these photocatalysts (Tong et al., 2012). A complete mineralization of the toxic organic compounds is essential to minimize the formation of byproducts, which in some cases could be more toxic than the initial pollutant (**Section 4.1**) (Calvete et al., 2019). Most of the studies discussed in this review lacked toxicity assessments of intermediate photoproducts. We recommend that researchers conduct toxicity studies along with studies of catalyst performance.

In addition, it is worth noting that most research on the modification of Titania and other semiconductors for AB degradation utilize laboratory-scale reactors containing synthetic solutions of antibiotics in distilled water rather than in real wastewater irrigation samples. However, the observed catalyst efficiency in these laboratory systems is an overestimate and does not reflect the real-world efficiency of the catalyst in contaminated water samples. Similarly, catalyst recovery in large-scale applications is expected to be more challenging than it is in small-scale laboratory experiments (Li R. et al., 2020).

To conclude, we recommend that further research is needed to bring Titania-based photocatalytic degradation of ABs into large scale application. An efficient and easily recyclable catalyst system should be coupled with an optimum reactor design and adequate light source to guarantee a feasible large scale application.

As for the impact on humans, we conclude that human consumption of AB-contaminated water and edible crops leads to health risks because it can potentiate antibiotic resistance in human pathogens. A clear assessment of the risks imposed by antibiotic contaminants on human health is lacking. The ecotoxicological effects of using antibiotic-contaminated irrigation water and/or animal manure fertilizer have not been fully investigated and understood. This would require a clear understanding of the physiochemical properties of the antibiotics in the soil and the mechanisms of their translocation and bioaccumulation in plants (Pan and Chu, 2017). Field studies are required to accurately assess antibiotic uptake by various crops under different environmental conditions, and the impacts of antibiotic bioaccumulation in these plants (Pan and Chu, 2017).

Well-defined dietary studies are urgently needed to evaluate the impact of consumption of antibiotic-contaminated crops from real-world fields on human health (Pan and Chu, 2017). These studies should include participants of different ages consuming different edible crops planted in soil treated with different concentrations of animal manure and irrigated with antibiotic-containing wastewater.

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Resilience Analysis Framework for a Water–Energy–Food Nexus System Under Climate Change

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Climate change impacts the water–energy–food security; given the complexities of interlinkages in the nexus system, these effects may become exacerbated when feedback loops magnify detrimental effects and create vicious cycles. Resilience is understood as the system's adaptive ability to maintain its functionality even when the system is being affected by a disturbance or shock; in WEF nexus systems, climate change impacts are considered disturbances/shocks and may affect the system in different ways, depending on its resilience. Future global challenges will severely affect all vital resources and threaten environmental resilience. In this article, we present a resilience analysis framework for a water–energy–food nexus system under climate change, and we identify how such systems can become more resilient with the implementation of policies. We showcase results in the national case study of Greece. Parametric sensitivity analysis for socioecological systems is performed to identify which parameter the model is the most sensitive to. The case study is based on the structure of a system dynamics model that maps sector-specific data from major national and international databases while causal loop diagrams and stock-and-flow diagrams are presented. Through engineering and ecological resilience metrics, we quantify system resilience and identify which policy renders the system more resilient in terms of how much perturbation it can absorb and how fast it bounces back to its original state, if at all. Two policies are tested, and the framework is implemented to identify which policy is the most beneficial for the system in terms of resilience.

Keywords: system resilience, engineering resilience, ecological resilience, sensitivity analysis, climate change, system dynamics modeling, causal loop diagrams, water–energy–food-climate nexus

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INTRODUCTION

Economic growth during the last century has positively affected many people, thus providing them with the main essentials resources for living—water, energy, and food (WEF) (UNDP, 2016). These accomplishments have adverse effects on environmental assets. Worldwide, aquatic and terrestrial ecosystems have been irreparably affected, natural deposits have been exhausted, some species are facing high risk of extinction, and susceptibility to disturbances has increased (Turner et al., 2003; Vörösmarty et al., 2020; Puma, 2019). Considering the current global situation, GHG emissions are projected to increase by 50%, primarily due to a 70% growth in energy-related CO_2 emissions (Kitamori et al., 2012). To prevent that, many countries have adopted Nationally Appropriate Mitigation Actions (NAMAs) to set limits to this increase, aiming at stabilizing global temperature increase by 2°C in the future (UNFCCC, 2011). However, if no major interventions are carried out, the global temperature is expected to rise by 3.5°C by 2035 (IEA, 2010), indicating the need for imperative and drastic implementation of solutions to address the problem in a timely manner. Water security will ensure both the reduction of energy needs for the agri-food sector and generation of renewable energy supply aiming at stabilizing the GHG emissions.

Both environmental burden and lack of the combined WEF security are expected to deteriorate in the next decades, driven by overpopulation, increasingly resource-intensive lifestyles, and susceptibility to disturbances under climate change (Hoekstra and Wiedmann, 2014; Steffen et al., 2018). A WEF nexus approach seems to be able to set limits to this ongoing problem since such an approach can enhance WEF security, leading to fewer CO_2 emissions by increasing resource efficiency and integrating management and governance across sectors and scales (Hoff, 2011). Applying the nexus approach to policymaking is based on the idea that WEF systems should be addressed collectively and holistically in order to achieve WEF security (WEF, 2011; Bleischwitz et al., 2018). To achieve sustainable development at a national and ultimately the global level, other aspects such as poverty, hunger, wellbeing, equality, and environment are of equal importance. To this extent, these aspects which constitute part of the 17 sustainable development goals (SDGs) are fully interconnected with the WEF nexus under climate change (SDG2-food, SDG6-water, SDG7-energy, and SDG13-climate) since the cross-sectoral management is vital to achieving the SDGs (Flammini et al., 2014). Integrating climate change adaptation strategies into the WEF nexus can obtain efficient resource cooperation, resulting in better environmental resilience (Mpandeli et al., 2018). As the nexus approach becomes more and more popular, a lot of research has been published on the WEF nexus concept (Laspidou et al., 2020; Albrecht et al., 2018; Finley and Seiber, 2014; Stephan et al., 2018; Ioannou and Laspidou, 2018), extended Nexus approaches, such as the water–energy–food ecosystem (Malagó et al., 2021), and including land use and climate in the nexus concept (Janssen et al., 2020; Laspidou et al., 2019), with some articles focusing on the combined WEF security and system resilience (Sukhwani et al., 2019; Mguni and van Vliet, 2020). One of the greatest challenges worldwide is to provide essential human needs and resources to all in an environmentally compatible, economically resilient, and socially inclusive manner that is capable to contend with disturbances and catastrophes (Sachs et al., 2019).

At the same time, the resilience analysis approach was discussed in scientific debates, evolved from the field of ecology, and is firmly linked with sustainability science and global change research (Folke et al., 2010; Scheffer et al., 2012; Anderies, 2015). In a world characterized by uncertainty and complexity, unexpected disturbances and disasters may affect systems in unpredictable ways, reducing system performance (Nyström et al., 2019). Hence, the resilience analysis approach accentuates the need to design, develop, and manage systems for resilience with the aim to withstand and absorb unavoidable disturbances; either short-term disturbances, such as a pandemic, or long-term disturbances, such as climate change (World Bank, 2013; Hall et al., 2014; Grafton et al., 2019). Resilience literature at its early stage often uses the metaphor of a stability landscape, where resilience measures the persistence of a system and its ability to absorb change and disturbance (Holling, 1973). The resilience analysis approach is progressively urged to tackle some of the great disputes of the current century: providing WEF security to all while maintaining natural resource availability at sustainable levels; this is a great challenge, considering the extensive environmental stress caused by exploitation and climate change.

Both nexus and resilience approaches are applicable to science and to policy- and decision-making, but it is still indefinite to what degree they are expected to accomplish what they stand for to make a significant contribution to WEF security goals. In resilience modeling, there is a great deal of diversity in the literature on disturbance conceptualization, methodology, and tools for implementing different approaches. (Grafton et al., 2016; Allen et al., 2019). Similarly, for the nexus, while aiming at identifying the WEF system interlinkages under climate change conditions, there are limited advanced analytical frameworks proposed in the literature for integrated WEF policy development (Laspidou et al., 2020; Papadopoulou et al., 2020; Scott et al., 2011; Leck et al., 2015; Albrecht et al., 2018). Therefore, the convergence of objectives and concepts in both contexts led researchers to consolidate the two approaches (Guillaume et al., 2015; De Grenade et al., 2016; Stringer et al., 2018).

System dynamics modeling (Forrester, 1961; Coyle, 1997; Ford, 1999; Kelly et al., 2013) is used with the intention of simulating and analyzing complex systems, thus offering policymakers a valuable tool to comprehend the potential impacts of policy implementation (Bakhshianlamouki et al., 2020). A system dynamics model (SDM) attempts to simulate the real-world system's behavior based on the principal concepts of flows, feedback loops, and time delays. Thus, when aiming at modeling any system, it is critical to develop the model based on the behavior of the system in real-world circumstances and apprehend the interaction of the parameters affecting the system's behavior in accordance with the real system (van Emmerik et al., 2014; Chen et al., 2016). In this study, the system dynamics modeling approach is adopted to model the WEF nexus interlinkages under climate change due to its adjustability and its ability to focus on the long-term characteristics (Robinson, 1998), and thus propose policies to improve the overall behavior of the system with the aim to enhance its resilience.

In this article, we identify and quantify the WEF nexus interlinkages of a system under climate change and develop an SDM that is conceptualized to be used as a framework for nexus system resilience analysis. We focus on the nexus approach at the national level combined with system resilience analysis and parametric sensitivity analysis (SA). We present a study of the systemic reaction to disturbance and quantify different measures of resilience of socio-ecological systems (SESs) (Walker et al., 2006) to climate change for different scenarios/policies for the national case study of Greece. Our goal is to set up a comprehensive resilience analysis framework of the WEF

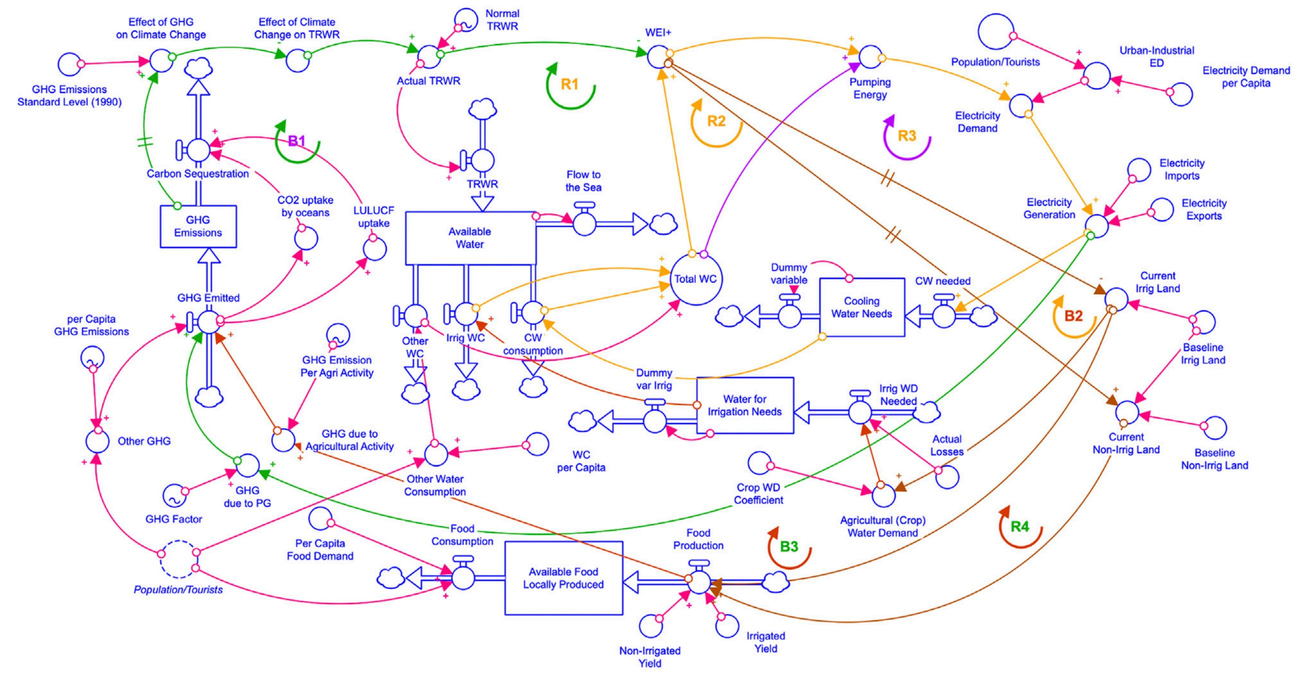

FIGURE 1 | Stock-flow diagram for the national case study of Greece.

nexus system under climate change through system dynamics modeling and causal loop analysis in order to assess and quantify causality and systemic resilience under environmental stress and shock, simulating extreme events under climate change. This analysis enhances the science-policy interface and translates the complexity of a WEF nexus system in terms that are easy to understand, thus communicating the effects of climate change and leading to informed policy-making. SA is also conducted on a system and sector level to identify variables that the system is most sensitive to. The energy and agricultural policies are modeled, and their effects on system resilience are investigated.

MATERIALS AND METHODS

The SDM was implemented in STELLA Architect (www.iseesystems.com/). We used the SIM4NEXUS project dataset (Mellios and Laspidou, 2020) that was developed for 2010 and ran simulations for 100 years (2010–2110) with a yearly time step. We focused on water for the case study of Greece (modeled as available freshwater) since water has been identified as the most vulnerable nexus sector and the one most prominently affected by the other sectors for Greece (Laspidou et al., 2019). In relation to energy, the water–energy interlinkage is monitored through cooling water (CW) since electricity is produced in thermal power plants in the country, requiring large amounts of freshwater. Hydropower is not considered in this study. The water–food interlinkage is presented through the quantities of water for irrigation and available food produced locally, while GHG emissions are produced from fossil-fuel power plants, human activities (transportation, households, services, etc.), and agricultural activity (**Figure 1**).

According to the Greek Statistical Authority (ELSTAT), Greece has a population of 10.4 million people (2020), which has been experiencing an ongoing decline since 2010 (Hellenic Statistical Authority, 2020). It is a popular touristic destination amassing over 30 million tourists per year, as was the case in 2019 (SETE, 2019). On the one hand, tourism is a significant factor for the Greek economy, and on the other hand, a demanding resource consumer, affecting resource availability and competing with antagonistic resource uses in the country. Furthermore, the agricultural sector in Greece has always been a reference point for economic and social life, thus contributing to 4% of the GDP, twice as much as in other European countries (Hellenic Statistical Authority, 2018), consuming close to 80% of all national freshwater resources and contributing to 7.84 million tons of GHG emissions (Our World in Data).

System Dynamics Model

System dynamics modeling has broadly been used as a simulator of complex real systems, helping researchers and policymakers to frame and understand the complexities of and interlinkages within the system, while at the same time, it provides information on how the system might evolve over time (Bakhshianlamouki et al., 2020). To conceptualize a complex dynamic system prior to simulation analysis, causal loop diagrams (CLDs) are used to identify the key variables in a system and indicate the causal relationship between them using links (Randers 1980). CLDs can perfectly describe the flow of the dynamic behavior of complex dynamic systems. A

CLD consists of variables connected with links showing their interdependence and corresponding signs on each link that mark the nature of the paired connection—increase or decrease of the dependent variable; the number of increases or decreases defines the nature of the system behavior as a whole—making loops either reinforcing (multiplying the change in one direction) or balancing (breaking the chain, counterbalancing explosive system behavior, and resulting in reduced outcomes) (Lannon, 2012). Balancing or stabilizing feedback loops (Chapin et al., 2009) act by altering variables in the reverse direction to their existing one, neutralizing the effects of the condition on the system (Morecroft, 2015). Balancing *the* feedback loop is crucial because it can contribute to system recovery after a perturbation disappears. Reinforcing or amplifying feedback loops intensify the effects of the perturbations that contribute to destabilizing the system. The policies aiming at enhancing resilience might be used in "vicious" amplifying feedback loops by counterbalancing them to diminish or delay their effects on the outcome function of the system and mitigate the impact of perturbations. Whether loops are reinforcing or balancing, it depends on the number of negative relationships in a feedback loop: an even number of negative relationships indicates that the loop is positive (reinforcing), while an odd number indicates a negative (balancing) loop. Ideally, in each SDM, the existence of both, reinforcing and balancing loops, ensures the overall balance of the system.

As the next step, to quantify the variables in the loop, the stock-and-flow diagram (SFD) is used since SFDs can perfectly capture the stock and flow behavior of a system. Stocks are variables that represent accumulations (Richardson, 2011), and the flow is changing by decisions based on the condition of the system and can be simulated to generate the dynamic behavior of the system. Crucial stocks can enhance system resilience due to the by-default delay created between the disturbance and its effect. Thus, the system outcome function is less affected by the disturbance and saves time for easier recovery. The SFD represents integral finite difference equations involving the variables of the feedback loop structure of the system and simulates the dynamic behavior of the system (Manetsch and Park 1982; Bala et al., 2017).

The SDM (**Figure 1**) starts by simulating the GHG emissions as a stock, so GHGs in the atmosphere are the sum of what is emitted (GHG emitted) minus what is sequestrated (carbon sequestration). The GHG emitted is the sum of GHGs produced due to power generation (PG), GHGs due to agricultural activity, and other GHGs (i.e., urban/household) coming mainly from the population and tourists using the per capita GHG emissions (industrial GHG emissions are excluded from this calculation as they are deemed minor—see Laspidou et al., 2020). Carbon sequestration, on the other hand, depends on land use, land-use change, and forestry (LULUCF) uptake and CO_2 uptake by the oceans. As the GHG emissions change over time, the effect of GHGs on climate change varies accordingly, while the effect of climate change on total renewable water resources (TRWRs) is affected inversely; thus, an increase in GHG emissions leads to a decrease in the *TRWR*, reflecting the fact that climate change will bring about water scarcity in the long run. The TRWR is the inflow that feeds the available freshwater stock, while its outflows are: flow to the sea, (CW) consumption, the irrigation water consumption (WC), and other WC (household/urban WC). The sum of all these outflows (except from flow to the sea) is the total WC.

We use the Water Exploitation Index plus (WEI+) as a measurement of water stress in the country (Casadei et al., 2020). Values greater than 20% indicate water scarcity, while values greater than 40% indicate situations of severe water scarcity (i.e., the use of freshwater resources is clearly unsustainable) (EUROSTAT). WEI+ is affected by both actual TRWR and total WC. The former inversely affects the WEI+ (a delay signal has been used herein, indicating that changes in TRWR will become visible in the WEI+ in the long run), while the latter directly affects the WEI+. When the WEI + increases, it means that we have increasing deficits in freshwater availability, which leads to a drop in aquifer levels and an increase in pumping energy (PE) as we have to go deeper and deeper to find water. In turn, the electricity demand (ED) associated with pumping increases, followed by increased electricity generation to meet demands, which leads to both increased GHG emissions (when fossil fuels are used) and increased demands in CW, and thus in total WC, and a further increase in WEI+, creating a reinforcing loop (R3).

An increased WEI+, which is a result of either increased water consumption, decreased TRWR, or both, will in the long run result in farmers switching to alternative crops that do not require irrigation. This is a natural adaptation to climate change practice that farmers will follow. As a result, irrigated land and associated irrigation water demand will decrease and nonirrigated land should increase; this is not expected to be an immediate response to water scarcity; thus, a delay is taken into account in the SDM. Naturally, both irrigated and nonirrigated land affect food production (FP) and GHG emissions due to agricultural activity. Finally, all human consumption is represented and regulated by the population/tourist parameter directly affecting the following quantities in the model: urban–industrial ED, food consumption, other (urban) water consumption, and other (urban) GHG emissions. The CLDs formed in this SDM are presented in the *Results* section.

Sensitivity Analysis

With the purpose of developing confidence and validity in the model and its results, unit consistency and SA were implemented in the developed SDM; this analysis aims to prove that this model is sufficiently accurate for its intended use (Robinson, 2004). To check the unit consistency of our model, each model variable in the SDM was separately selected and either confirmed or amended to ensure that it is correct and in consistent units. In this combined nexus–resilience analysis, we used the SA to identify the most important parameters affecting the basic variables of the system by quantifying the importance of each parameter.

We start by performing sensitivity runs based on Monte Carlo simulations implemented in the SDM for all model parameters. The initial values of the parameters were altered by ±10% to observe the corresponding changes on the variables of the greatest interest in our model. We present the analysis for three important

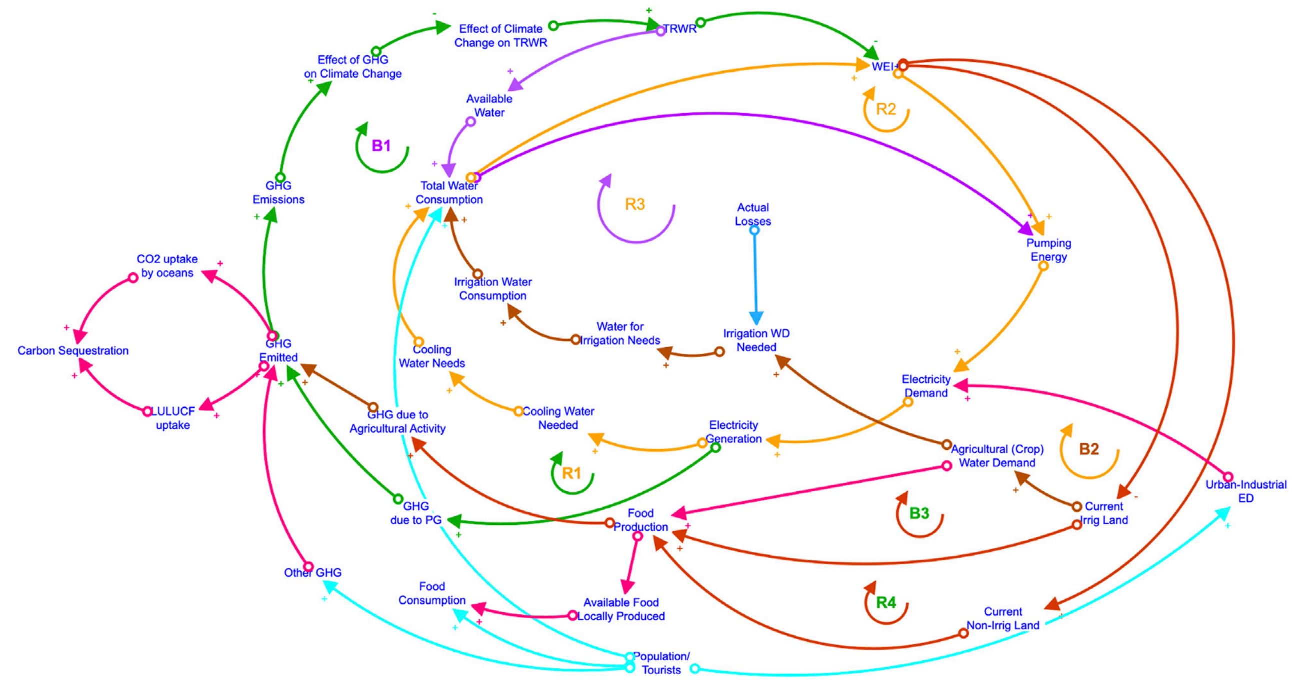

FIGURE 2 | Causal loop diagram (CLD) indicating the interconnection of Greece's water–energy–food system under climate change using the SDM.

quantities, namely, available freshwater, ED, and GHG emissions. Our interest is to show how these quantities change when all parameters vary by ±10% with a Monte Carlo analysis. For some parameters, we observed almost no change, while for some others, we had significant variability. We show the results for a selected set of seven parameters that our quantities show variable sensitivity to. These are: TRWR (m^3 of water), population/tourists (number), GHG emission factor for PG (kg of CO_2/GWh produced), per capita GHG emissions (kg of CO_2/capita due to human activity—mainly transportation), ED per capita (GWh electricity consumed/capita), irrigated land (m^2 of land), and actual losses in the agricultural irrigation system (m^3 water). All data come from the SIM4NEXUS dataset (Mellios and Laspidou, 2020) and are expressed on a yearly basis.

To quantify sensitivity, we used **Eq. 1**, where $S(p)$ is the estimated sensitivity value of a parameter, x is the selected variable, p is the selected parameter, and Δx and Δp denote the change in the variable and parameter, respectively (Jørgensen and Bendoricchio, 2001). The larger the $S(p)$ value of a given parameter, the more important that parameter is.

$$S(p) = \frac{\frac{\Delta x}{x}}{\frac{\Delta p}{p}}, \qquad (1)$$

System Resilience Analysis

In the context of implementing SRA, we investigated how our system responds to a disturbance (σ). In our case study, we chose disturbance (σ) to be the reduction of the TRWR (i.e., a drought) as a consequence of climate change. Our outcome function F(x) (i.e., available freshwater) indicates how the system responds to that disturbance. The purpose of this analysis is to investigate whether a system—after being affected by a disturbance (σ)—can recover or not and under which circumstances. More specifically, two things can happen to a system that has undergone shock or a very strong disturbance: it can either absorb the shock and result in maintaining its original behavior (no change) or it can change to a new state. When a system shifts to a new state, it can then either bounce back to its original state (a mechanical equivalent would be that the system "bends") or be forced to a completely new permanent state and never bounce back to its original state (corresponding to the system "braking" according to our mechanical analogy) (Herrera de Leon and Kopainsky, 2019). When assessing system resilience, it is important to identify "when the disturbance forces the system to change its behavior", or in other words, "how big a disturbance needs to be", "under which circumstances and after how long the system bounces back or breaks", and/or "how fast the system can recover", if at all. To address the aforementioned questions, we follow the Herrera (2017) methodology and quantify system resilience by measuring five resilience metrics. To do this, we consider the available freshwater as the outcome function F(x) and quantify the system behavior after being affected by disturbance (σ), which is an extreme drought, expressed as a steep reduction in the TRWR.

Engineering resilience and ecological resilience are both considered here. Engineering resilience is defined as the rate (how fast) at which a system resumes to its original state after a

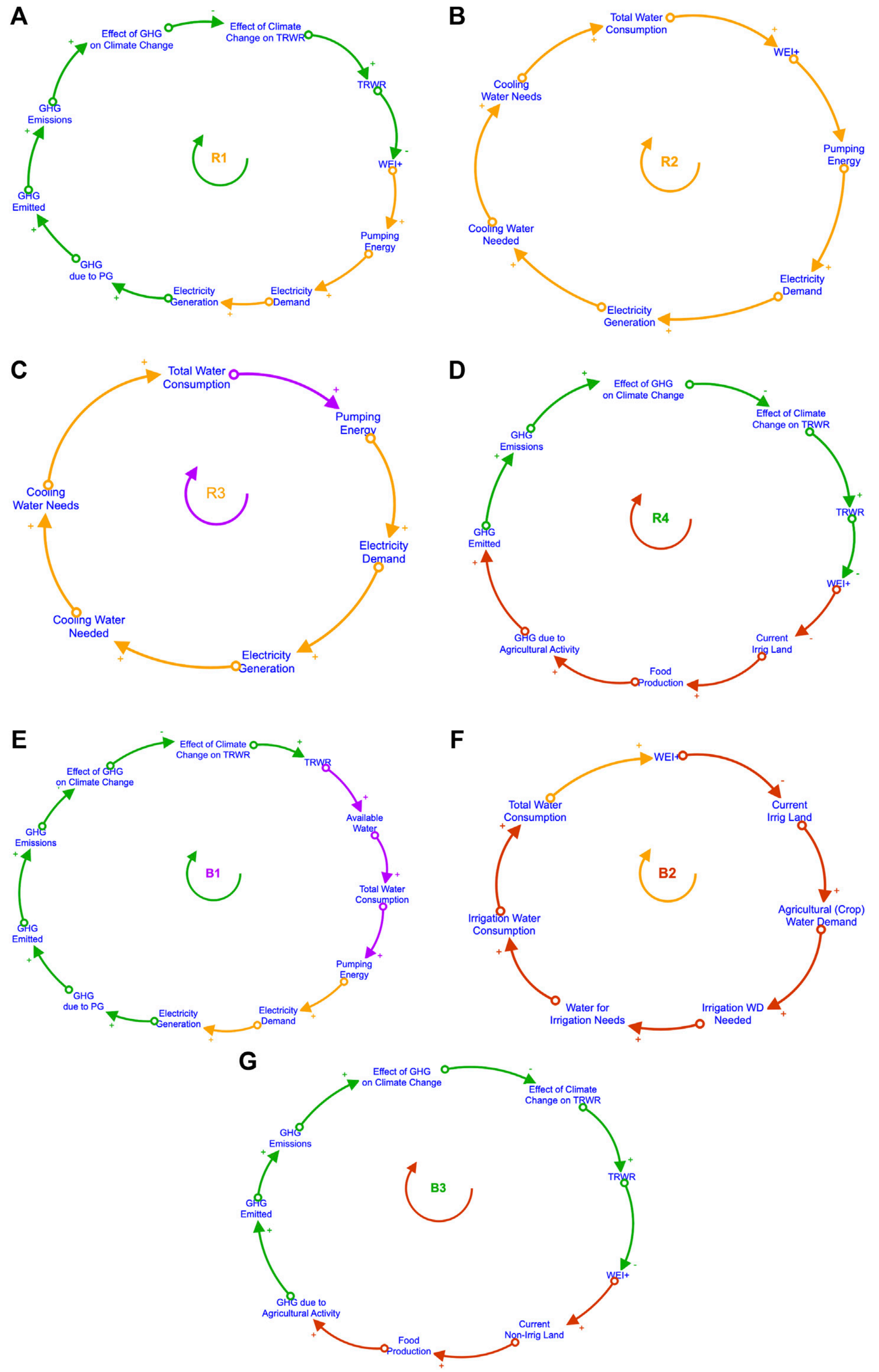

FIGURE 3 | Individual causal loop diagrams (CLDs) indicating the four reinforcing and three balancing loops. **(A)** Water–energy–climate reinforcing loop, **(B)** water–energy reinforcing loop, **(C)** water–energy reinforcing loop, **(D)** water–food–climate reinforcing loop, **(E)** water–energy–climate balancing loop, **(F)** competitive water uses the balancing loop, and **(G)** water–food–climate balancing loop.

TABLE 1 | Whole model's parameter importance in descending order.

Model parameter	Sensitivity parameter value
TRWR	0.440
Population/tourists	0.438
Baseline irrigated land	0.297
Electricity demand per capita	0.254
Per capita GHG emissions	0.200
GHG factor	0.184
Actual losses	0.047

perturbation (Pimm 1984), whereas ecological resilience is defined as the amount of disturbance a system can withstand and not change into a new condition (Carpenter and Gunderson, 2001). As also described by Herrera (2017), for this analysis, we assess engineering resilience by using hardness, recover rapidity, and robustness measures, whereas to assess ecological resilience, we use elasticity and index of resilience measures. To define the aforementioned measures, we consider the following characteristics:δ: magnitude of disturbance, t_c: time when the disturbance starts, t_d: time when the disturbance stops, and t_f: time when the system fully bounces back.

Hardness (σ_H) is the system's ability to withstand a disturbance (σ) without presenting a change in the performance of the outcome function $F(x)$. To measure hardness, we increase δ to find the smallest value of σ that produces a different outcome function $F(x)$, while keeping t_d and t_c constant.

$$\boldsymbol{\sigma_H = \delta_H \times (t_d - t_c)}. \tag{2}$$

Recover rapidity ($\bar{R}$) is the average rate at which a system bounces back to its original situation after a disturbance (σ) (Pimm, 1984; Martin et al., 2011; Herrera 2017). To measure $\bar{R}$, we continue increasing δ, keeping t_d and t_c steady, and estimate the $F(t_{d_1})$ for the current (original) situation and $F(t_{d_2})$ after the disturbance (σ):

$$(\bar{\boldsymbol{R}}) = \frac{(\boldsymbol{F}(\boldsymbol{t}_{d_1}) - \boldsymbol{F}(\boldsymbol{t}_{d_2}))}{\boldsymbol{t_f - t_d}}. \tag{3}$$

Robustness ($\bar{\rho}$) is the system's ability to resist big disturbances (σ) without significant loss of performance (Attoh-Okine et al., 2009; Herrera 2017) and is given by **Eq. 4**:

$$(\bar{\boldsymbol{\rho}}) = \frac{\boldsymbol{\sigma}}{(\boldsymbol{F}(\boldsymbol{t}_{d_1}) - \boldsymbol{F}(\boldsymbol{t}_{d_2}))}. \tag{4}$$

Elasticity (σ_E) is the system's ability to absorb a disturbance (σ) without changing to a different permanent state (Holling, 1996; Herrera 2017). Elasticity is calculated as the smallest disturbance σ_E that moves $F(x)$ to a different state. The bigger σ_E a system has, the more undisturbed it is

$$\boldsymbol{\sigma_E = \delta_E \times (t_d - t_c)}. \tag{5}$$

Index of Resilience (I_{res}) is the probability of the system to keep its current situation steady (Holling, 1996; Holling and Gunderson, 2002; Martin et al., 2011). High values of I_{res} indicate low probability of the system changing to a different state.

$$\boldsymbol{I_{res} = P(\sigma \leq \sigma_E)}. \tag{6}$$

RESULTS AND DISCUSSION

Causal Loop Diagrams

For this analysis, the conceptualization of the nexus system is presented through the construction of a CLD. The CLD (**Figure 2**) revealed seven interesting feedback loops–four reinforcing (R1, R2, R3, and R4) and three balancing ones (B1, B2, and B3). R1 is a climate–water–energy nexus reinforcing loop starting from the climate sector (**Figure 3A**). When the GHG produced due to PG is dealing with an increase, then the GHG emitted inflow is also increased, which in turn affects the GHG emissions the same way. An increase in GHG emissions causes a delayed increase on the effect of GHGs on climate change, while the effect of climate change on the TRWR is affected inversely, causing a decrease on the TRWR. When the TRWRs are reduced, WEI+—affected by *TRWR*—faces an increase which intensifies PE, ED, and EG, leading to a further increase in GHG produced due to PG. The R2 loop (**Figure 3B**) indicates the interconnection of total WC, WEI+, PE, ED, EG, and CW, where all are followed by successive increase, thus creating a water–energy nexus reinforcing loop. R3 in **Figure 3C**, is also a water–energy nexus reinforcing loop following the structure of R2, but in this loop, an increase in PE is caused by an increase in total WC due to the emerging need to extract more water to cover water demands (WEI+ is not part of this loop). In the R4 loop (**Figure 3D**), the GHG emissions affect the TRWR and WEI+ in the way described previously for R1. An increase in WEI + leads to a drop in water supply forcing the farmers to adapt to the new challenge by switching to nonirrigated crops, thus leading to an increase in nonirrigated land and FP. In turn, an increase in FP leads to a GHG emission increase through GHG due to agricultural activity, thus creating a reinforcing climate–water–food nexus loop.

In the B1 loop (**Figure 3E**), an increase in GHG emissions causes a decrease in the TRWR through the effect of climate change on TRWR; thus, both water availability and WC are also decreased, meaning the energy sector is also facing a decrease contributing to less GHG emissions (through GHG due to PG). Balancing loop B1 contributes to the limitation of climate change effects on the water and energy sector, creating a climate–water–energy nexus loop. In the B2 loop (**Figure 3F**), an increase in total water consumption means that water scarcity is deteriorating, so the WEI + values increase. When the country faces water scarcity, farmers will adapt to this situation by limiting the cultivation of irrigating crops; thus, the irrigated land, the associated irrigation WD, and irrigation WC will decrease. This behavior sets limits to reckless water use and creates a competitive water use balancing loop. In the B3 loop (**Figure 3G**), similar to B2, an increase in WEI + causes a decrease in irrigated land, FP, and GHG emissions through the GHG emitted due to agricultural activity, thus creating a climate–water–food nexus balancing loop. The system comes to a relative balance due to the existence of both kinds of loops–reinforcing and balancing.

Following the model's conceptualization, we then proceeded to the system's SFD as depicted in **Figure 1** to quantify the nexus

TABLE 2 | Parameter quantified importance/sensitivity for available water, electricity demand, and GHG emissions in a descending order.

Parameters quantified importance/ sensitivity for available water		Parameters quantified importance/ sensitivity for electricity demand		Parameters quantified importance/ sensitivity for GHG emissions	
TRWR	0.645	ED per capita	0.563	Population/tourists	0.704
Population/tourists	0.313	Population/tourists	0.531	GHG factor	0.509
GHG factor	0.196	Irrigated land	0.199	Per capita GHG emissions	0.423
Per capita GHG emissions	0.181	TRWR	0.175	ED per capita	0.276
Irrigated land	0.163	Per capita GHG emissions	0.090	Irrigated land	0.106
ED per capita	0.119	GHG factor	0.053	TRWR	0.085
Actual losses	0.048	Actual losses	0.034	Actual losses	0.015

interlinkages, find the most sensitive system parameters, and quantify system resilience for the three scenarios.

Sensitivity Analysis Results

Table 1 reveals the most important parameters that affect the whole system in a descending order based on parameter S(p) (**Eq. 1**). The TRWR and the number of people (population/tourists) seem to be the two parameters that our model is the most sensitive to, while the parameter actual losses in the irrigation network is the one that affects the model the least.

To quantify how much these seven model parameters affect the three basic quantities in the model, namely, available water, ED, and GHG emitted, we present a sector-specific SA, in which S(p) is calculated for each quantity, making it possible to compare and contrast the sensitivity of the important quantities to these parameters (**Table 2**). We observe that actual losses are at the bottom of the list, and the number of people (population/tourists) is close to the top of the list for all three quantities.

Next, a percentile analysis is performed. The most sensitive parameters are expected to bring about large variability in the quantities, while small variability indicates that the quantities do not change much, so they are insensitive to the parameters in question. Tornado diagrams are used to visually depict these results, showing the value of the quantity for the limiting values of the 5th and the 95th percentile of the parameter (Howard, 1988; Eschenbach, 1992). To show not only the limiting values but also the values of the quantities for the whole range of values that the parameter takes in the Monte Carlo analysis, we use sensitivity spread diagrams that were produced using the "ggplot2" plotting package in RStudio software. These results are shown in **Figure 4**. The climate sector is mostly affected by the population/tourists, GHG factor, and per capita GHG parameters (**Figures 4A,B**). The most important parameters of the water sector are TRWR and population/tourists (**Figures 4C,D**), while the energy sector is proved to be sensitive when ED per capita and population/tourists change (**Figures 4E,F**). Actual losses seem to affect these three sectors (and the whole system) the least.

The spread diagrams indicate the values of the quantities for the whole range of values that the parameter takes in the Monte Carlo analysis for: b) GHG emitted in kg CO_2, d) available water in m3, and f) electricity demand in GWh.

To validate the results of the model, we used the WEI + values. We simulated the WEI + values starting from year 1 (corresponding to actual year 2010), and we compared the two values—simulated and real—for the year 7 (corresponding to actual year 2017). We chose the year 2017 since this is the last value published by EUROSTAT. The actual WEI + value for the year 2017 is 39.37% (European Environmental Agency (EEA), 2020), while the simulated value is 38.7%, thus validating model results.

Resilience Analysis and Policy Evaluation

To assess SRA for our case study, we study the system behavior and quantify its ability to withstand shock under climate change; in this case, an extreme drought scenario is imposed on the system, and its ability to withstand it is investigated. The ecological and engineering measures of resilience (system resilience analysis) were applied to the developed SDM for the baseline scenario (with no interventions) and also for two suggested policies aiming to enhance WEF security; the implementation of renewable energy systems (RESs) (policy I) and increased stakeholder awareness and education, followed by increased funding to implement advanced irrigation systems with minimal losses in agriculture (policy II).

In **Figure 5**, we show the SFD that includes the implementation of policy I. The outer loop shown with black arrows is reinforcing loop R1, while the balancing loop B1 combines black and blue arrows and goes through the available water stock and through total WC and pumping energy. For policy I, we add the parameter fraction of RES in total energy generation mix (shown in the box in **Figure 5**), and this way, we reduce the GHG emissions due to power generation by **30%** as compared to the baseline scenario.

For policy II, we add extra variables in the SDM, and a new loop is formed (reinforcing loop R5). Here, awareness and education is designed to lead to stakeholders demanding and obtaining more funding for the implementation of efficient irrigation technologies that will lead to increased irrigation efficiency and reduced actual losses in agriculture (**Figure 6**). We expect both policies to lead to more resilient water systems overall through a WEF analysis; our goal is to compare the two policies in terms of systemic resilience using the metrics presented in the system resilience analysis. Therefore, we simulate and measure the resilience function $F(x)$ (which represents the quantity of choice, depending on our scenario) for the baseline scenario (with no policies yet implemented); in our case, $F(x)$ is available water. As the next step, the two proposed policies are applied separately to the system, and then the respective responses to the system are measured. "Before" and "after" results can then

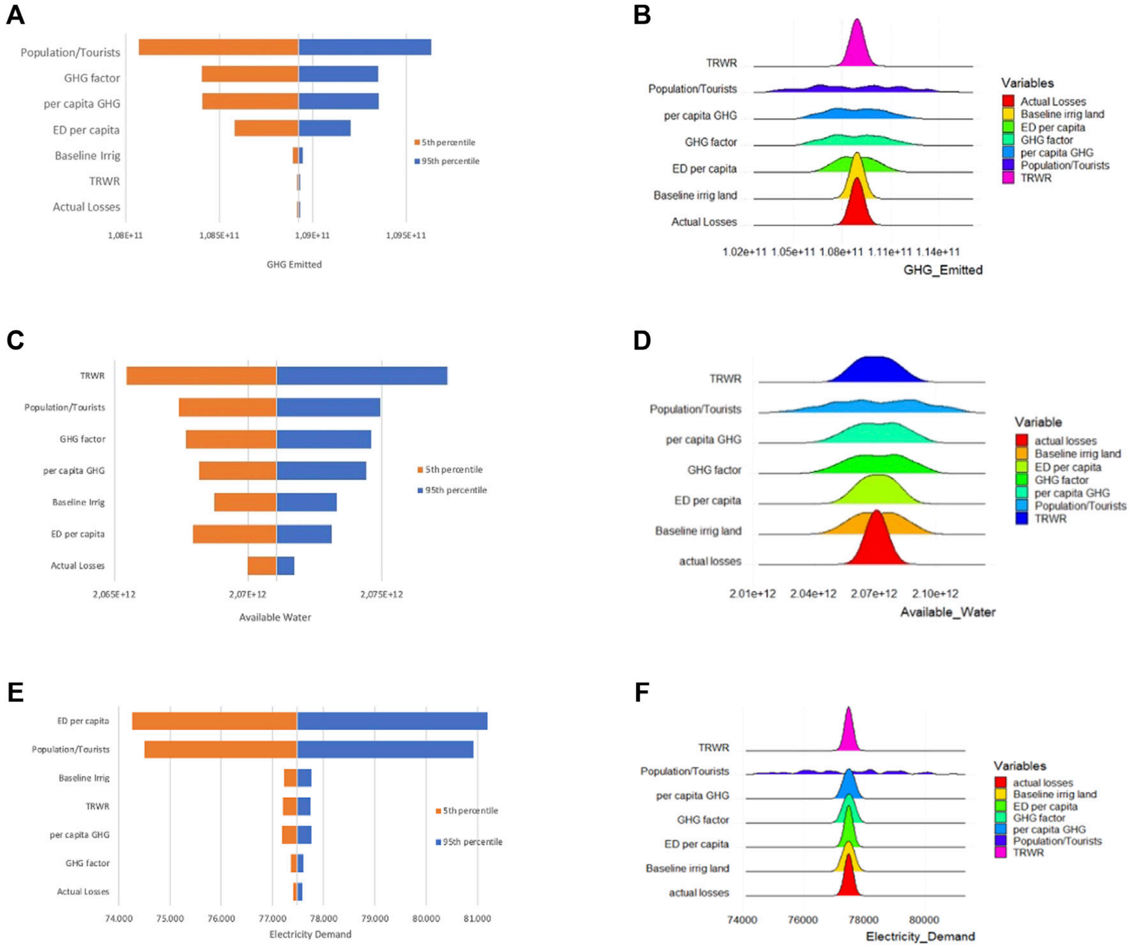

FIGURE 4 | Tornado diagrams showing the value of the quantity for the limiting values of the 5th and the 95th percentile of the parameters for: **(A)** GHG emitted in kg CO_2, **(C)** available water in m3, and **(E)** electricity demand in GWh. Spread diagrams indicating values of the quantities for the whole range of values that the parameter takes in the Monte Carlo analysis for: **(B)** GHG Emitted in kg CO_2, **(D)** Available Water in m3, **(F)** Electricity Demand in GWh.

be compared to identify which scenario enhances the system resilience aiming at WEF security under climate change.

We follow a methodology in order to define system hardness (σ_H) and elasticity (σ_E). To find system hardness, we keep increasing the magnitude of the system disturbance ($TRWR$ reduction) over a period of 10 years, specifically from 2014 to 2024, and we observe how $F(x)$—available water—changes. The highest disturbance/change in the TRWR that produces the least noticeable change in $F(x)$ is its hardness (σ_H), the engineering threshold (shown in **Table 3**). We observe that when all scenarios are compared, the baseline is the least resilient system, having the lowest hardness, while policy I has the highest. With the implementation of policies, the system can withstand bigger changes (higher hardness) in the TRWR, such as extreme droughts caused by climate change, before available water is affected. Variable $\bar{R}$ shows how quickly the system will recover from the disturbance, and it is the highest for policy I, while in terms of robustness, the two policies appear similarly robust and more robust than the baseline. Ecological resilience is assessed next with the calculation of system elasticity (σ_E) and Index of Resilience (I_{res}) for the same 10-year period (2014–2024). We now reduce the TRWR even more until the outcome $F(x)$—available water—changes significantly and to a new state, and we observe whether $F(x)$ bounces back or not. In a mechanical analog, we speak about the system "bending" and "not breaking", that is, eventually recovering to its original state after some time. Again, policy I seems to perform the best, showing higher system elasticity and a significantly higher Index of Resilience overall. The system shows a higher overall resilience under policy I.

In **Figure 7**, we show graphically the function $F(x)$ for the three scenarios (baseline and policy I and II) along with the initial values (blue), hardness σ_H (orange), and elasticity σ_E (green). The initial values are improved for the two policies, with policy I being slightly better (curve slightly higher than the other blue curves). For hardness and elasticity, we need to compare the difference with the initial values. For hardness, we observe that the biggest difference is found between initial

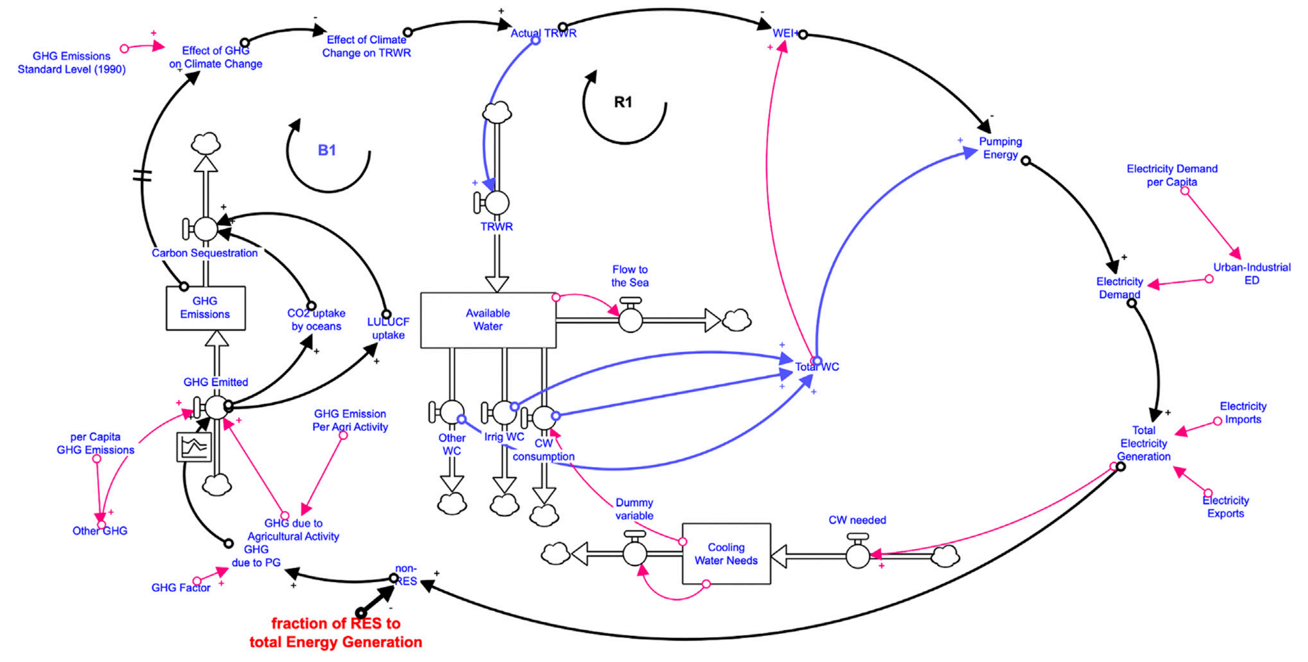

FIGURE 5 | Stock-and-flow diagram with the implementation of policy I—renewable energy systems (RES).

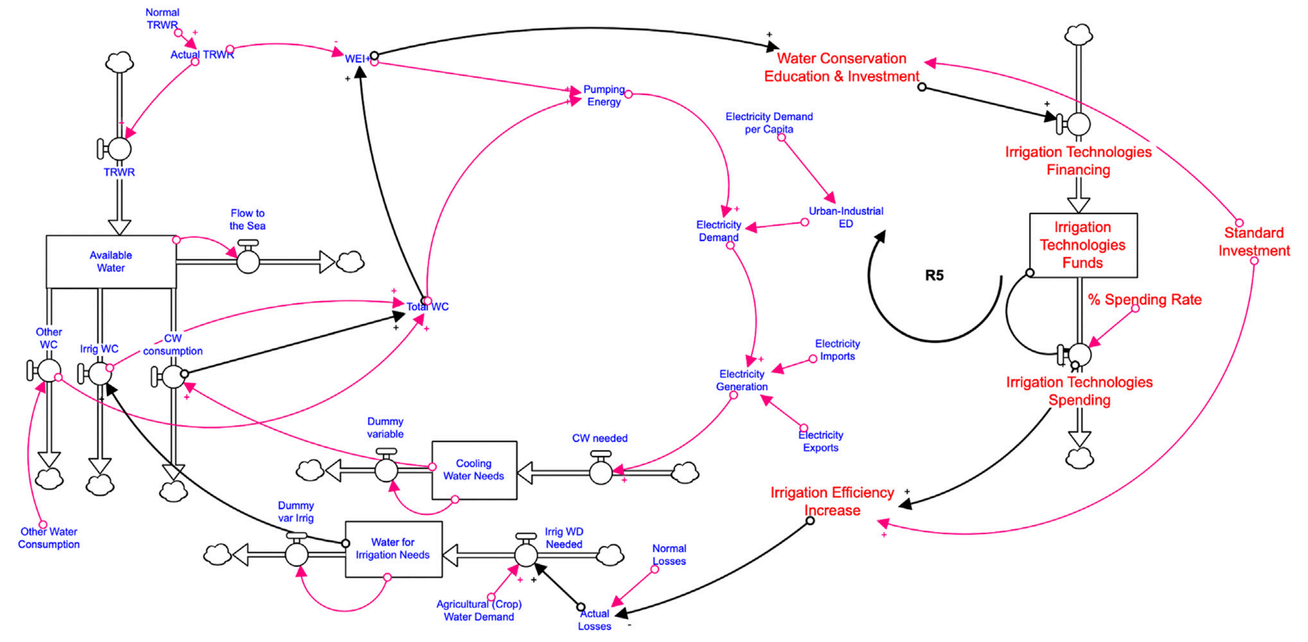

FIGURE 6 | Stock-and-flow diagram with the implementation of policy II—funding to reduce water losses in irrigation systems.

values and policy I, indicating that the system is the "hardest" with policy I. Policy II shows hardness that is improved from the baseline. For elasticity, again, policy I is the most "elastic" with the difference being significantly larger when comparing with policy II and baseline. This means that the system is more resilient, and even when there is a large perturbation, it is capable of "absorbing" it and bouncing back to its original state. When examining the baseline scenario, we observe that

TABLE 3 | Results of engineering and ecological resilience measures for the three scenarios; the baseline scenario, policy I—RES, and policy II—irrigation funding.

	Engineering resilience			Ecological resilience	
Scenarios	**Hardness** (σ_H)	$\bar{R}$	$\bar{\rho}$	**Elasticity** (σ_E)	**Index of Resilience** (I_{res})
Baseline	$2,54 \cdot 10^9 m^3$	$0,80 \cdot 10^9 m^3/year$	0.107	$5,08 \cdot 10^9 m^3$	33,4%
Policy I	$5,08 \cdot 10^9 m^3$	$2,38 \cdot 10^9 m^3/year$	0.108	$15,24 \cdot 10^9 m^3$	46,6%
Policy II	$4,06 \cdot 10^9 m^3$	$1,34 \cdot 10^9 m^3/year$	0.108	$10,16 \cdot 10^9 m^3$	40%

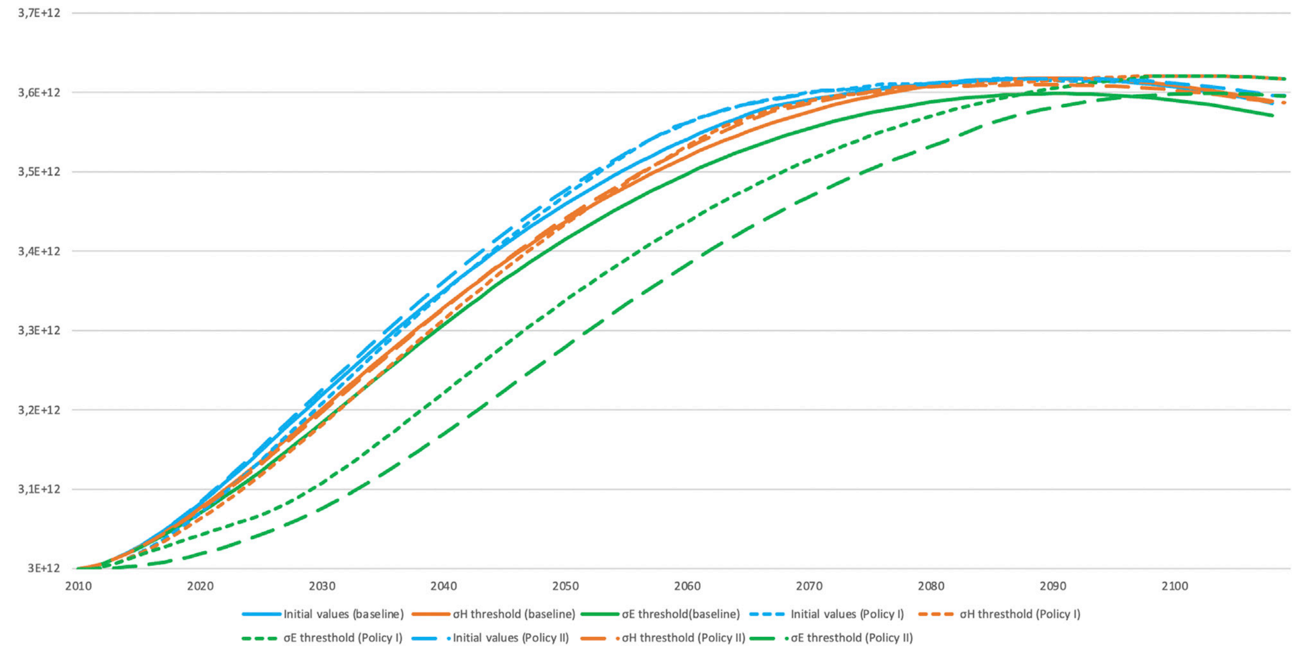

FIGURE 7 | Simulated behavior for the available freshwater constituted of initial values of the TRWR (with no disturbance) and system thresholds of hardness and elasticity referring to the three scenarios: baseline scenario, policy I, and policy II.

the system is capable of absorbing a small disturbance (indicated by hardness curve matching the initial value at 100 years), but it is not able to bounce back to its original state when a larger perturbation occurs. This is indicated when we observe that the green solid line (elasticity for baseline scenario) never meets the blue solid line (initial value, baseline scenario), but even 100 years later, it remains lower than the original curve. Thus, without the implementation of any policies, the system suffers a significant blow and never bounces back.

CONCLUSION

New approaches on natural resource policymaking need to be applied with the intention to provide essential human needs and resources to all in an environmentally compatible, economically resilient, and socially inclusive manner that is capable of contending with perturbations. SES adaptation to climate change requires a more functional approach of resilience use in policymaking. System dynamic modeling prevails over other simulation techniques by supporting the analysis of system structure and focusing on feedback loop relationships. This study combines WEF nexus analysis under climate change with SA and SRA that are said to have the potential to deliver on these grand development challenges. The proposed methodology describes how to simulate the WEF nexus system under climate change for the national case study of Greece using system dynamic modeling, identify the most important (sensitive) system parameters, and quantify five essential metrics of resilient behavior (for three scenarios), thus providing the policymakers with a quantitative basis to enhance the resilience of SESs. Engineering (σ_H, $\bar{R}$, and $\bar{\rho}$) and ecological (σ_E and I_{res}) resilience measures are quantified, and the respective thresholds are also identified. In this study, two proposed policies are compared to decide which one enhances the system resilience best. Evaluating the results, we conclude that the Greek simulated system can withstand an extreme drought event affected for a 10-year period under the allowing circumstances of engineering and ecological thresholds found for the two policies (policy I and policy II); the baseline scenario has little tolerance to such disturbance (reduction on *TRWR*) and easily breaks when it overcomes the ecological threshold without being able to recover. Policy I proposing the implementation of RES seems to be the most promising scenario as its resilience measures have the highest values, so the system can even recover from the shock for a more severe drought, while policy II is also a good scenario since it contributes to system recovery when affected by drought although having lower resilience measures values by enhancing water security through irrigation funding techniques.

DATA AVAILABILITY STATEMENT

Publicly available datasets were analyzed in this study. These data can be found here: https://data.mendeley.com/datasets/9x7wn24rrp/1.

AUTHOR CONTRIBUTIONS

AI: conceptualization, methodology, software, validation, formal analysis, visualization, data curation, and writing—original draft preparation. CL: conceptualization, methodology, resources, writing—reviewing and editing, supervision, project administration, and funding acquisition.

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Fe-Sensitized Zeolite Supported TiO_2 for the Degradation of Tetracycline Using Blue LED Irradiation

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In this study, we investigated the photocatalytic degradation as a potential treatment of tetracycline (TC) antibiotic contaminated water using TiO_2 semiconductor. To expand the activity of TiO_2 into the visible light region and to enhance its adsorption capacity for TC, we explored its modification *via* sensitization with Fe ions and *via* immobilization on beta (BEA) zeolite support. The nano-sized beta zeolite, synthesized using the seed-assisted procedure, was used to immobilize TiO_2 initially prepared by the sol-gel method. The immobilized TiO_2/BEA catalyst was further ion exchanged with Fe^{3+} ions using $FeCl_3$ precursor. Fe^{3+} modified TiO_2/BEA (Fe-TiO_2/BEA) catalyst was characterized using SEM, XRD, BET, UV-VIS DRS, and FTIR. After the immobilization of TiO_2 over BEA, the surface area of TiO_2 increased from 90 to 530 m^2/g and similarly its TC adsorption efficiency increased from 10% to 33%. The photocatalytic performance of the Fe-TiO_2/BEA was evaluated under blue LED light for TC degradation. Fe-TiO_2/BEA exhibited higher TC removal efficiency (100%) compared to TiO_2 (80%) after 90 min of irradiation using 50 W blue LED light for a 250 mg/L initial catalyst concentration and 20 mg/L TC concentration. The enhanced performance of the final catalyst was a result of the expanded surface area due to the immobilization of the TiO_2 on the BEA zeolite, which resulted in an improved TC adsorption. Moreover, the presence of Fe^{3+} ions reduced the band gap energy of the TiO_2, hence led to a red shift in its absorption spectrum to the visible light region and minimized the extent of the recombination of the charge carriers.

Keywords: tetracycline, photocatalytic degradation, beta zeolite, immobilized TiO_2, Fe-sensitized TiO_2, blue LED light

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1 INTRODUCTION

Antibiotics (ABs) are antibacterial compounds used to treat bacterial infections both in humans and animals (Torres-Palma et al., 2020). Tetracyclines (TCs) are one of the most prescribed families of ABs and are widely used in medical, agricultural, and poultry sectors. TCs are poorly absorbed by the body (20%–50%), hence they are excreted to the environment *via* urine and feces (Liao et al., 2021). TCs continuous presence in the environment, both in water sources through urine and in soil through animal manure, have created adverse effects on the aquatic and agriculture ecosystems and have led to the development of antibiotic resistant bacteria (ARB) (Chong et al., 2015).

Photocatalytic degradation is an advanced oxidation process (AOP) that uses light activated catalysts for the removal of persistent organic contaminants from water (Chong et al., 2015; Saqib et al., 2019). Titanium dioxide (TiO_2) semiconductor has been reported to efficiently degrade ABs due to its attractive properties such as: high thermal and chemical stability, commercial availability, low cost and toxicity, and high specific surface (Foura et al., 2017; Behravesh et al., 2020; Ebrahimi et al., 2020). Nevertheless, several challenges limit the large-scale application of TiO_2 in the photocatalytic degradation of ABs under visible light: 1) TiO_2 has a band gap energy of (3.2 eV) which limits its activation to mere UV light that accounts only for 3%–5% of the solar spectrum, 2) TiO_2 nanoparticles used in slurry reactors require expensive, energy consuming, and complicated recovery for further reutilization, 3) the finely dispersed TiO_2 particles suffer from aggregation which hinders its efficiency in slurry reactors (Chong et al., 2015; Foura et al., 2017; Saqib et al., 2019; Behravesh et al., 2020; Hu et al., 2021). In order to red-shift TiO_2 light absorption, researchers have investigated several methods to decrease its band gap energy or to introduce new intra-band gap energy states *via* doping with transition metals such as Cr, Fe, Co, Mo, Mn, and V, or their ions (Foura et al., 2017). In metal doped-TiO_2, upon visible light excitation the electrons in the metal dopant are excited and are transferred to the conduction band of TiO_2 leading to its activation (Zhang et al., 2019). Specifically, iron metal-ion doping of TiO_2 can minimize the back recombination of electrons (e^-) and holes (h^+) and therefore maintain a high stable degradation efficiency (Foura et al., 2017; Saqib et al., 2019). Many studies in literature have reported on the visible light sensitization of TiO_2 *via* Fe metal ion doping. For example, Tsiampalis et al. (2019) reported successful degradation of the sulfamethoxazole antibiotic using 0.04% Fe/TiO_2 under simulated solar radiation. Furthermore, the UV-VIS DRS results confirmed an enhanced visible light absorption of the doped TiO_2 and a decrease in its band gap energy from 3.2 eV to around 2 eV with an increase in the Fe content from 0.04% to 2%. The visible light photocatalytic degradation efficiency of the metal ion doped TiO_2 was 95% after 90 min compared to only 45% by the undoped TiO_2. Another study by Suwannaruang et al. (2020) reported visible light induced degradation of ciprofloxacin AB over Fe-N-TiO_2 mesoporous photocatalyst using visible light emitting diode (LED) as illumination source. With the increase in Fe content, the morphology of the doped catalyst was gradually converted from spindle to spherical shape. For the same nitrogen content (2.5%), increasing the Fe content from 0.5% to 1.5% decreased the band gap energy of TiO_2 from 2.9 eV to 2.7 eV. Nearly, 70% of the antibiotic was removed after 6 h radiation compared to only 17% using the undoped TiO_2 (Suwannaruang et al., 2020).

TABLE 1 | BET specific surface area and external surface area (m^2/g) and micro and meso pore volumes (cm^3/g) of BEA, TiO_2, and Fe-TiO_2/BEA.

Sample	S_{BET}	V_{micro}	S_{ext}	V_{meso}	V_{total}	d
BEA	620	0.26	120	0.44	0.70	25
Fe-TiO_2/BEA	530	0.22	170	0.40	0.62	22
TiO_2	90	0.04	190	0.08	0.12	49

S_{BET}, specific surface area (m^2/g), V_{micro}, micropore volume (cm^3/g); S_{ext}, external surface area (m^2/g), V_{meso}, mesopore volume (cm^3/g); d, crystallite size (nm).

In addition to metal ion doping of TiO_2 for enhanced photocatalytic activity, immobilization of TiO_2 particles on porous and inert supports has been widely investigated by researchers to control its morphology and improve adsorption capacity for the organic pollutant. TiO_2 immobilization further improves its stability, and ease of recovery specially when applied in large-scale slurry reactors. Several inorganic TiO_2 immobilizing substrates such as magnetite core, activated carbon, clays, ceramic, silicates, sands, glass, carbon nanotubes, polymers, and zeolites have been investigated (Lei et al., 2012; Mozia et al., 2012; Bel Hadjltaief et al., 2015; Chong et al., 2015; Cunff et al., 2015; Nawawi et al., 2016; Foura et al., 2017; Wang et al., 2017; Cunha et al., 2018; Mohd Adnan et al., 2018; Oblak et al., 2018; Radwan et al., 2018; Mahdavi et al., 2019; Saiful Amran et al., 2019; Scaria et al., 2020; Hu et al., 2021). Among the mentioned supports, zeolites have gained superior attention due to their desirable properties such as: high specific area and excellent adsorption ability for pollutants (surface area: 350–950 m^2/g and pore volumes >0.1 cm^3/g) (Yilmaz et al., 2013). Beta zeolite (BEA) is one type of zeolite with an interesting architecture of 3D open framework pore structure, high adsorption ability, shape/size selective properties, high hydrothermal stability, easily reachable large micro-pore volume, wide pore channel network, and strong acid sites (Taufiqurrahmi et al., 2011; Yilmaz et al., 2013). Researchers have reported many examples on TiO_2/zeolite systems of enhanced photocatalytic activities due to the enhanced and stable adsorption of pollutants on the catalyst over long reaction times. Titania/zeolite composites have been investigated for the removal of various pollutants in water, including dyes and pharmaceuticals (Al-Harbi et al., 2015; Saadati et al., 2016a; Foura et al., 2017; Liu et al., 2017; Maksod et al., 2017; Rahman et al., 2018; Sun et al., 2018; Aghajari et al., 2019; Liu et al., 2019; Saqib et al., 2019; Behravesh et al., 2020). For antibiotics removal, Behravesh et al. (2020) prepared zeolite-supported TiO_2 to degrade acetaminophen and codeine pharmaceuticals under sunlight irradiation. The FTIR characterization confirmed the absence of chemical bonds between the TiO_2 and the support, while the SEM-EDX analysis combined with XRD patterns showed that TiO_2 particles were mainly uniformly dispersed on the external surface of the zeolite and partially in its pores. Zeolite immobilization of TiO_2 increased the surface area of TiO_2 from 50 m^2/g to 98 m^2/g, and therefore the photocatalyst was able to degrade 39% of the initial concentration of these pharmaceuticals after 120 min. In addition, Saadati et al. (2016b) used TiO_2-P25/Semnan natural zeolite for tetracycline degradation under visible light irradiation. The immobilized TiO_2-P25 exhibited a specific area of 93 m^2/g, which was two times larger than that of TiO_2-P25. This catalyst was able to degrade 87% of the initial tetracycline concentration within 90 min of radiation as compared to only 10% degradation efficiency by the TiO_2-P25. In this study, TiO_2 particles were deposited on the external sites of the zeolite leading to an

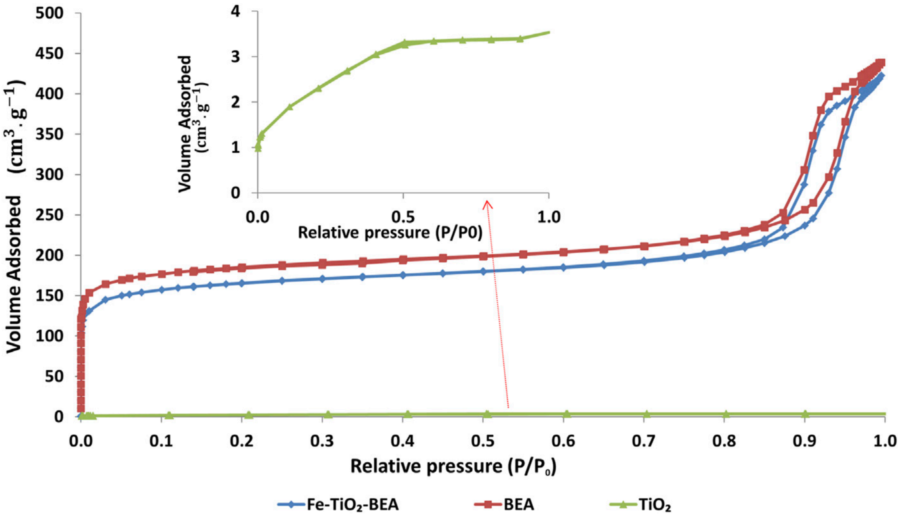

FIGURE 1 | N_2 adsorption-desorption isotherms at 77 K of BEA, TiO_2, and Fe-TiO_2/BEA. Inset: N_2 adsorption-desorption isotherms at 77 K of TiO_2.

improved adsorption of tetracycline. The XRD characterization of the final catalyst indicated that the structure of the zeolite was conserved and the crystallite size of TiO_2-P25 increased after the deposition of TiO_2 on zeolite, while the FTIR spectrum of the final catalyst exhibited a new absorption band proving the presence of a chemical bond between TiO_2 and the zeolite. The presence of such a chemical bond, however, was not always present in other reported TiO_2/zeolite systems (Foura et al., 2017; Maksod et al., 2017; Behravesh et al., 2020; López et al., 2021).

Additionally, both iron-modified and zeolite immobilized TiO_2 was used for the degradation of organic dyes under visible light. For example, Foura et al. (2017) used Fe-doped TiO_2 over HY zeolite for methylene blue degradation under visible light illumination and reported >98% removal efficiency after 60 min for the optimum 10 wt.% Fe-doped TiO_2/HY. In this particular work, FTIR characterization results indicated the absence of chemical interaction between the TiO_2 and the HY zeolite and BET analysis confirmed the deposition of TiO_2 in the pores of the zeolite. The UV-VIS DRS characterization proved that the addition of Fe into TiO_2/HY zeolite caused a red shift in its absorption spectrum towards the visible light region due a decrease in its band gap energy from 3.12 to 2.55 eV.

Recently, light-emitting diodes (LEDs) have gained interest in photocatalysis as efficient and economic light sources for the photocatalytic degradation of ABs and organic pollutants (Alpatova et al., 2015). The following characteristics of LEDs make them attractive for use: low power consumption, practical configuration, high energy efficiency, robustness, long life expectancy (50,000 h), flexibility of adjustment in various reactor designs (Casado et al., 2017; Liu et al., 2017). Many papers reported on the use of LEDs as efficient light sources for ABs removal in general (Malkhasian et al., 2014; Sarafraz et al.,

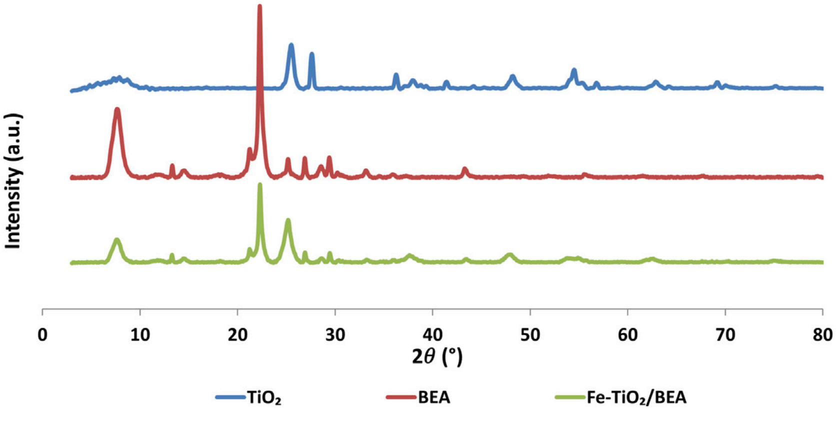

FIGURE 2 | XRD patterns of the prepared catalysts.

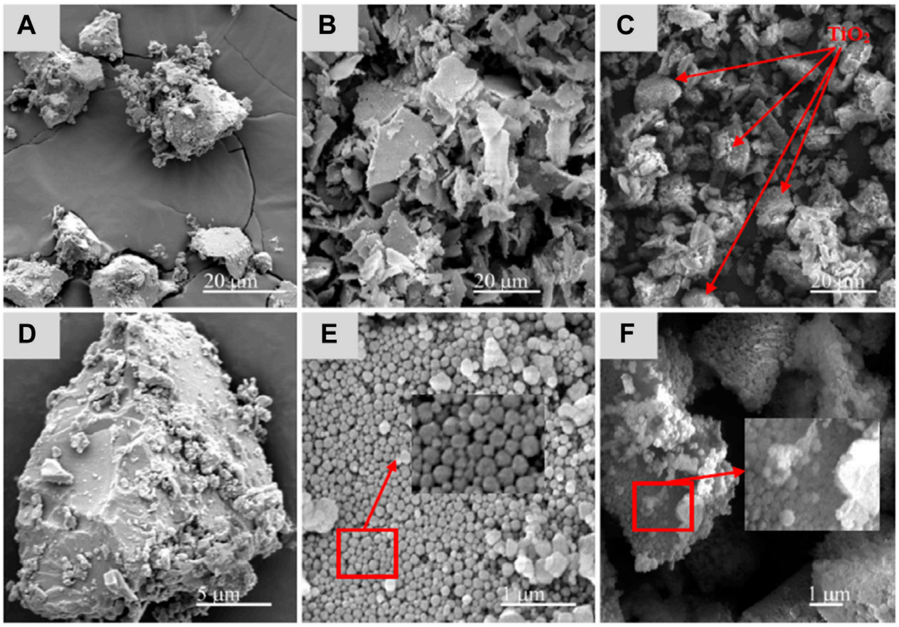

FIGURE 3 | SEM images at different magnification scales of TiO_2 **(A,D)**, BEA **(B,E)**, and Fe-TiO_2/BEA **(C,F)**.

2020; Zhong et al., 2020; AttariKhasraghi et al., 2021; Varma et al., 2021; Wang et al., 2021; Das and Ahn, 2022), and for tetracyclines removal in specific (Alpatova et al., 2015). For example Moshoeu et al. (2020), reported ~92% degradation efficiency of TC using TiO_2 nanofibers under LED strip with a wavelength ranging from UV to infrared region. Blue LED was also previously used to degrade TC using CdS semiconductor nanorods (Das and Ahn, 2022), where 92% efficiency was reported after 120 min for a 50 W lamp.

Particularly, the role of Fe ions has been investigated for the sensitization of TiO_2 under blue LED light ($420 < \lambda < 495$ nm). Impellizzeri et al. (2014) applied iron-modified TiO_2 in the form of Fe ion-implanted TiO_2 thin film for the photocatalytic degradation of methylene blue under blue LED light (420–470 nm). In this work, the introduced Fe ions lowered the band-gap energy of TiO_2 from 3.2 eV to 1.6–1.9 eV, resulting in an enhanced visible light absorption, hence in an improved photocatalytic efficiency. Similarly, both Tsiampalis et al. (2019) and Foura et al. (2017) modified titania *via* iron ion doping, and successfully expanded its activity to the visible light range between 420 and 490 nm.

In this work, we investigated both Fe^{3+} ion sensitization and zeolite immobilization routes to enhance the photocatalytic activity of TiO_2 for the degradation of tetracycline antibiotic under blue LED light. Sol-gel synthesized TiO_2 was immobilized on beta zeolite and further ion exchanged with iron. The structural, morphological and visible light properties of the prepared Fe-ion-exchanged BEA/TiO_2 (Fe-TiO_2/BEA) catalyst was studied in relation to the observed photocatalytic performance. Moreover, in order to achieve optimum degradation efficiency of the prepared catalyst for TC removal, the effect of various process conditions such as initial TC concentration, catalyst's concentration and light intensity were studied.

2 MATERIALS AND METHODS

2.1 Materials

LUDOX® SM colloidal silica 30 wt.% suspension SiO_2 in H_2O, (Sigma-Aldrich, 30%, particle size 3–4 nm), sodium hydroxide (Sigma-Aldrich), aluminium iso-butoxide (Sigma-Aldrich, 97%), tetraethylammonium hydroxide (Sigma-Aldrich, 35%), Titanium (IV) n-butoxide (Alfa Aesar), ethanol (Fisher Chemical, 99%), nitric acid (BDH Laboratory supplies, 69%), sodium hydroxide (Sigma-Aldrich), Tetracycline (Sigma-Aldrich), Iron (III) anhydrous chloride (BDH Laboratory supplies). All chemicals were used without further purification.

2.2 Preparation of the Catalysts

2.2.1 Preparation of TiO_2 Sol-Gel

TiO_2 was prepared using the sol-gel method as described previously (Bazargan et al., 2012). A mixture (A) of 4 ml of titanium (IV) butoxide and 2 ml of ethanol was stirred for 30 min. A second mixture (B) composed of 0.4 ml of nitric acid, 2 ml H_2O and 17 ml of ethanol was simultaneously prepared. Mixture (B) was gradually added into mixture (A) using a dropper (approximately 3 ml/min) under vigorous stirring for an hour during after which the clear solution turned into a gel. The obtained gel was then dried in an oven at 80°C for 3 h to remove traces of ethanol and H_2O. Then the dried sample was subjected to calcination in a muffle furnace for 4 h at 450°C to induce crystallization of TiO_2. The crystalline mass obtained after calcination was approximately 0.6 g.

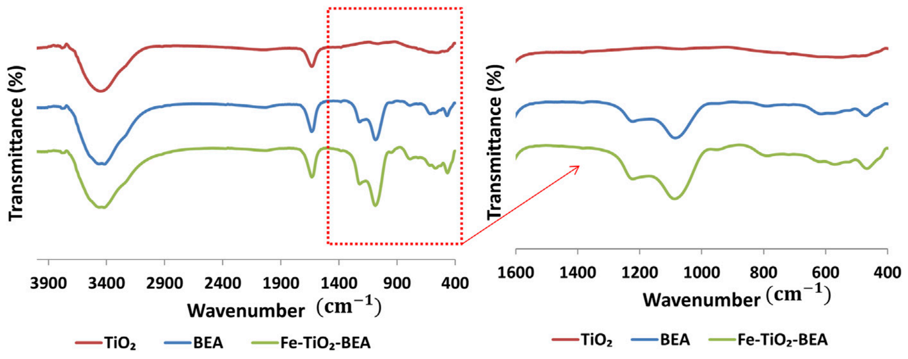

FIGURE 4 | FTIR of TiO_2, BEA, and Fe-TiO_2/BEA. Inset: Magnified FTIR of TiO_2, BEA, and Fe-TiO_2/BEA.

2.2.2 Preparation of BEA Zeolite

BEA zeolite was prepared *via* seed assisted approach. The BEA seeds were prepared from clear precursor suspensions with molar compositions: 9TEAOH: $0.5Al_2O_3$: $25SiO_2$: $295H_2O$, where TEAOH stands for tetraethylammonium hydroxide (Sigma-Aldrich, 35%). Initially, aluminium iso-butoxide (Sigma-Aldrich, 97%) was dissolved in a solution containing TEAOH and distilled water, and then the Silica source, colloidal Silica (LUDOX® SM 30 wt.%), was added into the mixture under stirring. After mixing the precursor suspensions for 60 min, a hydrothermal treatment was carried out at 100°C for 3 days. The obtained crystalline suspensions were purified by multistep high-speed centrifugation (20,000 rpm, 60 min); then the solid product was dried at 40°C and calcined at 550°C prior to being used as seeds.

The synthesis of BEA zeolite was carried out using the following suspension: $9.5Na_2O$:$0.25Al_2O_3$:$40SiO_2$:$570H_2O$ by dissolving LUDOX® SM colloidal silica (30 wt.% SiO_2, pH = 10, Aldrich) in a sodium hydroxide solution followed by heating at 100°C for 5–7 min in order to transform the turbid solution into clear water suspension. After cooling down to ambient temperature, BEA seeds (8 wt.%) were slowly added to the solution, and the mixture was homogenized by vigorous stirring for 30 min, followed by the addition of aluminum isopropoxide (Sigma-Aldrich, 98%). The obtained precursor suspension was further homogenized for 20 min before being transferred into a stainless-steel autoclave and subjected to the hydrothermal treatment at 100°C for 5 days under static condition. The resulting product was filtered, washed, and purified by double deionized water and then dried at 50°C. The yield of the sample was calculated with respect to the SiO_2, Al_2O_3, and the BEA seeds were included. A yield between 18 and 22% was obtained for BEA zeolites.

2.2.3 Modification of the TiO_2 Sol-Gel (Preparation of Fe-TiO_2/BEA Zeolite)

TiO_2/BEA Zeolite was prepared *in-situ* during the synthesis of the TiO_2 sol-gel, as previously reported (Sponza and Koyuncuoglu, 2019). After the preparation of TiO_2 sol-gel suspension, an appropriate amount of BEA zeolite nanoparticles was added into the transparent sol-gel to obtain 20% TiO_2/Zeolite composite. The obtained suspension was kept under stirring for 24 h. The final product was dried at 80°C for about 3 h followed by calcination at 450°C for 4 h. The as-synthesized zeolite supported TiO_2 (TiO_2/BEA) was then subjected to ion exchange treatment. Typically, 1.0 g of BEA/TiO_2 composite was stirred in 40 ml of 0.05 M iron chloride ($FeCl_3$) solution. The exchange process was repeated three times by separating supernatant from the mother liquid, re-dispersing it in new solution and repeating the procedure with the aforementioned ion exchange process to ensure that the highest possible exchange was achieved. The obtained sample after ion-exchange was washed thoroughly with double deionized water then dried in an oven at 80°C for 4 h followed by calcination in a muffle furnace at 450°C for 4 h. The final obtained sample was named Fe-TiO_2/BEA.

2.3 Characterization and Analysis Methods

Various analysis techniques were applied to characterize the surface morphology, structure and optical properties of each of the Fe-TiO_2/BEA, TiO_2, and BEA. Fourier transform infrared (FTIR) spectra in the range of 400–4,000 cm^{-1} were obtained using JASCO FTIR 6300 spectrometer using DTGS detector (resolution 4, 128 scans; KBr: sample = 99:1 mg) to study the structure of the prepared catalysts. X-ray powder diffraction (XRD) (BRUKER, D8) was used for the identification of crystalline phases. Fe-TiO_2/BEA, TiO_2, and BEA were analyzed in the range of $5^\circ < 2\theta < 80^\circ$ with a step size of 0.02°. The Scherrer Formula (**Eq. 1**) was used to calculate the average crystallite size of all samples;

$$d = \frac{0.89\lambda}{\beta cos\theta} \tag{1}$$

where d is the average crystallite size, λ is wavelength of the X-ray, 0.89 is the Scherrer's constant, β is the broadening at half the maximum intensity, and θ is the diffraction angle (Ali et al., 2017). **Table 1** presents results of these calculations. Scanning electron microscope (SEM) using MIRA3 LMU by TESCAN was used to investigate the morphology and structure of the three samples. Brunauer–Emmett–Teller (BET) coupled with

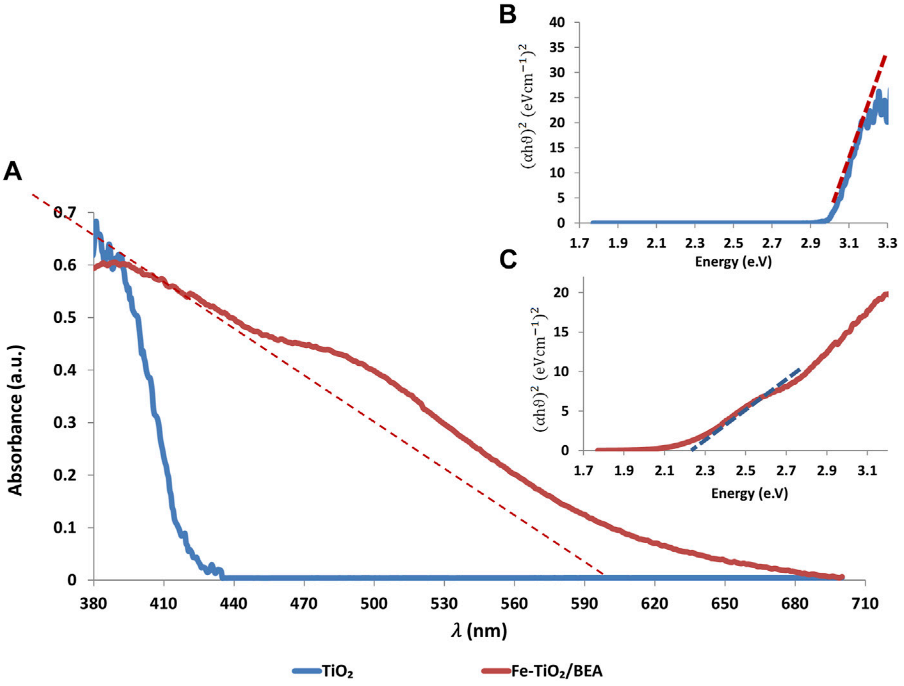

FIGURE 5 | (A): UV-VIS DRS of TiO_2 and Fe-TiO_2/BEA. Inset: Tauc's plots of **(B)**: TiO_2 and **(C)**: Fe-TiO_2/BEA.

Dubinin–Radushkevich method was used for the analysis and calculation of the surface area and pore volume of all samples. Nitrogen adsorption/desorption isotherms at 77 K (GEMINI VII 2390) in the relative pressure (P/P_0) range of 0.04–0.99 were applied. Diffuse reflectance spectroscopy (UV-VIS DRS) using (JASCO, V-570) in the range ($350 < \lambda < 700$ nm) was applied to study the optical properties of the prepared samples. To estimate the band gap energy of the samples, Tauc's formula (**Eq. 2**) was applied using the absorbance data of the UV-VIS DRS plot; where, α is the absorption coefficient, α_0 and h are constants, n is constant with a value of 0.5 or 2 for indirect and direct band gap semiconductors respectively, and (Eg) is the band gap energy of the sample. To find E_g, a linear plot of $(\alpha\ h\vartheta)^2$ vs. $h\vartheta$ is extrapolated ($n = 2$) and Eg estimated from the x-intercept (Khairy and Zakaria, 2014; Saadati et al., 2016b).

$$\alpha = \frac{\alpha_0 \left(h\vartheta - E_g\right)^n}{h\vartheta} \tag{2}$$

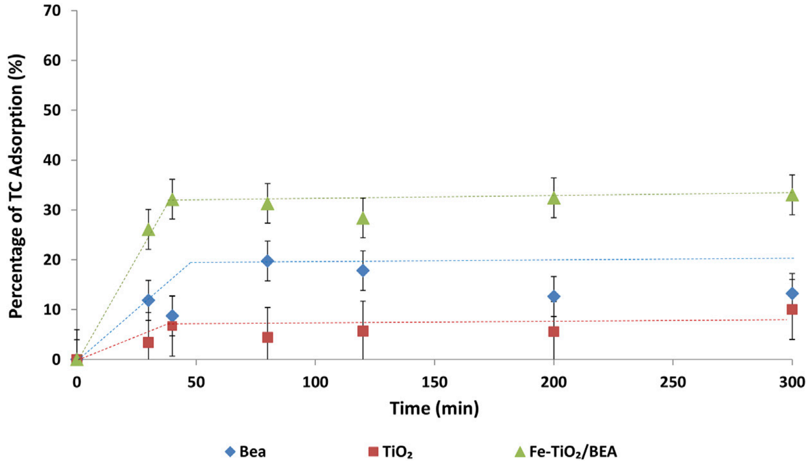

FIGURE 6 | Adsorption percentage of TC (20 mg/L) on BEA, TiO_2, and Fe-TiO_2/BEA (250 mg/L).

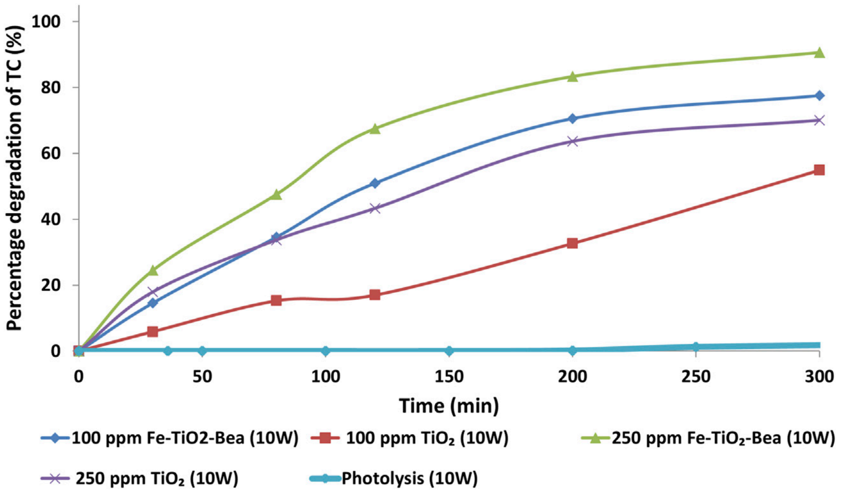

FIGURE 7 | The photolysis and photocatalytic degradation efficiencies of TC (20 mg/L) by TiO_2 and Fe-TiO_2/BEA catalysts at catalyst concentrations of 100 and 250 mg/L.

2.4 Photocatalytic Degradation Experiments

The photocatalytic degradation setup was composed of a 500 ml reactor beaker containing the TC solution and the photocatalyst. A blue LED light ($450 < \lambda < 495$ nm), used as the light source, was mounted at the top of the 500 ml beaker. The reactor was initially filled with 300 ml of TC solution with different weights of the photocatalysts; 30 mg or 75 mg of TiO_2 or Fe-TiO_2/BEA to obtain 100 mg/L and 250 mg/L initial concentration of the catalyst. The reaction mixture was kept at ambient conditions under stirring at 700 rpm. Prior to photocatalytic tests, the reactor was kept in the dark for 30 min to ensure adsorption/desorption equilibrium of TC on the catalyst's surface after which the light was turned on. A 2 ml sample was taken at pre-determined times (30, 40, 80, 120, 200, and 300 min), transferred into a Falcon tube and then centrifuged at 10,000 rpm for 15 min. High performance liquid chromatography (HPLC) (Agilent Technologies with ChemStation software), was used to analyze the concentration of the TC using a calibration curve previously prepared for TC. To calculate the degradation efficiency of each catalyst **Eq. 3** was applied, where C_0 and C_t are the initial and final concentration of TC at time t, respectively (Saadati et al., 2016a). Adsorption tests were performed using the same procedure as the photocatalytic degradation tests, but the reactor was kept in dark during the entire experiment without any use of light.

$$TC\,degradation\,\% = \frac{C_0 - C_t}{C_0} \times 100 \tag{3}$$

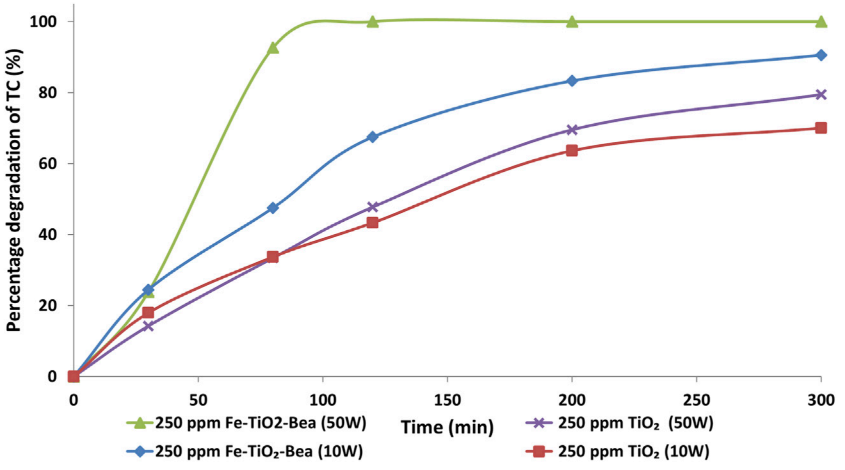

FIGURE 8 | The photocatalytic degradation efficiencies of TC (20 mg/L) by TiO_2 and Fe-TiO_2/BEA under 10 and 50 W light power.

TABLE 2 | Previous photocatalytic degradation work using zeolite immobilized titania.

Catalyst	Pollutant	Source of light	Efficiency	References and year
Zeolite immobilized TiO_2	Methylene blue dye	compact fluorescent light (36 W 400 < λ <750 nm)	92% after 180 min	Saqib et al. (2019) 2019
Fe-doped TiO_2 over HY zeolite	Methylene blue dye	Visible light	>98% 60 min	Foura et al. (2017) 2017
Au- modified TiO_2-BEA	Malachite green dye	Visible light	92% after 60	Maksod et al. (2017) 2017
TiO_2-Fe_2O_3/Fe-doped zeolite X	Oxytetracycline antibiotic	200 W 455 nm LED	98% after 60 min	Liu et al. (2019) 2019
TiO_2-Fe_2O_3/zeolite with persulfate	Ciprofloxacin antibiotic	50 W 455 nm LED	100% after 3.5 h	Liu et al. (2017) 2017
TiO_2-P25/Semnan natural zeolite	Tetracycline antibiotic	Visible irradiation	87% in 90 min	Saadati et al. (2016b) 2016
Ag-TiO_2 supported by artificial zeolite	Methylene blue dye	500 W high-pressure xenon light cut-off wavelength of 420 nm	93% within 90 min	Sun et al. (2018) 2018
Fe-TiO_2/BEA	Tetracycline	50 W Blue LED (450 < λ <495 nm)	100% after 90 min	Our work

3. RESULTS AND DISCUSSION

3.1 Characterization of the Catalysts

3.1.1 Specific Surface Area

Figure 1 shows the N_2 adsorption-desorption isotherms at 77 K of each of the BEA, TiO_2, and Fe-BEA/TiO_2 sample. The adsorption-desorption isotherm of the BEA nanocrystals showed a combination between Type I and Type IV isotherms. The isotherm was demonstrated by a steep uptake of N_2 gas at the low partial pressure due to the presence of micropores, followed by a plateau and a slight inclination with the increase in the partial pressure and was terminated with a large hysteresis loop at the relatively high partial pressure. Such a feature was associated with textural pores formed by the close packing of mono dispersed and well-shaped nanosized crystallites, which gave rise to the characteristic mesoporous structure of the BEA. The N_2 adsorption-desorption isotherm of the Fe-BEA/TiO_2 showed a comparable result to that of the BEA zeolite, while TiO_2 did not show any microporous structure with a pore volume of only 0.08 cm^3/g. This was a clear evidence that, in the Fe-BEA/TiO_2, no additional micropores were added to the BEA zeolite nanoparticles and the mesoporous structure of the BEA was preserved without any changes in its morphology or intergrowth as a result of TiO_2 dispersion.

As shown in **Table 1**, the calculated Brunauer-Emmett-Teller (BET) surface area of BEA zeolite was 620 m^2/g while its total pore volume was 0.70 cm^3/g. The BET surface area and the total pore volume of the Fe-TiO_2/BEA were 530 m^2/g and 0.62 cm^3/g, respectively. The decrease in the BET surface area of the final catalyst is explained by TiO_2 dispersion in its micropores leading to a partial blockage of these pores. Our results were in accordance with literature studies (Liu et al., 2018; Shokrolahi et al., 2019); for example, Shokrolahi et al. (2019) and Liu et al. (2018) reported that TiO_2 deposition on the surface and in the pores of the zeolite reduced its surface area and pore volume. Similarly, Foura et al. (2017) concluded that the specific surface area of the zeolite support decreased linearly as the amount of immobilized TiO_2 increased. This happened due to partial clogging of the micro-pores of zeolite as TiO_2 could enter these pores. In contrast, as demonstrated in N_2 sorption, we observed a huge increase in the external surface area of the BEA from 120 to 170 m^2/g in the Fe-TiO_2/BEA catalyst. This was in agreement with previous work (Tayade et al., 2007; Sun et al., 2018; Liu et al., 2019; Behravesh et al., 2020) and confirmed that TiO_2 dispersion occurred mainly on the external surface of the zeolite and only partially in its pores. The external surface area of a zeolite/TiO_2 composite was previously reported to increase when TiO_2 particles were dispersed on the external surface of the zeolite and not in its internal pores (Saadati et al., 2016b). This happened when the pore diameter of the zeolite was too small for TiO_2 molecules to enter.

3.1.2 X-Ray Powder Diffraction

Figure 2 shows the XRD patterns of BEA zeolite, TiO_2, and Fe-TiO_2/BEA catalysts. The XRD pattern of the zeolite substrate exhibited two main diffraction peaks at $2\theta = 7.6^\circ$ (75%) and 22.4° (100%). These peaks were in agreement with those of BEA zeolite, according to JCPDS 48-0038 standard and confirmed that our prepared zeolite exhibited nanocrystallite size as reported by Maksod et al. (2017). The XRD patterns of TiO_2 showed diffraction peaks at $2\theta = 25^\circ$ (80%), 37.9°, 48.2°, 55° (44%), and 62.5°, corresponding to the (101), (200), (211), (004), and (204) crystallographic planes for anatase phase, and 27° (80%), 36°, and 41.0°, corresponding to (110), (101), and (111) crystallographic planes of rutile phase according to spectrum standards (JCPDS 21-1272) and (JCPDS 21-1276). These results showed that our sol-gel prepared TiO_2 was mainly present in anatase polymorph with small portion present in rutile polymorph (Ebrahimi et al., 2020; Rahman et al., 2018; Saadati et al., 2016b; López et al., 2021; Liu et al., 2018). According to Kanakaraju et al. (Kanakaraju et al., 2014), a mixture of anatase and rutile phases was obtained when calcining at intermediate temperatures 200°C < T < 550°C. For the modified catalyst, Fe-TiO_2/BEA, the obtained X-ray diffraction patterns showed characteristic diffraction peaks of the BEA zeolite both at $2\theta = 7.6^\circ$ (31%) and 22.4° (100%) and that of TiO_2 at $2\theta = 25^\circ$ (54%). This confirmed that both TiO_2 and zeolite were well incorporated in the final catalyst, and that the framework structure of the zeolite remained unmodified after the deposition of TiO_2 and after the ion exchange with Fe^{3+} ions, which is in well agreement with previous studies on TiO_2/zeolites (Saqib et al., 2019; Foura et al., 2017; Maksod et al., 2017; Liu et al., 2019; Liu et al., 2017; Saadati et al., 2016a; López et al., 2021; Shokrolahi et al., 2019; Liu et al., 2018; Tayade et al., 2007). Also, as obvious from XRD, Fe-TiO_2/BEA catalyst exhibited peaks at lower intensities than those of the BEA zeolite. This was further confirmed from the calculations of the crystallite sizes. As shown in **Table 1**, the average crystallite size of the TiO_2 based on the Scherrer Equation was found to be 49 nm while the average crystallite size of BEA was 25 nm. After the immobilization of TiO_2 on zeolite, the average crystallite size of the final catalyst was 22 nm, which was lower than the values of both TiO_2 and BEA. Moreover, the differences in the XRD peak ratios of the unmodified and modified TiO_2, could be attributed to a decrease in the phase transition of the TiO_2 in the final catalyst, from the anatase to the rutile phase. The absence of peaks associated to the presence of any crystalline iron oxide phases in the XRD spectra, was due to the low iron content (less than 5 wt.%), hence to the small crystallite sizes of these iron phases, which stayed below the detection limit of XRD (Ali et al., 2017).

3.1.3 Scanning Electron Microscope (SEM)

Figure 3 shows the SEM images at different magnification scales of all the prepared samples. The SEM images of the BEA zeolite showed rough sphere-shaped surfaces contributing to its high surface area and making it an excellent adsorbent for many organic molecules (Liu et al., 2018; Liu et al., 2019). The SEM images of the Fe-BEA/TiO_2 catalyst confirmed the distribution of TiO_2 on the surface of the BEA zeolite as nanoparticles and clusters, in well agreement with previously reported studies on zeolite immobilized TiO_2 (Saadati et al., 2016b; Liu et al., 2019; López et al., 2021). Based on the shown SEM images, we may also confirm that TiO_2 immobilization was nearly uniform over the entire surface of the zeolite leaving no uncovered exposed sites. The SEM characterization also indicated that although the surface of the BEA zeolite exhibited higher roughness upon immobilization with TiO_2, its morphology and structure remained unchanged. The same observations were previously reported by Saadati et al. (2016b) and Aghajari et al. (2019).

3.1.4 FTIR Spectroscopy

In order to demonstrate the nature of the interaction of TiO_2 with the zeolite in the photocatalyst, samples were characterized by FTIR. **Figure 4** presents the FTIR spectra of the Fe-TiO_2/BEA in reference to both unmodified BEA and TiO_2 samples. The intense vibration obtained in the spectrum of the BEA zeolite at 3,730 cm^{-1} corresponds to the stretching and bending of OH present at the surface of the inorganic material (Foura et al., 2017; Liu et al., 2018), while peaks at the 1,634 cm^{-1} region are attributed to the bending vibration of H–O–H bonds of the adsorbed water molecules, as reported in various literature articles (Foura et al., 2017; Maksod et al., 2017; Liu et al., 2018; Rahman et al., 2018; Ebrahimi et al., 2020). The band at 950–1,250 cm^{-1} corresponds to the antisymmetric stretching vibration of the Si(Al)-O in the tetrahedral $Si(Al)O_4$ skeleton of the zeolite (Taufiqurrahmi et al., 2011; Saadati et al., 2016b; Foura et al., 2017; Liu et al., 2018; Behravesh et al., 2020). The observed band at the 520–570 cm^{-1} range corresponds to the T–O, T–O–T, and O–T–O (T: Si or Al atom) symmetric stretching vibrations and confirms the presence of ring-shaped tetrahedral SiO_4 and AlO_4 units (Taufiqurrahmi et al., 2011; El-Sherbiny et al., 2014; Foura et al., 2017; Maksod et al., 2017; Liu et al., 2018). In general, the observed vibration bands in the FTIR spectra of the BEA zeolite, corresponding to Si, Al, and O bonds, confirmed the successful synthesis of the BEA zeolite and illustrated the degree of crystallinity of the zeolite substrate along with the order of its structure (Maksod et al., 2017). The FTIR spectrum of the TiO_2, showed two clear peaks, a broad peak at 3,500 cm^{-1} corresponding to the symmetric and asymmetric stretching vibrations of the hydroxyl group (Ti–OH) of the TiO_2 particles and another at 1,634 cm^{-1} corresponding to the bending vibrations of adsorbed water molecules (Praveen et al., 2014; Maksod et al., 2017). The FTIR spectrum of the final catalyst Fe-TiO_2/BEA, showed new peaks at the 945 to 900 cm^{-1} range that might correspond to anti-symmetric stretching vibrations of Ti–O–Si and Ti-O-Al as similarly reported by Li et al. (2005). The conserved FTIR peaks of the zeolite BEA in the final catalyst indicated that the structure of the zeolite was stable and partially affected by the TiO_2 immobilization, which led to the formation of Ti-O-Si or Ti-O-Al, and this confirmed the incorporation of Ti in the zeolite structure in the final sample. The incorporation of Ti was due to the high calcination temperature, which caused the condensation of Si-OH or Al-OH bond with Ti-OH.

3.1.5 UV-VIS DRS Analysis

Figure 5 represents the UV-VIS diffuse reflectance spectra of Fe-TiO_2/BEA and TiO_2 applied to study the optical properties of the catalysts BEA, Fe, and TiO_2. The wavelength of the spectral onset increased from around 400 nm for TiO_2 to around 595 nm for the modified TiO_2 in a similar manner as reported previously for iron-modified TiO_2 (Foura et al., 2017; Tsiampalis et al., 2019; Ali et al., 2017). The light absorbance of the final Fe-TiO_2/BEA catalyst in the visible region of the light spectrum (400–575 nm) was higher than that of unmodified TiO_2. **Figure 5** presents the Tauc's plot of both the TiO_2 and the Fe-TiO_2/BEA photocatalysts. The band gap energy of TiO_2 was found to be 3.05 eV and was found to decrease to 2.23 eV after its immobilization on the BEA zeolite and applying the ion exchange process of the iron ions. We attribute this decrease in the band gap energy and eventually the increase in visible light absorption of the final catalyst, to the presence of the Fe^{3+} ions on the Fe-BEA/TiO_2 in a similar manner as reported in other studies (Impellizzeri et al., 2014; Foura et al., 2017). We propose that, during the ion exchange process of the BEA/TiO_2 with $FeCl_3$,

Fe^{3+} ions replaced the sodium compensating ions in the BEA zeolite, and since TiO_2 was dispersed on the zeolite (confirmed by SEM images), we propose that Fe^{3+} ions were also impregnated on the surface of TiO_2. Since XRD results confirmed the absence of any changes in the TiO_2 lattice parameters of the Fe-TiO_2/BEA catalyst, we confirm that the improved visible light absorption of the final catalyst was due to the role of the Fe^{3+} ions in reducing the band gap energy of the TiO_2 as confirmed by Tauc's plots and resulting in a red shift in its absorption spectrum to the visible light region (Ali et al., 2017; Maksod et al., 2017).

3.2 Experimental Results

3.2.1 Adsorption of Tetracycline

During photocatalytic degradation process, pollutants migrate into the surface of the catalyst and adsorb on it, then they are mineralized and eventually desorbed from the surface of the catalyst (Ibhadon and Fitzpatrick, 2013). In fact, poor adsorption of TC on the surface of the catalyst can limit the rate of the adsorption; hence eventually limit the rate of the degradation. **Figure 6** presents the adsorption of TC antibiotic on each of the BEA, TiO_2, and Fe-TiO_2/BEA under dark conditions, at room temperature with a catalyst dose of 250 mg/L. The obtained adsorption patterns by all samples followed the Langmuir adsorption isotherm, similar to what has been reported earlier by Liu et al. (2018). The Langmuir adsorption assumes a monolayer homogeneous adsorption that attains equilibrium saturation when a molecule occupies only a vacant adsorption site (Foo and Hameed, 2010), and the adsorption isotherm is characterized by an initial linear increase followed by a plateau reflecting the attained equilibrium saturation. After 300 min, the adsorption percentage of the tetracycline was the highest (33%) for the Fe-TiO_2/BEA. Our observations were in agreement with the work of Liu et al. (2018) who also reported enhanced overall adsorption percentages of sulfadiazine antibiotic onto TiO_2/zeolite compared to those of unmodified zeolite. In our work, the immobilization of TiO_2 over BEA zeolite enhanced its adsorption capacity for TC from 10% to 33%. This was mainly due to the higher specific surface area (530 m^2/g) of the Fe-TiO_2/BEA catalyst as compared to TiO_2 (90 m^2/g). Similar results were reported in previous studies (Saadati et al., 2016b; Saqib et al., 2019), where TC adsorption over TiO_2 was enhanced after the dispersion of TiO_2 photocatalyst over the zeolite support.

3.2.2 Photocatalytic Degradation of Tetracycline

3.2.2.1 Effect of the Initial Concentration of the Catalyst

Figure 7 shows the photolysis and photocatalytic degradation of tetracycline over TiO_2 and Fe-TiO_2/BEA under 10 W blue LED light at two different initial concentrations of the catalyst; 100 and 250 mg/L. The photolysis results indicated that nearly no TC was degraded in the absence of any catalyst under 10 W blue LED light. Almeida et al. (2022) reported no photodegradation of TC under visible light while Zarazua et al. (2017) reported very low degradation efficiency (~15%) of TC photolysis. As shown in **Figure 7**, at all catalyst concentrations, Fe-TiO_2/BEA resulted in higher degradation efficiency of the TC than the unmodified TiO_2 at both 100 mg/L (77% compared to 54%) and 250 mg/L (90% compared to 70%) initial catalyst loading. Based on our obtained results, we could deduce that both the Fe-metal ion insertion and the zeolite support immobilization enhanced the degradation activity of the TiO_2 under blue LED light. The simultaneous presence of Fe^{3+} ion exchanged zeolite of a large surface area synergistically enhanced the efficiency of the final catalyst by improving its TC adsorption and enhancing its visible light absorption (Foura et al., 2017). Previous studies (Ali et al., 2017; Foura et al., 2017) reported enhanced photocatalytic activity of the Fe-modified TiO_2 under visible light by the presence of the Fe^{3+} ions. For example, Foura et al. (2017) reported that Fe-modification of TiO_2/zeolite enhanced its photocatalytic degradation activity (98% after 60 min) for methylene blue dye under visible light as compared to TiO_2/zeolite (30% after 60 min). An optimum concentration of the Fe-dopant was reported to be crucial to minimize the recombination effect of the charge carriers, *via* creating trapping species within the transfer route of the charge carriers (Ali et al., 2017; Foura et al., 2017). In order to better illustrate the role of the Fe^{3+} ions in enhancing the light absorption capacity of the BEA/TiO_2, hence enhancing its photocatalytic activity, we propose a localized surface plasmon resonance mechanism (LSPR) as previously reported by Maksod et al. (2017). Fe^{3+} ions exchanged with Na^+ cations in the zeolite and impregnated on the surface of the TiO_2 absorb the visible light irradiation and form excited electrons. These electrons, due to LSPR, move into the conduction band (CB) of the TiO_2 creating positive holes in the iron ions. The transferred electrons result in the formation of the superoxide anion radicals $O_2^{\bullet-}$ that are eventually converted into •HO_2 radicals. These •HO_2 radicals are further transformed into hydroxyl radicals (•OH), which are key radicals for the photocatalytic degradation and complete mineralization of the TC (Jalloul et al., 2021).

In regard to the role of the zeolite, we explain that its presence enhanced the performance of the TiO_2 by increasing its surface area, hence increasing the adsorption of the pollutant molecules on the surface of the catalyst. Moreover, we propose that the zeolite had possibly as well inhibited the recombination effect of the charge carriers. For example, it was suggested that the surface of the zeolite can get saturated with electrons, hence can eventually act as a positive hole entrapper, which would consequently enhance the electron transfer into TiO_2 (Rahman et al., 2018). Another significant role of the zeolite support was to prevent the aggregation of the TiO_2 particles. Liu et al. (2018) and Saadati et al. (2016b) reported that the immobilization of TiO_2 on the zeolite enhanced its efficiency as a photocatalyst by minimizing the aggregation of the TiO_2 particles due to their uniform dispersion on the zeolite.

Moreover, **Figure 7** shows that an increase in the catalyst concentration from 100 mg/L to 250 mg/L under 10 W, enhanced the overall photocatalytic performance of both the unmodified and modified TiO_2, from 54% to 70% and from 77% to 90%, respectively. We mainly attribute this to the increase in the active sites of Fe-TiO_2/BEA due to the increase in the catalyst's concentration; which in turn led to an increase in the absorption of the light photons as well as the adsorption of the pollutant molecules. Higher number of hydroxyl and superoxide active radicals were then eventually generated by the increased number of charge carriers, leading to an increase in the number TC molecules degrading during the same reaction time (Ebrahimi et al., 2020). Kanakaraju et al. (2014) reported enhanced efficiency of zeolite supported TiO_2 in the degradation of amoxicillin with an increase in the catalyst concentration up to 2 g/L, in agreement with the reporting of Ebrahimi et al. (2020) on the degradation of microcystin by zeolite immobilized TiO_2.

3.2.2.2 Effect of Light Intensity

Figure 8 shows the photocatalytic degradation of tetracycline over TiO_2 and Fe-TiO_2/BEA under 10 W and 50 W blue LED light at an initial concentration of 250 mg/L. As compared to 10 W blue light, the performance of both catalysts under 50 W LED light was higher while the effect was more significant for the Fe-TiO_2/BEA. The efficiency of the Fe-TiO_2/BEA under 50 W was 100% after 90 min compared to only 60% under 10 W. For TiO_2, its photocatalytic degradation efficiency under 50 W was only slightly higher, ~40% after 90 min compared to 38% under 10 W light, which was in agreement with the UV-VIS DRS results, where Fe-TiO_2/BEA exhibited a higher light absorption as compared to the unmodified TiO_2.

Specifically for the Fe-TiO_2/BEA, increasing the intensity of the light improved the photocatalytic degradation efficiency of the system. We attribute this to the generation of more electron/hole pairs in the iron metals, higher number of transferred electrons into the CB of TiO_2, and eventually to the increased number of the active radicals. The effect of light intensity was previously discussed by Hussein (2012), who reported that under low (0–20 mW/cm^2) and intermediate (25 mW/cm^2) light intensities, the rate of the photocatalytic degradation increased linearly with a first order and half order, respectively. Similar results were obtained by Chen et al. (2019) and Das and Ahn (2022) who reported improved photocatalytic degradation of trichloroethylene and TC respectively as a result of increasing the power of the LED light.

To compare our observations with other results reported in literature, we collected and listed in **Table 2** various studies including modified TiO_2 for the photocatalytic degradation of pollutants under visible and Blue LED lights. When analyzing the reported results by other studies using zeolite immobilized catalysts for the degradation of antibiotics like ciprofloxacin (Liu et al., 2017), and oxytetracycline (Al-Harbi et al., 2015), we observe that increasing the power of the LED light source from 50 W (Liu et al., 2017) to 200 W (Al-Harbi et al., 2015) while using the same catalyst greatly enhanced the overall efficiency of the catalyst. In our work, we achieved 100% degradation efficiency for TC after 90 min, employing relatively low-power blue LED light of 50 W. These results are considered to be better when compared to those reported by Liu et al. (2017), for example, who reported 98% degradation of the oxytetracycline over TiO_2-Fe_2O_3/Fe-doped zeolite X catalyst employing 200 W of blue LED light or Liu et al. (2017), who achieved 100% degradation of the ciprofloxacin antibiotic using 50 W LED, with a single wavelength of 455 nm after 3.5 h.

4 CONCLUSION

In this work, we prepared Fe^{3+}-ion sensitized BEA zeolite supported TiO_2 catalyst for the photo-catalytic degradation of tetracycline antibiotic under blue LED visible light. XRD, FTIR, and SEM confirmed the deposition of TiO_2 mainly on the external sites of the zeolite and partially in its internal sites without modifying its morphology. The immobilized TiO_2 catalyst exhibited higher surface area and better adsorption capacity as compared to the unmodified TiO_2. The presence of Fe metal ions in the final catalyst enhanced its visible light absorption as confirmed by UV-VIS DRS. The photocatalytic degradation performance of Fe-TiO_2/BEA was higher and faster under blue LED light as compared to pure TiO_2. The improved efficiency of Fe-TiO_2/BEA was mainly due to its enhanced visible light absorption, higher surface area, better TC adsorption, and lower charge carriers recombination effect. The photocatalytic degradation results of the TC, over the as-prepared catalyst, confirmed that the coupling of Fe^{3+} ion exchange with zeolite immobilization of TiO_2 can be a promising method to extend the photocatalytic application of TiO_2 semiconductor into visible light and enhance its overall adsorption and harvesting capacity for the pollutant. (Zhao et al., 2013).

DATA AVAILABILITY STATEMENT

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

AUTHOR CONTRIBUTIONS

Conceptualization, CB, and HA; Experimental work, GJ, AA-M, FC, and AM; Writing—original draft; GJ and AA-M; Review and editing; CB and HA; Supervision, CB and HA; Funding acquisition, CB. All authors have read and agreed to the published version of the manuscript.

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Opportunities and Challenges for Establishing a Resource Nexus Community of Science and Practice

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The American Chemical Society's Division of Environmental Chemistry symposium Toward Creating a Water-Energy-Food (WEF) Nexus Community of Practice, brought together 25 cross-disciplinary speakers in five thematic areas: *1*) state of the art models and approaches, *2*) WEF Nexus initiatives and case studies, *3*) WEF governance and stakeholder engagement, *4*) chemical processes and WEF Nexus, *5*) WEF education, community, and practice. Discussions included diverse perspectives from different areas of expertise and provided key take-home messages toward building a WEF community of practice. This paper summarizes those messages, drawing conclusions regarding the anticipated challenges and opportunities moving toward establishing a resource-nexus community of science and practice that includes the chemical societies. We define the community of science and practice as a bottom-up approach of formal and non-formal scientists, policy makers, practitioners, technology providers, and civil society members concerned with any aspect of water, energy, food, ecosystem resources allocation, management, governance, and financing. The roles of chemistry and chemical processes in understanding the interlinkages of nexus systems must not be overlooked. Chemistry plays an important role in the circularity of the food and agriculture system, and in providing cleaner energy, cleaner water, and more sustainable food production. The question is how to better engage the chemical society in the WEF nexus moving forward? The paper proposes the resource of health, highlighting major challenges and opportunities in the Water-Energy-Food-Health-Ecosystems (WEFH) Nexus, and highlights future steps for fostering dialogue among this broad, multidisciplinary, multi-stakeholder community toward establishing an inclusive community of science and practice.

Keywords: water-energy-food (WEF) nexus community of practice, resources allocation, resources management, governance, financing, circularity of the food and agriculture system

CHALLENGES AND OPPORTUNITIES

This section summarizes the issues raised at the symposium and deliberated in the WEFH Nexus literature.

Modeling and Tools

The nexus concept is useful for developing integrative indices that require multiple attributes, such as resilience. System Dynamic modeling tools (https://systemdynamics.org/tools/) are a good means for teaching systems concepts in the classroom; they allow students to explore scenarios, look at interactions, and design sustainable interventions to the resource nexus. Several types of models exist which offer opportunities for the resource nexus portfolio mix. These include optimization models, system dynamics models, heuristic algorithms, and process-based models, among others (Laspidou et al., 2019; Laspidou et al., 2020). Future nexus work will include complex and simple models, process-based and optimization models, scenario-based models, and more. Each type of model has advantages and disadvantages, depending upon the questions asked, the challenges presented, and the stakeholders involved in its use (Dargin et al., 2019). The System Dynamics Society lists various type of tools for research and education available commercially, open source, stand alone and online tools. Huang and Worboys (2001) were among the first wave of scientists to demonstrate how dynamic modelling and visualization can be conducted on the Internet. The question is how to validate these complex system models. There are no simple, easy solutions with complex systems: they involve a web of interactions that cut across biophysical, social, and political systems. Finding a simple way to validate the models is difficult. Laspidou et al., 2019; and Laspidou et al., 2020 observed that the less traditional but more qualitative methods, social acceptance and stakeholder perspectives, play an important role. Laspidou et al., stated that advanced visualization techniques are important for communicating complex scientific information in layman's term and maintaining citizen engagement.

Regardless of adopted models, we should seek a principled, pragmatic, science-guided framework for complex problem-driven solutions. The framework (or Nexus) of shared tools, such as network analysis for social and physical sciences and their role in WEFH dynamics, is important to facilitate some of the principles that will be used to catalyze actionable solutions (Daher et al., 2019). Several components contribute to the formulation of the framework. As an example, virtual water is a critical component of the Nexus that involves the private sector, the political economy, subsidies, and policies. Virtual water is an important element that must not be overlooked given the quantity of water, transport energy, land use, and land processes that are embedded in each product and production location (Lee et al., 2016). Free food does not exist; someone must pay for it, whether farmer, consumer, or human/ecosystem health. Within this context, soil health and conservation is a major resource to support food security, as such preventing soil degradation as a threat to achieve food security targets. These externalities in the cost of food must be looked at carefully for they impact the long-term sustainability of human security. Thus, the question becomes **what externalities in the cost of food are appropriate to and should be embedded in the system?** This is a question of geography, geology, space, and time and opens our thinking to the notion that a universal magical solution does not exist. As those externalities vary in space and time, so does our strategies and solutions.

Implementation of the Sustainable Development Goals (SDGs)

The role of the Nexus in implementing the SDGs will become more critical (Stephan et al., 2018). Already, some governments see the interconnectivities as they struggle to implement all 17 goals without compromising the implementation of any single goal. The connection between knowledge and tools is essential to help guide the implementation of the SDGs (Malagó et al., 2021). We must identify those policy makers who are ready to engage in and champion the necessary policy changes that will enable appropriate and integrated national plans for implementing the SDGs. Pappas et al., 2022, presented a modelling for key performance indicators for waste management which encompasses several of the SDGs. Daher and Mohtar (2021) presented a study assessing the government of Morocco plans for water, energy and agriculture plans. They highlighted the need for better coherence at the national level for achieving the national targets.

Water, Water Quality, and Green Water Management

In the future, green water management must include water quality, treatment levels, and the role of chemistry in designing personalized water treatments that keep the end users in mind. Green water is referred to rainwater stored in the soil matrix and responsible for evapotranspiration processes. Green water management is an important aspect of the nexus of water, food, energy, sustainability and recycling, and the circularity of food and agriculture systems (Jones et al., 2021). Effective management of green water can reduce the energy used for pumping and irrigation, save water, and allow sustainable food production (Mohtar and Assi, 2019). Green water management is one of the many approaches that place soils at the heart of the nexus in supporting food security, water security, climate resilience, energy security, reduced emissions, and long-term regenerative solutions. Likewise, regional integration and cropping systems can provide a win-win scenario that considers the water footprint, water productivity, allocation, diet, and other choices using cost-benefit analyses.

Human and Ecosystem Health

Health, in the context of the physical resources of food, energy, and water, is essential in the development of a nexus model. We must develop nexus-inspired health indices and transform the narrative on health from an "implicit burden" on resources into a manageable resource in and of itself. The U.S. Global Change Research Program (USGCRP, 2016) presented a comprehensive account of human health and how it is being impacted by climate change. They addressed issues of temperature-related death and illness, air quality impacts, extreme weather events, vector-borne diseases, water-related illness, food safety, nutrition, and distribution, mental health and well-being, and health and minority and under represented groups as they are preferentially impacted.

Interdisciplinary Theory

At its core, interdisciplinary theory supports the WEFH nexus principles. Still, there are many theories that must be woven into the theoretical background of the nexus community as we move forward. Generalized, generalizable, and actionable knowledge is important. As we learn more, we must guide the public sector and the community at large using easily implementable and actionable knowledge. This will not be an easy task, especially as we are dealing with a complex system that couples the natural, social, practitioners, and policy domains. Moreover, in academic circles, interdisciplinarity is very expensive: while young professionals are needed to propel the interdisciplinarity of the nexus work, they are often held back by the need to be acknowledged for their disciplinary work and to seek tenure within their own disciplines (Mohtar and Daher, 2019). These concepts are being propelled by the convergence research that emerged recently out of the National Science Foundation as a mean of solving complex societal problems.

THE NEXUS COMMUNITY OF SCIENCE AND PRACTICE

As discussed above, the nexus community should be built from the bottom up and have a distributed organization structure that promotes the Nexus community and discipline while also promoting equity and social wellbeing. We must engage the health community while keeping these principles in mind. Communication and anthropological expertise will be necessary to induce changes in consumption and the ways in which we interact with the resource nexus.

Governance of Nexus Community of Science and Practice

The Community of Nexus Practice of science and practices has an advisory role in the community. The leading core group provides leadership for the network, playing a lead role that facilitates the network's vision and orientation. The CoP should be managed by an executive team responsible who will be responsible for engaging dialogue between all the members.

Sustainability in Nexus Community of Science and Practice

Many communities of practice have chosen to practice sustainable development, which is an offshoot of the standard community development process that considers issues of sustainability at different level economically, socially, and environmentally. The process basically addresses the community's current and future needs for long-term, sustainable development that is not going to compromise later generations.

FIGURE 1 | The nexus community of science and practice.

HOLISTIC, MULTI-SCALE, MULTI-STAKEHOLDERS, NEXUS APPROACH

At this stage, we must consider the principles of a holistic, multi-scale, multi-stakeholder, *Nexus* approach. This begins with an **integrative view** of water, energy, food, and health resources management, which must prevail at all levels and be founded in inclusiveness for all sectors: governance, academic, civil society, and the private sector. We must **define** and **quantify** the interconnectivity between *Water*, *Energy*, *Food*, and *Health* systems to create the tools, data, and knowledge for use in policy and planning. Finally, we must better engage the **private sector** for its role in **supply-chain** management, **mobilization** of resources, **conservation**, and **responsible investment.** Additionally, we must support R&D for **enhanced business opportunities** and **technology development**.

The **Community of Science and Practice** will become a platform for the engagement and dialogue. It will allow multiple tiers of *Education*, *Research* and *Engagement*, and consider several thematic areas of data policy engagement, including the data, tools, as illustrated in **Figure 1**.

FUTURE AGENDA OF THE COMMUNITY OF SCIENCE AND PRACTICE (COP)

The Symposium was of great interest and raised a wide range of questions. There are remaining questions that need addressing by the WEFH Nexus community including:

1. How do we maintain the Nexus principles given their complexity?
2. What type of representation and modeling will emerge to solve Nexus problems and what type of Data will be required?
3. Do we need special NEXUS professional societies, keeping in mind the distribution of disciplines, geographies, thematics, *etc.*?
4. Should we publish a new NEXUS Journal?
5. Is it time for a new NEXUS discipline?
6. What needs exist to educate and train a future Nexus/system workforce?
7. How can convergence between opportunities and Nexus-ready graduates be secured?
8. What and how can ACS members and Society contribute to this evolving discussion?
9. What structure would be the most appropriate for a CoP?
10. Can such a community make us more resilient to pandemics and shocks?
11. Who would be interested in funding such an effort? NSF, NAS, AAAS, FAO, IDRC?
12. How can we make the Nexus communicated inclusively?

Whatever the future of the Nexus and Nexus community is, we can say that the genie is out. The system's thinking is here to stay whether we call it "Nexus" or give it some other name.

DATA AVAILABILITY STATEMENT

The original contributions presented in the study are included in the article/Supplementary Material, further inquiries can be directed to the corresponding author.

AUTHOR CONTRIBUTIONS

All authors participated in a technical session at the ACS annual conference and engaged in a discussions following Mohtar as a speaker. The paper is a summary of this discussion.

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The Water, Energy, and Food Nexus: Health is yet Another Resource

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This perspective highlights a place for Health (H) in the Water, Energy, and Water (WEF) nexus. It reviews the reference to health in the WEF nexus literature and makes the case for its inclusion into the WEF Nexus. We argue that although the nexus concept of water, energy, and food is relatively recent, it has been adopted by several UN agencies and international organizations and it will continue to draw emphasis in research, politics and communications of the scientific community. Now is the time to integrate health.

Keywords: WEF-health nexus, nexus and human health, health-water interface, food-health interface, ecosystem-health, sustainable development

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INTRODUCTION: WHERE IS HEALTH IN THE WEF NEXUS?

The concept of the WEF Nexus is relatively recent and it presents a framework for the analysis of the interrelatedness and interconnectedness between the water, energy, and food resources. Over the last decade, the concept was studied extensively and it exhibited much flexibility. In spite of a controversy about its novelty and practical application, it was adopted by many UN and international organizations (Mohtar, 2011) and it encompassed many disciplines (Simpson and Jewitt, 2019) and will continue to draw emphasis in research, politics and communications of the scientific community (Finley, 2000). Proctor et al. (2021) stated that researchers from various disciplines "engage with and study the nexus from differing perspectives with distinct motivations and analytical methodologies." Several researchers recently recommended the inclusion of additional and new resources to the WEF Nexus, such as forests (Melo et al., 2021) and land (Wolde et al., 2021).

Despite the engagement of multiple disciplines, the interactions between the WEF Nexus and human health have not been widely studied (Calder et al., 2021) and current Nexus studies "do not capture (its) effects on human health" (Slorach et al., 2020). To illustrate, we conducted a preliminary search of a health/medical database of publications to explore how frequently the Nexus concept was discussed in relationship to Water, Energy, and Food (WEF) and of these, how many engaged concurrently with the theme of health. We searched Ovid MEDLINE®, Epub Ahead of Print, In-Process, In-Data-Review and Other Non-Indexed Citations, and Daily data bases (Ovid MEDLINE, 2021). We searched for all peer-reviewed papers published between 1946 and 16 August 2021 that contained each of the following terms in the title, abstract, or text of the article: water, energy, food, nexus, health, wellbeing/well-being. Over one million publications referenced "water," 785,373 referenced "energy," and 641,850 referenced 'food'. The term "nexus" was used in 4,842 publications. Yet, when we searched the publications that addressed the three resources (water, energy, and food) and the concept "nexus" concurrently in the same paper, only 180 records were identified. Similarly, we identified 3,180,787 publications that used the word 'health' and an additional 110,000 publications that used the term 'wellbeing'. We then combined the two searches and found that only 33 articles referenced food, energy, water, and health in the same paper together

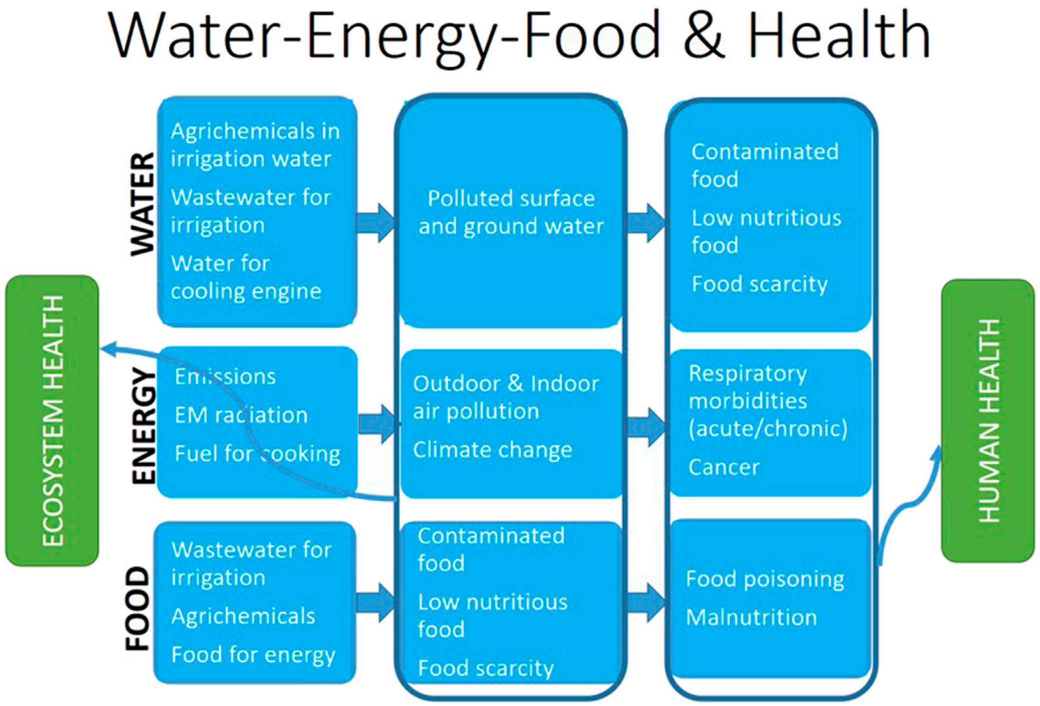

FIGURE 1 | Diagrammatic scheme of how health is part of the WEF Nexus.

with the concept "nexus." We realize this is a very preliminary analysis that could have missed on publications that adopted a nexus approach to water, energy, and food with or without health without using the term nexus, yet we are interested in documenting whether the nexus concept is consciously addressed or adopted. Our analysis confirmed as noted by Slorach et al. (2020) that the interaction between health and the WEF Nexus is not well studied, begging the question: *how is health perceived or approached in the context of the Nexus?*

PROPOSAL: HEALTH AT THE HEART OF THE WEF NEXUS

It is safe to assume that health is not perceived as a resource or component of the WEF Nexus. Instead, when health is linked to elements of the environment (water, energy, or food resources), it is perceived as a burden. The burden of the environment (its pollution or degradation) on health translates into an unavoidable health care cost that must be paid. Globally, the World Health Organization reports that 22.7% of deaths and 21.8% of the disability-adjusted life years (DALY) were attributed to environmental risks (Prüss-Üstün et al., 2016). In other words, health is implicit in the Nexus.

At the interface of health and water, are agrichemicals that seep into irrigation water, the water table, wastewater used in irrigation, and cooling water used for engines. Each of these practices pollute surface and ground water and has health outcomes, such as diarrhea, blue baby syndrome, or chemical poisoning. At the interface of health and energy are gas emissions, electromagnetic radiation, and fuels used for cooking. These lead to indoor and outdoor air pollution, climate change, and consequently, to health outcomes such as acute and chronic respiratory morbidities and cancers. As for the food-health interface, the use of wastewater in irrigation, agrichemicals, and food for energy lead to contaminated food, foods with low nutritional value, and food scarcity as outputs and to food poisoning and malnutrition as health outcomes. The outputs associated with the interfaces of water-health, energy-health, and food-health reflect the health of the ecosystem (ecosystem health), while the different health outcomes associated with these outputs reflect the health of affected populations (human health). **Figure 1** shows how human and ecosystem health are part of the nexus.

More recently, the literature has proposed new WEF Nexus models that implicitly include health. The International Water Association presented an approach in which people, landscape, and ecosystems are placed at the center of nexus model, implicitly integrating health (https://www.iwa-network.org/wp-content/uploads/2018/05/sfs.jpg). Melo et al. (2021) presented a new model in which forest security is recommended as a fourth, foundational dimension of a water, energy, food, and forest security nexus framework.

While we have made a lot of progress in linking health to the WEF Nexus, we need to be more explicit. It is time to integrate H into the WEF Nexus, where H stands both for human and ecosystem Health. It is time to place Health at the core of the Nexus in our search for resource security. Why?

First, because health is the culmination of our management of the resource nexus. Second, because it humanizes the nexus by placing people and ecosystem at the center of the dialogue. Health should be addressed as a renewable resource, an asset that involves behavior, policy, choice, and values. Our premise is that only fulfilled individuals, who live with dignity in a participatory setting, can contribute to their imagined communities. Hence, we need to transition from individual health into community and population health, and to transition away from the frameworks of 'disease' and "burden" into an asset of wellbeing.

As we integrate Health into the Nexus, we must embrace it as a holistic, social, and political concept with which we must engage at three levels. At the individual level, it encompasses mental and spiritual health, dignity, and self-expression. At the community or population level, it relates to social determinants, such as poverty, low education, gender inequity, and lack of participation or agency. After all, poor health outcomes undermine peoples' appreciation of WEF resources. Finally, at the macro or global level (be it governments, multinational corporations, or dominating global economic model), global health inequities are the outcome of greed, nepotism, self-interest, economic disparities, injustice, and the unrestrained exploitation of WEF resources.

CONCLUSION

We need a different approach. Only when we manage and invest in health as a resource, can we achieve and nourish healthy societies and healthy ecosystems. It is all about context: the social, the political, and the economic. We must understand and alter the context if we are aiming to achieve healthier communities and properly manage our water, energy, and food resources. This can be accomplished through engaging people in responsible decision making and allowing space for innovation. Only people experiencing socio-economic wellbeing have the capacity to promote sustainability and defend ecosystem health.

DATA AVAILABILITY STATEMENT

The original contributions presented in the study are included in the article, further inquiries can be directed to the corresponding author.

AUTHOR CONTRIBUTIONS

IN prepared the initial manuscript and conducted the MEDLINE data search. RM contributed to, edited, and consulted in all aspects of the work. Both IN and RM were and are actively involved in the Water-Energy-Food Research and Action for Health (WEFRAH) Initiative of the American University of Beirut.

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Examining Lebanon's Resilience Through a Water-Energy-Food Nexus Lens

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Lebanon faces a mix of underlying political and economic challenges, shocks, and triggering events that threaten the sustainability and resilience of its interconnected resource systems. The complex nature of these pressures begs for a systems approach to better understand the existing interconnections and to support the co-creation of cross-sectoral solutions to address them. This article specifically aims to: 1) conduct a scoping review of the existing literature and current events to identify interconnections between water-, energy-, and food-related challenges as they relate to the underlying conditions and triggering events at play in the context of Lebanon; 2) highlight ways in which the Water-Energy-Food (WEF) Nexus is a useful lens through which to understand and act upon issues at different scales; and 3) identify emergent themes including decentralization and systems thinking and their roles as catalysts toward more resilient resource systems. The examination concludes with two main recommendations: first, to create platforms and opportunities for interactive resource planning and decision making to facilitate systems-thinking for top-down WEF management; and second, to empower decentralized initiatives at the local level to build resilient, bottom-up solutions to WEF challenges.

Keywords: security, integrative planning, decentralized approaches, compound shocks, systems thinking

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INTRODUCTION

Viewing water, energy, and food (WEF) resources as an interconnected system of systems has become a increasingly popular among researchers and policymakers during the past decade (Gain et al., 2015; Garcia and You, 2016; Hogeboom et al., 2021). At the same time, the WEF Nexus is still broadly defined and can be applied in many contexts. Through providing different conceptualizations and frameworks of the resource system interconnections, trade-offs and opportunities for cooperation between sectors can be identified. That is happening at a time of growing awareness and consideration among governments and international organizations about the role of the sustainability of interconnected resource systems in impacting security and resilience, at different scales. Resilience, a newly popularized term, has been defined in a variety of ways. Some see resilience as the potential of a system to maintain its functionality, structure, and feedbacks by reorganizing in response to disturbances (Walker et al., 2002, 2004), while others define resilience as the ability of a system to remain within critical thresholds while adapting and changing (Folke et al., 2010). Resilience has been defined as a set of categorical reactions to disturbances (Béné and Doyen, 2017) or used to describe specific system features or specific types of shocks (Carpenter et al., 2001). The link between resilience and the interconnected resource systems warrants further delineation. For this research, we consider resilience as the ability of a system to withstand and recover from shocks, in this case, with a specific focus on the ability of water, energy, and food systems to recover from both natural and manmade shocks in Lebanon. As resilience becomes a topic of greater interest within WEF Nexus research, it is important to identify examples of resilience across the interconnected resource systems. It is also important to identify the connections between shocks and resource systems to determine when and how an integrated nexus approach is useful. The context of Lebanon is one with many challenges and factors affecting interconnected resource systems, and thus, it is an ideal case study for integrative evaluation of these resource systems as relates to the underlying political, economic, and social factors present in the country. The recent social, political, and financial shocks affecting Lebanon make it a unique study to see resilience, or lack thereof, in action.

This paper has three main objectives: first, it aims to conduct a scoping review of the existing literature and current events to identify interconnections between water-, energy-, and food-related challenges as these relate to the underlying conditions and triggering events at play in the context of Lebanon. Second, it will use the review to highlight the ways in which the WEF Nexus is a useful lens through which to understand issues at the national, local, and even individual level. Third, it identifies emergent themes including decentralization and systems thinking and their roles as catalysts toward more resilient resource systems by drawing from existing examples that highlight successful strategies and useful opportunities.

THE WATER-ENERGY-FOOD NEXUS

The past decade has seen a growth in the body of literature exploring water, energy, and food security interconnections (Sims and Dubois, 2011; Rogers, 2017; Simpson and Jewitt, 2019; Hogeboom et al., 2021). The concept first arose with a focus on water: understanding how the technical processes related to energy production utilize water, and how water management processes utilize energy (Siddiqi and Anadon, 2011). This interdependency soon spread to include the agricultural sector, which depends on both water and energy (Sims and Dubois, 2011; Rogers, 2017). Understanding the interconnectedness of these key resources provides valuable insights into the factors supporting human, social, and political security (World Economic Forum, 2017). Policy makers have increasingly recognized the value of a WEF Nexus approach in understanding complex resource challenges, even though its application remains limited (Gain et al., 2015; Garcia and You, 2016).

One trend over the past decade is the securitization of the WEF Nexus, as described by Leese and Meisch (2015). This dialogue demonstrates a shift from a normative focus on distributional justice to a focus on the sustainability of water, energy, and food systems for the sake of long-term security. Security often describes the overarching durability of the WEF Nexus, while resilience describes the ability to endure and recover on a smaller scale (Allouche et al., 2014; Leese and Meisch, 2015; Simpson and Jewitt, 2019). Resilience is a term used in many disciplines and is applied to the WEF Nexus to describe systems that are sustainable and capable of quickly recovering from shocks. An in-depth review of WEF resilience literature by Hogeboom et al. (2021) found that resilience sometimes describes holistic sustainable ecological systems and, at other times, describes the specific resilience of a single feature of the system. Much of the literature focuses on creating theoretical conceptualizations of resilience for the WEF Nexus or describing management and infrastructure for resilience (Hogeboom et al., 2021). For this research, we consider resilience as an aspect of security that describes the ability of a system to withstand and recover from shocks.

In addition to the different systems with which the WEF Nexus interacts, there is the question of scale. Although the WEF Nexus was originally conceptualized with a normative focus on fair distribution of resources for the most vulnerable, much of the current literature emphasizes large-scale security issues at the national and international level (Leese and Meisch, 2015). Sustainability at the system level rarely incorporates sustainability of the livelihoods interacting with the nexus, although the literature has recently begun analyzing how it applies to smaller scales. Biggs et al. (2015) argue that the WEF Nexus approach often looks at "top-down," large-scale resources, which may not predict results at the livelihood level. Consequently, the authors argue that incorporating a livelihood perspective can reveal bottom-up approaches and local opportunities to strengthen the operationalizing of nexus solutions. Simpson and Jewitt express concern that the "securitization" of the WEF Nexus has led to a neglect of livelihood and local-level results and reveal a tension between a security-oriented approach and an approach that considers fair distribution of resources. They argue that both perspectives must be considered to achieve the best results (Simpson and Jewitt, 2019). It is especially important at the local level, where the water, energy, and food systems may never have been conceptually separated (Allouche et al., 2015). WEF Nexus thinking is also vital for rural areas not reached by centralized systems (Leck et al., 2015; Terrapon-Pfaff et al., 2018).

Although the WEF Nexus focuses on supply and demand, resource limitation, and competition between the three sectors, analyzing small units of societal demand can clarify consumptive patterns and inform the most effective management policies and recommendations (Hussien et al., 2017). There has already been research done to this effect, both in developing models for understanding consumption and in regarding the usefulness of specific household-level recommendations (Hussien et al., 2017; Foden et al., 2019). In this study, we aim to build on the WEF Nexus literature and explore critical questions at the interfaces of the interconnected resource systems in the context of Lebanon, and to highlight both small- and large-scale themes.

METHODOLOGY

This research was carried out as a purpose-specific scoping review of Lebanon's current context. This method, based on the methodological framework described by Arksey and O'Malley (2005), prioritizes exploring a broad topic with a wide range of source types. The purpose of this review is to explore the usefulness of the WEF Nexus lens for understanding system interconnections and issues at different scales. This review identifies and maps key characteristics or factors (Munn et al., 2018) related to the WEF Nexus lens in Lebanon. In order to capture relevant literature from a broad set of topics related to our specific purpose, the characteristics and factors found in the initial reviews were mapped to inform additional review. The method can be broken down into two parts (**Figure 1**). First, reviews of topics related to water, energy, and food in Lebanon and to the underlying factors affecting water, energy, and food in Lebanon were done. Next, an evidence summary of more recent works on the current situation in Lebanon was done. Evidence summaries are part of the "continuum of rapid reviews" and are appropriate for this topic because they "serve as an informative brief that prepares stakeholders for discussion on a policy issue" (Khangura et al., 2012).

The methodology of a scoping review is to identify the research questions, identify relevant studies, select studies to review, and chart the data (Page et al., 2021). The questions that guided this review are: 1) what are the interconnections between water-, energy- and food challenges as they relate to the underlying conditions in Lebanon?; and 2) what are the interconnections between water-, energy-, and food challenges as they relate to the current situation and recent events in Lebanon? The process for identifying relevant studies to review was different for each part and is described further below.

Part 1: WEF and Underlying Factors

Relevant studies were identified to determine the characteristics of the interconnections related to the guiding questions. The Texas A&M EBSCO Discovery Service was used to find relevant academic literature. The search terms "water," "food," "agriculture," "energy," "electricity," and "WEF Nexus" were paired with "Lebanon." Reports from recognized international organizations, such as the International Monetary Fund (IMF), the United Nations (UN), and the World Bank that were related to the search terms and Lebanon, as well as documents from Lebanese government entities related to the search terms were also collected. Next, backward citation searching was used to identify additional relevant literature from the sources identified. If the authors identified gaps in the information or narrative, additional searches for relevant sources were done through Google Scholar. Literature that was not relevant to the search terms was excluded. Literature was not excluded based on year or document type. Only English language sources were used.

In addition to collecting literature relating to Lebanon's water, energy, and food, the authors mapped the underlying political and economic factors that were either identified in the literature or identified by the authors as longstanding challenges to WEF Nexus management in Lebanon. Lebanon's unique confessional system of government has been highlighted in much of the academic literature on political factors in Lebanon (Bieber, 2000; Bordenkircher, 2020; Ramadan, 2020). By reviewing literature on the political system and the literature gathered from the WEF Nexus review of Lebanon, the authors identified additional themes, including reliance on external actors, corruption, and mismanagement. Once the authors agreed on the set of underlying political and economic factors affecting Lebanon, the same steps to identify relevant literature for the underlying challenges were done using the search terms "corruption," "management," "confessional," "political," and "economic," which were all paired with "Lebanon."

Part 2: Triggering Events, Impacts, and Outcomes

Next, the authors identified salient events that had triggered the multifaceted crisis in Lebanon. Many of these events were ongoing or recent, with new information being published daily. As a result, the authors concluded that a rapid scoping review was warranted to capture as much relevant, up-to-date information as possible. This part takes after elements of the method outlined by Khangura et al. (2012) to create an evidence summary, which include a systematic literature search, screening and selection of studies, and narrative synthesis.

The need for rapid study is based on the policy relevance of the findings and the recent nature of the events being analyzed. There is a need for a systematic organization of the many current and interconnected factors and characteristics outlined by the review. Furthermore, academic and gray literature is slow to capture many of the current details relating to the situation in Lebanon. The key allowance of the rapid review is the flexibility to use recent, non-academic sources, such as news articles to summarize the current context of Lebanon (Munn et al., 2018). The authors continued to search for information on current events through July of 2021, when the article was submitted.

To answer the second research question, the same steps were carried out to search for literature, this time using the search terms "refugee," "financial," "COVID-19," "port explosion" and "geopolitical," each paired with either "Lebanon" or "Lebanon news." Searches of well-known news sources (such as the New York Times, Al Jazeera, Reuters, and the Associated Press) and Google searches were done for additional relevant sources. Sources were excluded if they did not provide information relevant to the search terms. Only English language sources were used.

To determine the reliability of the non-academic sources, the authors determined if the source met one of three additional inclusion criteria: 1) The source written by a well-known news organization, non-profit organization, or research organization, 2) The facts provided by the literature were corroborated by at least one other piece of literature from a different author, or 3) If neither of the first two criteria were true, and the literature presented information that no other source had described, the authors evaluated if the source should be included.

Given the contemporary nature of the events covered in this part, there is a lack of up-to-date academic literature. As a result,

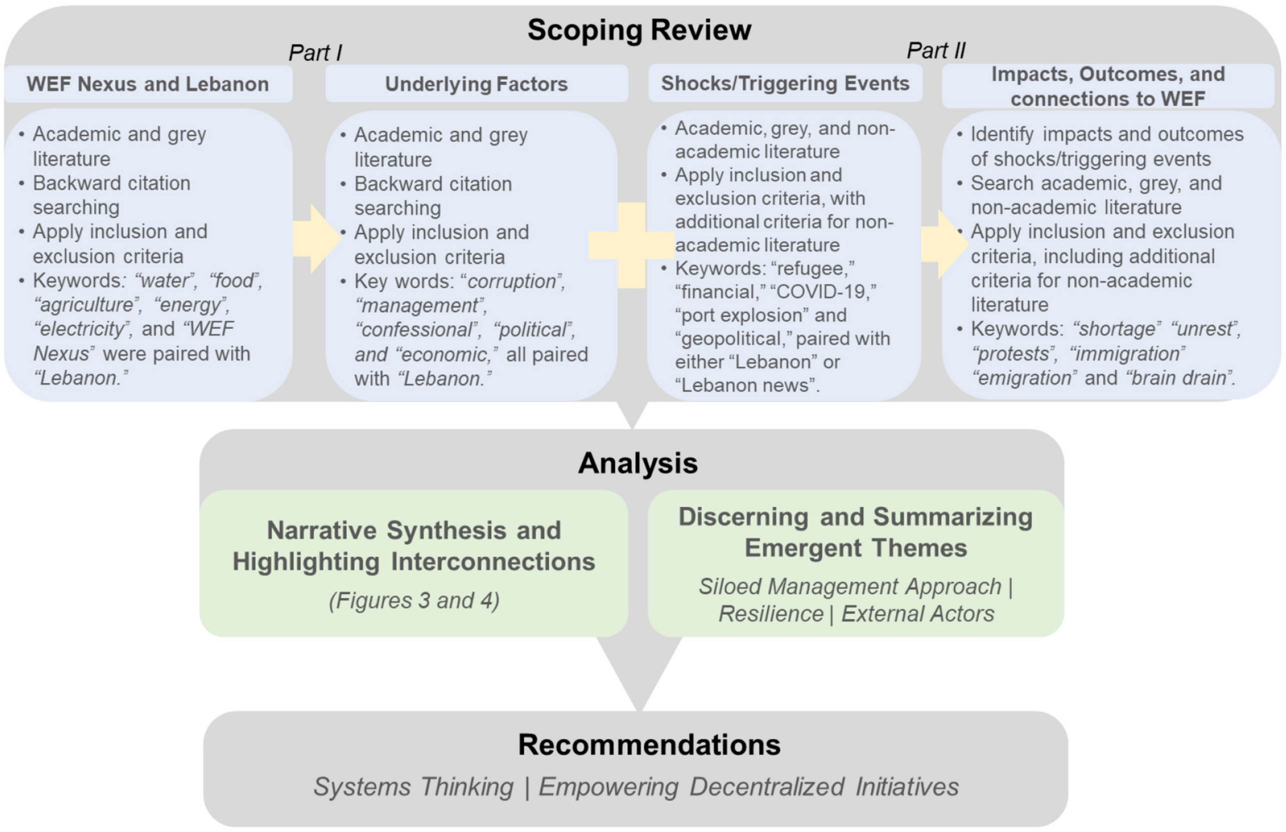


FIGURE 1 | Overarching methodological approach.

this review includes non-academic sources that may have bias. The authors limited bias in the report by 1) including a broad array of sources and 2) using the sources to gather facts or narrative details, rather than opinions or analysis. Despite the heavy reliance on news articles and gray literature, this evidence summary of the current crisis offers a significant contribution by organizing recent information that has not yet made its way into the academic realm.

Finally, the authors identified impacts and outcomes of the events based on the review. Because of the interconnectivity of recent events, factors could be both triggering events and impacts. Additional searches were then done pairing the identified impacts, outcome, and event terms with water, energy, and food terms to find sources that highlighted WEF Nexus connections. Additional terms were searched for relating to the impacts and outcomes. Terms included "shortage," "unrest," "protests," "immigration," "emigration," and "brain drain." Results were evaluated with the same inclusion and exclusion criteria.

The findings are presented according to Khangura et al.'s methodology, which calls for a narrative synthesis of the literature. The synthesis does not present information in the order it was found, instead, information is presented in the order that builds a cohesive narrative. This organization of existing knowledge is a key contribution that highlights connections between complex and constantly changing issues in Lebanon. After the whole scope of the information was organized, prevalent emergent themes were highlighted, with a focus on themes that are relevant to policymakers.

THE CONTEXT OF LEBANON

The underlying political and economic challenges, shocks, and triggering events highlighted in **Figure 2** show the complex web of intertwined factors influencing the water, energy, and food sectors. The impacts and outcomes listed result from a culmination of many challenges. Addressing any of the issues affecting Lebanon requires a system-level understanding of the relevant interconnections.

Underlying Political and Economic Challenges in Lebanon

Although Lebanon faces many challenges in managing its water, energy, and food resources, underlying political and economic challenges lay the foundation of Lebanon's current situation and continue to hinder the establishment of an integrated approach to natural resource management. Lebanon's political structure is one such underlying factor: the **confessional system** requires the president, prime minister, and speaker of the parliament

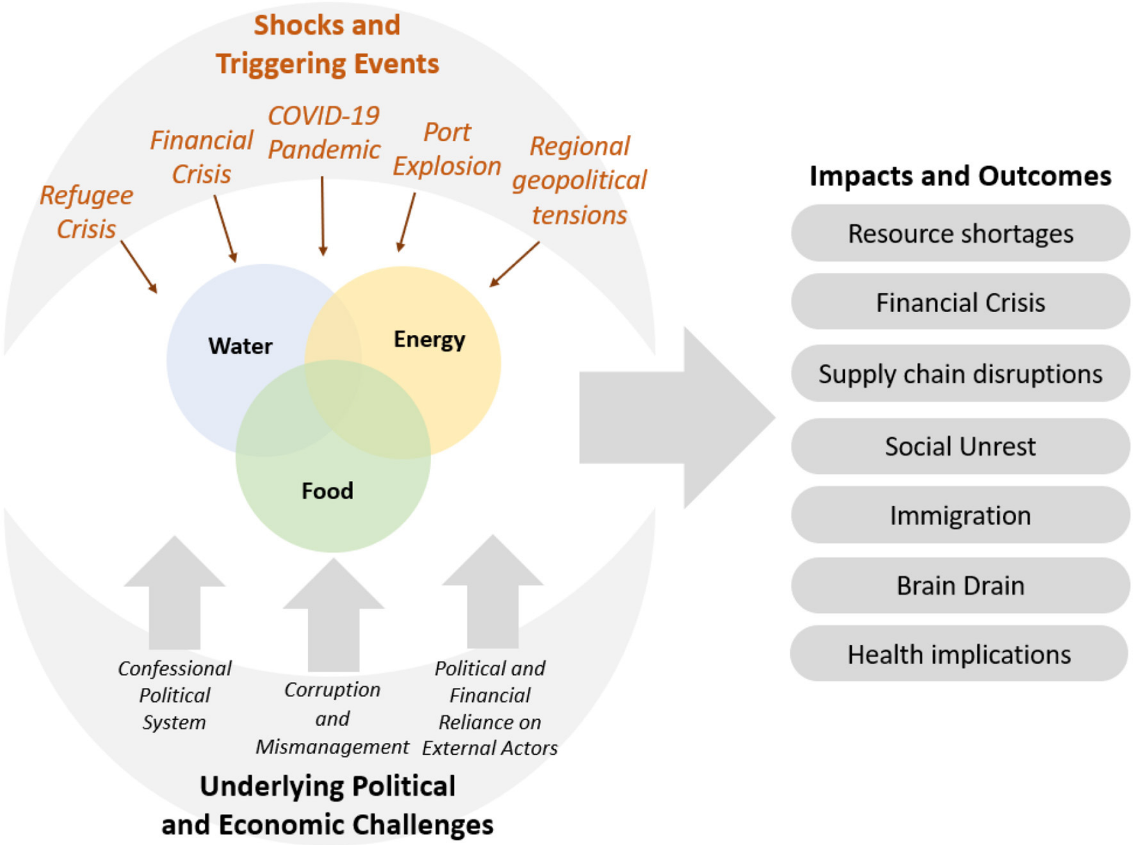


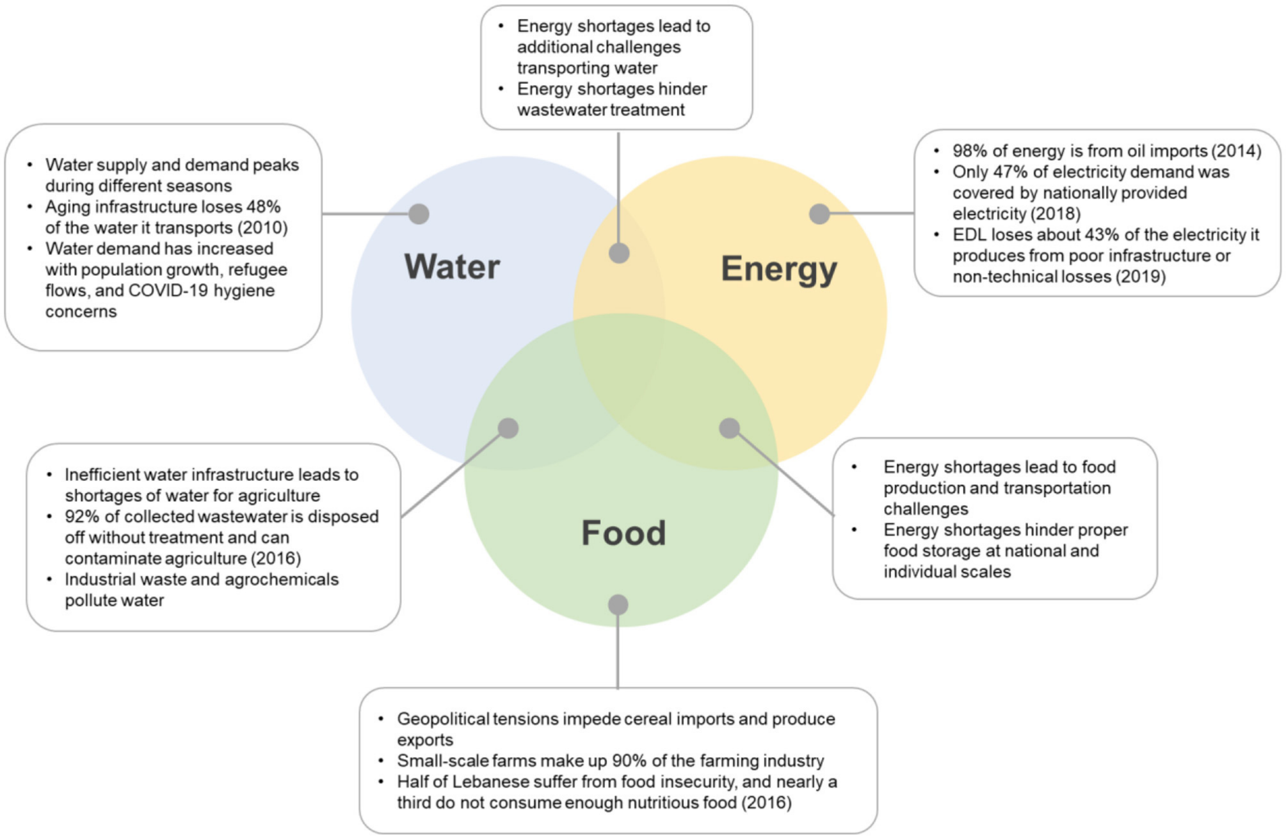
FIGURE 2 | The long-term underlying conditions, compound shocks and triggering events, and impacts and outcomes.

to be a Maronite Christian, Sunni, and Shi'a, respectively. An early attempt to strengthen national identity after the 1958 civil war failed because it was not backed by political reforms to address changing demographics and the balance of power between the confessions (Bieber, 2000). Although there were national dialogues during the 1975 Civil War, these did not establish permanent inter-confessional discussion platforms (Wählisch, 2017). While national dialogues resumed in 2006, and have occurred more frequently since then, demographic and confessional identities are far stronger than the national identity, hindering political cohesion at all levels of government (Bieber, 2000; Wählisch, 2017).

Politics in Lebanon have been characterized by many parties, but parties are often centered on a single leading politician, rather than on set structures or specific platforms. While the Lebanese electoral system recognizes politicians according to their religion, constituencies are regional. This makes politicians representative of one religious group but sometimes requires them to cater to other groups within their region. Although this arrangement sometimes fosters cooperation, it often weakens the legitimacy of politicians in the eyes of their constituencies. Because of this, the coalitions that form between parties are often the result of individual agreements between leading politicians rather than representative of broader political cooperation (Bieber, 2000). The confessionalist system has many limitations; major policy decisions must be approved by the president, prime minister, and house speaker. Generating such consensus often leads to political impasse. Other features of the system, such as the ability of the cabinet minority to veto policy decisions, encourage political standstills and prevent the government from effective action (Ramadan, 2020).

Another related factor is the longstanding "patron-client syndrome," common in Lebanese politics and dating back to Lebanon's time under French mandate. Due in part to the lack of a cohesive national identity and in part to the general inefficiency of domestic institutions, **political groups rely on outside actors** for support and forego reliance on national enforcement mechanisms to strengthen the state's legitimacy. As a result, inter-group conflicts and division are exacerbated: Lebanon is frequently involved in external actors' interests, and political accountability and enforcement are weakened (Bordenkircher, 2020).

The weak state and confessionalist system have fueled **corruption**, which is common in Lebanon. Political elites have used political fragmentation to justify corrupt practices, arguing that corruption is necessary to ensure favorable distribution of resources and power (Kechichian and Cortes, 2021). Without existing ethical norms surrounding corruption in the political



- Energy shortages lead to additional challenges transporting water
- Energy shortages hinder wastewater treatment

- Water supply and demand peaks during different seasons
- Aging infrastructure loses 48% of the water it transports (2010)
- Water demand has increased with population growth, refugee flows, and COVID-19 hygiene concerns

- 98% of energy is from oil imports (2014)
- Only 47% of electricity demand was covered by nationally provided electricity (2018)
- EDL loses about 43% of the electricity it produces from poor infrastructure or non-technical losses (2019)

- Inefficient water infrastructure leads to shortages of water for agriculture
- 92% of collected wastewater is disposed off without treatment and can contaminate agriculture (2016)
- Industrial waste and agrochemicals pollute water

- Energy shortages lead to food production and transportation challenges
- Energy shortages hinder proper food storage at national and individual scales

- Geopolitical tensions impede cereal imports and produce exports
- Small-scale farms make up 90% of the farming industry
- Half of Lebanese suffer from food insecurity, and nearly a third do not consume enough nutritious food (2016)

FIGURE 3 | Summary of the key challenges within and across the interconnected resource systems (El-Fadel et al., 2000; Bassil, 2010; OECD IEA, 2014; UNDP, 2014; ESCWA, 2016; Karnib, 2016; Soyres and Nakhle, 2019; MOA, 2020; Moore and Collins, 2020).

system, corruption has become common among political elites, both as a practice and as an issue to decry (Kechichian and Cortes, 2021). The clientelism between firms and regulatory institutions has been shown to decrease job creation and productivity (Diwan and Haidar, 2019). In the face of the ineffective governance system, corruption in its many forms has become a remedy for bureaucratic stagnation. Petty bribery and corrupt arrangements are often seen as necessary mechanisms to function in the judicial and welfare systems, political administration, and regulatory institutions (Poverty Corruption in Lebanon, 2021).

Even during times when Lebanon has experienced economic growth, misrepresentative political elites, religious fragmentation, and classism have ensured that the economic benefits are not evenly distributed (Bieber, 2000). The central bank of Lebanon (BdL) has also played a significant role in bringing about Lebanon's economic situation. Until recently, the BdL has contributed to financial stability and surpassed many shocks and crises, in part due to deposit inflows, remittances, and an exchange rate that was consistently pegged to the dollar (IMF, 2017). However, at the same time the BdL **prioritized building foreign reserves** and drawing in foreign capital while weakening its balance sheet and risking exchange rate pressures (IMF, 2017). This "reserve Ponzi" financial engineering policy meant that the BdL was attracting dollars without the ability to pay back the high interest rates (Panizza and Hassan, 2019). A 2017 IMF country report warned that severe scenarios of low growth or rising interest rates could lead to difficulty restoring capital and high liquidity stress (IMF, 2017).

WEF Nexus Challenges in Lebanon

Water, energy, and food systems have many inherent and man-made challenges in Lebanon, including poor governance, mismanagement, and economic challenges. Understanding the context of these challenges highlights how shocks, such as those affecting Lebanon recently, can have cascading effects on interconnected resource systems (**Figure 3**).

Water

Compared to other Middle Eastern countries, Lebanon has an abundant water supply. Despite this, it is considered to be a country experiencing water stress (Shaban, 2011; Shaban et al., 2021). Lebanon's water supply comes from precipitation, rivers, and springs that provided a water supply estimated at 1,350 m^3 per capita, annually, in 2011. In contrast, water demand was <220 m^3 per capita the same year (Shaban, 2011). Although there is no nation-level water stress quantification, UNDP environmental assessments have shown that water supply from springs and aquifers has decreased (UNDP, 2014; Jaafar

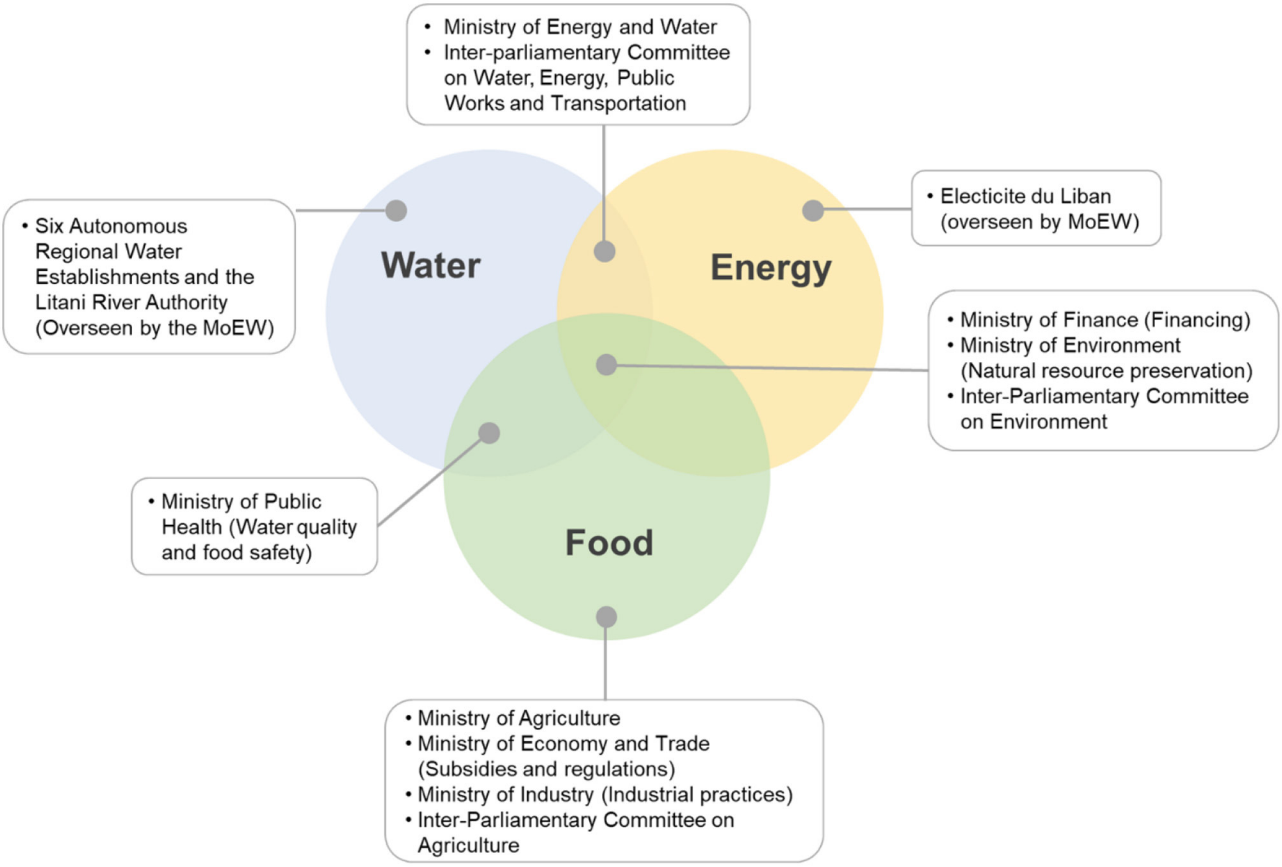


FIGURE 4 | Summary of key actors across the interconnected resource systems.

et al., 2020). One of the main reasons for the frequent water shortages experienced in Beirut and the surrounding areas is the inability and lack of infrastructure to capture water from mountains and store or transport the water to other areas. Lebanon's aging water infrastructure has resulted in 48% losses according to the most recent National Water Strategy, released in 2010 (Bassil, 2010). Additionally, demand for water has increased due to population growth, and other activities affecting water replenishment conditions, such as over pumping or deforestation, have diminished supply (El-Fadel et al., 2000; UNDP, 2014; Shaban et al., 2021).

Lebanon is fortunate to have two rivers—the Orontes and Litani—that originate in the agricultural Bekaa valley and support agriculture in the region (Quba'a et al., 2017; Conker and Hussein, 2020). To utilize the water from these sources, water is harvested through mountain lakes, dams, and individual storage (Shaban et al., 2021). However, these processes are underutilized and often less efficient than they could be. The lack of appropriate infrastructure to cater to the semi-arid and agricultural regions of Lebanon and general mismanagement have increased water stress (Sujud and Hamieh, 2018), with implications for both individual-level water needs in rural areas and for food production. Another underlying cause of Lebanon's water scarcity is that water supply peaks in the winter while demand peaks in the summer. With poor storage capacity, Lebanon experiences water shortages and rationing in the summer (UNDP, 2014).

Lebanon's focus on managing its water supply has drawn out long standing national challenges with wastewater management (Geara-Matta et al., 2010). In 1991, only 4 of 165 Mm^3 of raw sewage generated each year was treated; as of 2016, 92% of collected wastewater in Lebanon is disposed of without treatment (Karam et al., 2013; Karnib, 2016). Estimates in 2013 indicate that 35-50% of untreated urban sewage was filtering into aquifers, eventually making its way into marine environments (Karam et al., 2013). Furthermore, many areas are not connected to a sewer system and use open sewers, septic tanks, or no disposal infrastructure at all (World Bank, 2011). Therefore, many rivers and well sources are contaminated at the source by sewage disposal and by pollution from industrial waste and agrochemicals (El-Fadel et al., 2003). This contamination has repercussions for most water applications, including the availability of safe water for agriculture. Through agriculture, water contamination can negatively affect the health of domestic consumers and favor of international markets, which often have their own standards for produce. Water salination is another problem that occurs when low water tables cause salt-water intrusion during the summer's high water demand (El-Fadel et al., 2000).

Water quality issues affect both rural and urban areas. A 2010 study on rural water supplies found that although water gathered directly from a local spring was free of bacteria, water from private wells or stored in storage tanks was well above recommended WHO bacteria levels (Massoud et al., 2010). A 2008 study on water quality in Beirut found that all three water sources catering to the sampling site (well water, municipality water, and bottled water) were contaminated with fecal matter and had less than ideal physiochemical profiles (Korfali and Jurdi, 2009). In nearly all settings, residents rely on multiple sources of water, both informal and formal, to fulfill their water needs (Korfali and Jurdi, 2009; Massoud et al., 2010; Yassin et al., 2016).

Energy

Lebanon's extreme reliance on imported energy has implications and tradeoffs that affect all other systems dependent on it, including water and agriculture. Lebanon gets 98% of its energy from oil imports, and half of the oil imported is used for electricity production (Ibrahim et al., 2013; OECD IEA, 2014). Energy supply in Lebanon has been unable to meet demand since the civil war, and since then, population growth has continued to exacerbate the disparity. Historically, Lebanon imported much of its fuel from Syria, but this fuel source has been disrupted by the latter's civil war. As a result, Lebanon has turned into an "electricity island," where disruptions to imports and growing demand has led to significant shortages (Bouri and El Assad, 2016, 1). In 2013, Lebanon rented two Turkish power-generating ships to address the decreasing imports and continued demand for electricity (Bouri and El Assad, 2016). Lebanon's quickly aging energy infrastructure produces far below its intended capacity and was never repaired after damage during the civil war (Julian et al., 2020). Aside from private generators, most of the energy generated in Lebanon is from thermal power plants, with a small amount from hydraulic power plants (Ibrahim et al., 2013). Initiatives to find alternative sources of energy have been rare: there have been few attempts to search for oil within Lebanon, and none have seen results (Ibrahim et al., 2013; Azhari, 2020). Lebanon has opportunities to generate renewable energy, especially solar, wind, and hydro power, but these options have not been explored (Ibrahim et al., 2013).

Electricity is subsidized in Lebanon, but due to insufficient supply, only 47% of electricity demand was covered by nationally provided electricity in 2018 (Moore and Collins, 2020). Insufficient supply and poor infrastructure cause frequent power outages, and private diesel generators, technically illegal, are normal and necessary for adequate power provision (Julian et al., 2020). Power outages vary from daily three-hour blocks in Beirut to eight-hour or longer blocks in districts outside of Beirut. Outages are exacerbated at times when there is additional demand, such as during the heat of summer or when Lebanon's large diaspora community returns over holidays (Abi Ghanem, 2018). A 2017 study found that 66% of Lebanese use energy from diesel generators, either renting from a municipal generator or from an informal neighborhood electricity provider (IEP) (Harajli and Chalak, 2018).

On an individual scale, managing the routine power outages involves a complex array of alternative power sources, preparing specific chores to be done when power is available and managing which appliances use power when IEP electricity is in use (Abi Ghanem, 2018). Electricity cuts have been shown to negatively impact economic growth on a national level and add significant strain on individual finances (Dagher and Yacoubian, 2012; Bouri and El Assad, 2016; Abi Ghanem, 2018). The financial strain caused by having to pay multiple electricity bills creates pressures and trade-offs at the household level, including ability to afford more nutritious food or quality water. Much of the literature considers the effect of power outages on Beirut specifically. Abi Ghanem analyzes the junctions of living with power outages in Beirut——the rearranging of physical surroundings, adjusted their routines, and embedded IEP infrastructure—noting that these mitigation strategies normalize the everyday interactions with IEPs. This entrenchment is such that the public does not expect the formal system to improve, thus normalizing the dysfunctionality of official infrastructure (Abi Ghanem, 2018). Furthermore, Verdeil finds that the effects of sectarian splits on politics and urban demographic distribution both exacerbate and reinforce Beirut's current electricity arrangements by reinforcing reliance on neighborhood IEPs and perpetuating political stagnation that prevents power system reforms (Verdeil, 2016).

Food

Food and agricultural production offer a significant opportunity for Lebanon: about a quarter of Lebanon's land is agricultural and its climate is ideal for many crops (UNEP, 2005). Over time, Lebanon has transitioned from low-input extensive farming to intensive high value-added crops (Ghadban et al., 2013; MOA, 2014). The result of this transition has been twofold: more intensive farming has led to soil quality degradation; and the focus on high value-added crops has made Lebanon more dependent on imports to fulfill food demands. Currently, Lebanon's most common cultivated crops are fruits, such as tomatoes, oranges, apples, lemons, bananas, and grapes, as well as potatoes, cucumbers, wheat, and olives (MOA, 2014; Skaf et al., 2019). Lebanon is self-sufficient in fruits and close to being self-sufficient in vegetables but is highly dependent on imports for cereal products (ESCWA, 2016). Lebanon is self-sufficient in poultry but imports almost all its dairy and other meat products (UNEP, 2005).

Lebanon has a paradoxical comparative advantage in fruits and vegetables: climate and water availability make fruits and vegetables the ideal produce, while cereals and livestock are less cost-efficient, more water- and land-intensive, and provide fewer micronutrients (ESCWA, 2016). Consequently, it is generally agreed that Lebanon should not focus on full self-sufficiency in food production and should focus on strategically managing food production and decreasing import-shock vulnerabilities (Ghadban et al., 2013; ESCWA, 2016).

At the farm-level, the agricultural sector suffers from lack of planning, outdated technologies, and the use of untreated water for irrigation. Farms are either large-scale commercial agriculture (<25%), or non-commercial smallholder farms partly focused on subsistence agriculture (MOA, 2020). As input and production costs increase, small-scale farming becomes a less sustainable form of employment. As a result, 90% of the industry comprises small-scale farms that are unorganized and rarely participate in international value chains (MOA, 2020). Agricultural and livestock market infrastructure is poorly managed, with unimplemented international agreements hindering efficient foreign trade (MOA, 2014).

Small-scale rural farmers often grow wheat, subsidized by the government. A 2014 survey found that of 63 farmers in West Bekaa growing wheat, only 8.5% would continue growing wheat if the government stopped subsidizing it. Many of the poorest farmers cannot wait for the slow bureaucratic process to disperse payments for subsidized wheat and are forced to sell directly to the market. Without cooperatives to help rural farmers with marketing and communication, it is difficult for farmers to get the best prices for direct-to-market sales or alternative crops. this dynamic reveals that the most vulnerable farmers are often producing the least efficient crops and are motivated mainly by government subsidies. Additionally, 83% also grow livestock or other crops in addition to wheat (Tawk et al., 2019). Through local cooperatives or initiatives, the government of Lebanon could improve the efficiency of wheat production to mitigate import dependency, or facilitate the transition to more valuable crops, but is currently doing neither.

Because Lebanon is dependent on food imports, it is vulnerable to food price shocks that directly affect consumers. After the food price crisis of 2007/2008, Lebanon introduced national food subsidies for consumers on flour, wheat, and bread, and non-processed foods have value-added tax (VAT) exemptions (Makdissi and Edine, 2020). The results of a 2016 ESCWA survey found that half of Lebanese suffered from food insecurity and nearly a third were unable to consume enough nutritious food (ESCWA, 2016). Analysis of the 2004 and 2008 food crises also found that food price increases led to decreased consumption of macronutrients, micronutrients, and vitamins (Zaki et al., 2014). Although some have argued that social transfer programs would be preferable to food subsidies, food subsidies are currently the most functional solution, given Lebanon's government structure (Makdissi and Edine, 2020).

Water, Energy, and Food Management in Lebanon

The institutional responsibility for water, energy, and food in Lebanon is distributed around multiple organizations (**Figure 4**). The Ministry of Energy and Water (MoEW) manages and plans for water and energy sectors and some related projects. Laws, codes, and strategies for water management have been frequently implemented and reformed, but approval is often delayed. Existing policies often lead to fragmented decision making and overlapping responsibilities (Gharios et al., 2020). Within the MoEW, the General Directorate of Hydraulic and Electric Resources (GDHER) houses the Department of Planning, which has three units: water planning, energy planning, and a unit for projects, which usually works alongside external organizations such as the Council for Development and Reconstruction and the UNDP (Farajalla et al., 2016). As of 2016, the Department of Planning was 90% vacant, and the GDHER was 85% vacant. The department makes up for these vacancies by outsourcing their staff (Farajalla et al., 2016).

The MoEW also oversees the Electricité du Liban (EDL), the state-owned electricity company responsible for providing 90% of the nation's energy needs, among other responsibilities (Farajalla et al., 2016). EDL electricity tariffs are based on 1996 fuel prices and consequently do not cover the cost of electricity production (Kinab and Elkhoury, 2012; Julian et al., 2020). In 2018, tariffs only covered about 37% of EDL's operating costs (Moore and Collins, 2020) and EDL takes on huge operating losses ($1.4 billion USD between 2008 and 2017) and relies on government subsidies to keep from going bankrupt (El-Jamal et al., 2014; Moore and Collins, 2020). Energy sector subsidies cause significant financial stress to Lebanon's public finance, accounting for nearly half of Lebanon's overall external debt (World Bank, 2019; Moore and Collins, 2020). Additionally, EDL loses 43% of the electricity it produces: 17% are technical losses stemming from poor infrastructure, 21% are non-technical losses from incorrect billing, energy theft, and meter tampering, and 5% are losses from uncollected payments (Soyres and Nakhle, 2019).

In contrast, water operations are less centralized. Water supply and wastewater treatment are run by four autonomous regional authorities and the Litani River Authority. These entities have no policy-making authority, and their relationship with the MoEW is unclear because of the lack of implementation decrees (Farajalla et al., 2016).

The Ministry of Agriculture (MoA) manages the food sector through a handful of departments including the Lebanese Agricultural Research Institute, the Green Plan, and the Higher Council for Agriculture. The ministry's work ranges from scientific research to agricultural production strategies and methods (Farajalla et al., 2016). The MoA administers the agriculture sector, including setting crop safety and quality standards, overseeing international trade, and laying out natural resource management guidelines. There are various planning committees and groups that work under the MoA, but compared to the MoEW, there is less applicable oversight at the ground level for agriculture. From the household and individual perspective, the Ministry of Economy and Trade (MoET) has more impact on food provision, as the MoET decides and manages food subsidies.

Throughout the three sectors, it is common to see overlapping strategies, plans, and jurisdictions, as well as delayed approval of proposals. These bureaucratic hindrances make policy implementation difficult and stymie system reform.

The MoEW and MoET subsidize electricity and flour production, respectively, by subsidizing the purchase of fuel and wheat from international markets. The MoET also purchases flour and bread from local firms and sets prices for wheat products (ESCWA, 2016). In 2019, the MoET subsidized basic food goods and essential products such as fuel and medicine for consumers. The subsidy arrangement, though impactful during the financial crisis, has been criticized as unable to target poorer households. Due to the higher purchasing power for more affluent households, subsidies benefit affluent households more than the poorest (ESCWA, 2016). MoET also subsidizes wheat by purchasing wheat from international markets and selling it to flour mills at low prices (ESCWA, 2016). These subsidies are costly and have only been sustainable by lowering the mandatory foreign reserve threshold to maintain the subsidy programs (Chehayeb, 2021).

Inter-parliamentary committees exist to discuss proposals and amendments, such as the Committee on Water, Energy, Public Works and Transportation; the Inter-parliamentary Committee on Environment; and the Inter-parliamentary Committee on Agriculture. Other water, energy and food-related entities include the Lebanese Center for Energy Conservation, the Ministry of Environment, the Ministry of Finance, and the Ministry of Public Health (which oversees food safety, and water quality). These entities often work at the intersection of water and food or water and energy, but usually only facilitate a bilateral connection (either water and food or water and energy), or focus on specific programs and jurisdictions, such as natural resource preservation or financing (Farajalla et al., 2016).

Entities that facilitate dialogue and coordination between multiple sectors are critical for nexus-oriented management, but most entities have limited authority to make policy, and slow approval processes inhibit timely and effective policy implementation at the regional and local levels.

Shocks and Triggering Events

Given the turbulent situation in Lebanon, it is important to consider how recent shocks have triggered additional issues. One notable shock that has affected Lebanon for over a decade is the **Syrian Refugee Crisis** which, in addition to its humanitarian aspects, has strained both supply and demand for water, energy, and food. Recently, COVID-19 and related supply chain disruptions have made government assistance more necessary for vulnerable refugees and Lebanese citizens. Lebanon's recent financial crisis has drastically affected consumers' ability to buy food and the government's ability to subsidize essential goods and services.

The conflict in Syria, although no longer a recent event, has had unexpected and long-lasting effects on Lebanon. Primarily, demand for water, energy, and food has increased with the growing population of refugees from Syria. Lebanon hosts more refugees per capita than almost any other country in the world, with an estimated 1.5 million Syrian refugees living in Lebanon as of 2019 (Vulnerability Assessment of Syrian Refugees in Lebanon, 2020). Refugees have high unemployment rates and consequently represent a population highly vulnerable to food insecurity, unsanitary living conditions, and poor health (ESCWA, 2016). Vulnerable refugee populations have contributed especially to water demand and, in cases where wastewater infrastructure is poor, to water quality issues.

The Syrian conflict also represents a geopolitical tension with significant impacts on the supply side for many industries. Prior to the conflict, around 20% of exports and many imports passed through Syria (ESCWA, 2016). Lebanon imported up to 7.5% of electricity demand from Syria and Egypt through the regional grid (Bouri and El Assad, 2016). The resulting import disruptions had significant and long-lasting impacts on the energy sector. Food trade was also impacted: before the conflict, about 6% of agricultural imports flowed through Syria (ESCWA, 2016). These supply routes continue to be inaccessible, in part due to the continued conflict in Syria and in part due to the U.S.'s Caesar Syria Civilian Protection Act of 2019, which imposes sanctions on anyone doing business with the Syrian government.

More recently, the **financial crisis** in Lebanon has exacerbated nearly every other strain. Lebanon's financial policy began to break down when depositors started moving their funds out of Lebanon in 2017 (Panizza and Hassan, 2019). As foreign confidence—and deposits—declined, interest rates increased, bank lending declined, and GDP growth dropped (Panizza and Hassan, 2019). Banks limited dollar withdrawals to maintain liquidity. The government passed reforms to address the crisis, but these were harsh to citizens and failed to address the widespread corruption present in Lebanon (Panizza and Hassan, 2019). This led to social unrest, frustration with the government, and a perilous financial situation, which have continued to the present day.

The **COVID-19 pandemic** has been harsh in Lebanon, with lockdowns still common and vaccination rates low (Lebanon Goes into COVID-19 Lockdown for Orthodox Easter Weekend, 2021). Lockdowns have been particularly harsh as electricity has become less consistent (McCaffrey and Todman, 2021). Health professionals left the country as the health system struggled to manage the pandemic. Few people can afford healthcare, many hospitals are unable to afford staff or supplies (McCaffrey and Todman, 2021). Water supply and quality have become especially important, as COVID-19 made sanitation and hygiene practices more vital.

The August 2020 **Beirut port explosion** is another noteworthy shock that triggered social demonstrations against corruption and poor management. To understand the full results of the port explosion, an analysis of Lebanon's food supply chains is instructive. In 2016, when the Syrian crisis began, Lebanon's food supply, which had largely arrived over Syrian land routes, faltered briefly. Much of the trade transitioned to maritime routes, and Lebanon's food availability soon returned to pre-crisis levels (ESCWA, 2016). In 2020, the Beirut port explosion damaged grain silos and disrupted imports coming through the Port of Beirut. However, food stores in Beirut had already been low, and maritime trade had already slowed along with the slowing economy. Additionally, the port in Tripoli was able to receive imports for the week it took to bring the Port of Beirut back into service, so the impact of the explosion on food was brief (Ibrahim, 2020). More importantly, the explosion publicly and globally underscored the gross mismanagement of the nation's largest port and vital gateway for international trade. The explosion was the result of highly dangerous material that had sat, neglected, at the port for seven years. The blast killed more than 190 people, injured thousands, and caused significant infrastructure damage (Hubbard et al., 2020). In the aftermath of the explosion, social unrest led to the resignation of Lebanon's cabinet (Hubbard, 2020). The IMF and western donors showed unwillingness to assist Lebanon until it addresses finances and establishes a new cabinet (Dahan and El, 2021).

Geopolitical tensions play a complex role in Lebanon. Tensions with geographic neighbors lead to trade barriers and supply shortages, some of which directly impact water, energy, and food management. Given Lebanon's historic ties with a variety of external actors, it is often affected by outside conflicts. These geopolitical tensions have recently been exacerbated by the financial crisis, the weak value of the Lira, and the turbulent state of Lebanon's economy, leading to a general international hesitancy to do business with Lebanon. Tensions between Lebanon and the international community, including international organizations, have stalled infrastructure maintenance, and inhibited international assistance.

Impacts and Outcomes

The results of recent events and shocks in Lebanon have been broad. Understanding the full effects of the impacts and outcomes will take long-term attention, as many are still evolving. However, an overview of the outcomes and how they connect to preexisting challenges in Lebanon is instructive for identifying WEF Nexus resilience opportunities.

The outcomes and impacts of recent events in Lebanon are tightly interconnected. One of the most evident is the collection of **resource shortages** in water, energy, and food that Lebanon is experiencing, which is especially connected to the financial crisis and geopolitical tensions. The **financial crisis** is both a shock affecting the WEF Nexus and an outcome of other shocks and underlying factors. As conceptualized above, the financial crisis is the result of many years of financial engineering that has impacted the functionality of the interconnected resource systems. Simultaneously, the crisis can be conceptualized as an outcome of other shocks, such as geopolitical tensions and the COVID-19 pandemic. The financial crisis has connections to other outcomes. For example, COVID-19 has exacerbated financial struggles at both the national level and the individual level, and social unrest has been fueled by continuation of the financial crisis.

Of the sectors, water was least affected by the financial crisis as it is not an imported resource. Although water prices have increased drastically, much like other essential goods, the quality and quantity of water available has not been significantly reduced by recent events. In contrast, energy in Lebanon is almost entirely import-dependent, and the financial crisis has exacerbated energy challenges greatly. In March 2021, Lebanon's parliament approved a loan of $200 million to be used for fuel because the EDL had run out of funds. The loan was only fully approved in June, when power plants had shut down and outages were exacerbated due to lack of fuel (Houssari, 2021; Reuters, 2021; Reuters Staff, 2021). Additionally, the Turkish energy company that rented power-generation ships to Lebanon shut off supply following 18 months of outstanding payments totaling $100 million.

Food has been substantially affected by the financial crisis, the conflict in Syria, and geopolitical tensions. The refugee crisis has not only increased overall demand for food, it has impacted the amount of agricultural land available for food cultivation. A 2014 evaluation predicted that informal tented settlement growth would eventually encroach on agricultural lands and that the wastewater discharges created by Syrian refugee would add to untreated wastewater and would eventually contaminate crops (UNDP, 2014). The COVID-19 pandemic increased unemployment and household expenditures generally, making it more difficult to afford food and leading to the creation of subsidies for basic goods, which many now rely on. As the financial crisis lingers, Lebanon's ability to continue to fund these subsidies decreases; the Minister of Finance argued in April 2021 that subsidies for fuel and food would soon need to be restricted, leading to fears that both food production and consumption in Lebanon would soon face major strains (Mathur-Ashton, 2021). On the consumer side, many with limited access to dollars are unable to afford the food that is available. These business and **supply chain disruptions** have also affected infrastructure functionality, especially in the energy sector, where power plants now sit unused.

The government's reactions to COVID-19, the financial crisis, and the resulting impacts have drawn much criticism from the public, who have voiced protests that the government is not addressing fundamental problems of corruption and mismanagement. The protests and general **social unrest** were heightened following the port explosion. Protesters have demanded many changes, but generally call for the removal of the corrupt government officials and reform of ineffective institutional systems (Sherlock, 2020). The effects of COVID-19 and the government's slow response to the pandemic have also led to heighted unrest, frustration, and increasing emigration from Lebanon (Pearlman, 2013; Nakhoul, 2020). The government has been accused of using COVID-19 as an excuse to shut down protests (Rose, 2020).

The pandemic, financial crisis, and resource shortages have all led to increased **emigration**. While emigration from Lebanon is not uncommon, recent shocks have increased and shaped emigration. There are indicators that the more vulnerable demographics are seeking ways to leave Lebanon, sometimes despite significant risks (Hendrix and Durgham, 2020). Furthermore, Lebanon's vast diaspora and largely well-educated populace make emigration an attractive option to find better opportunities, especially as the financial crisis continues. **Brain drain**, or the movement of the most educated out of the country, has significant long-term repercussions for Lebanon. This outcome is connected to each of the others, as strains on health, food and water availability, and financial stability are all highly motivational factors that push residents toward emigration.

The **health implications** of recent shocks, though broader than many of the other outcomes analyzed here, are highly interconnected and offer a useful picture of impacts at the individual and local levels. Health implications are often traced to issues with the underlying water, energy, and food sectors. Most evident is COVID-19, which also impacted water supply, food availability, and energy, all of which affect sanitation, nutrition, and the population's ability to adhere to lockdowns. Lebanon's health sector was especially affected by emigration: medical professionals in Lebanon found themselves without pay and inadequate supplies to face the global pandemic, disrupted supply chains, and the financial crisis. Many Lebanese medical professionals took advantage of high demand to relocate outside of the country (Abdallah and Nakhoul, 2020; Karam and Tawil, 2021).

Analysis of water intake, infant health, and the prevalence of waterborne diseases in Lebanon indicate that water availability and affordability in Lebanon are also connected to health outcomes (El-Fadel et al., 2003, 2012; Korfali and Jurdi, 2009; Jomaa et al., 2016; Schuster et al., 2020). Because Lebanon is experiencing food shortages, particularly in cereal crops like wheat, inaccessibility of macronutrients will have increasing effects on health. Although Lebanon's domestic produce is nutritionally rich, much of the food grown in Lebanon is exported (ESCWA, 2016). Electricity shortages strain existing health infrastructure. Reliance on diesel generators leads to frequent exposure to airborne carcinogens: a study on carcinogenic emissions found that the use of generators for only 3 hours a day creates damage equivalent to smoking a few cigarettes per day (Shihadeh et al., 2013).

The port explosion was another notable trigger that compounded existing issues and exposed clear health implications: the explosion damaged more than half of health facilities in Beirut, making them non-functional, and injuries from the blast caused the remaining facilities to consume months of medical supplies within days (Landry et al., 2020). Damage to housing forced many into unsafe living situations (Abouzeid, 2021). The explosion is a specific example of the interconnectedness of many shocks and highlights the myriad of health implications.

DISCUSSION AND RECOMMENDATIONS

The review portion of this work covers a wide scope of information relevant to Lebanon's current situation and organizes this information into three categories—underlying challenges, shocks and triggering events, and impacts and outcomes. From this review, we highlight three recurring, emergent themes, and consider their implications for water, energy, and food policy. Finally, two recommendations are presented based on our findings.

Emergent Themes

The expanse of information presented here underscores many recurring themes in the case of Lebanon. There are a handful of salient themes that can be useful for the purpose of exploring WEF Nexus resilience and considering policy reactions to the current situation.

Siloed Approaches to Management

Considering themes of resilience in Lebanon can point out both areas of resilience and areas where resilience is lacking. The current context of Lebanon and its longstanding issues highlight the WEF Nexus's lack of resilience: the current systems of management are neither sustainable, nor have they facilitated recovery from the many shocks Lebanon has faced. In exploring the many causes of this lack of resilience, one theme is most apparent: Lebanon's water, energy, and food systems are managed within silos, run by many actors with differing priorities, capabilities, and jurisdictions. The Ministry of Economy and Trade, for instance, purchases wheat from international markets and sells it to flour mills at low prices while also purchasing local flour at fixed prices (ESCWA, 2016; Tawk et al., 2019). The result is that local farmers grow a different, hardier but less valuable wheat (ESCWA, 2016). The Ministry of Agriculture, which should manage agricultural production strategies, has no formal way of influencing these subsidies. Perhaps the most obvious split is the management of water supply for agricultural purposes, which is run largely by autonomous regional authorities. The role of the Ministry of Energy and Water is unclear, and the role of the Ministry of Agriculture is minimal (Farajalla et al., 2016). These artificial splits in management underscore the siloed approach to water, energy, and food administration before even considering the excessive bureaucracy, corrupt politics, and challenges with staffing public service roles. Although entities exist to facilitate cross-sector dialogue, most entities have limited power, or are focused on specific aspects of management. There are many layers of disconnect, which results in a siloed approach.

Pockets of Resilience

In contrast, resilience can be seen in Lebanon in areas where water, energy, and food systems continue to function despite numerous challenges. In cases where governance is necessary but absent, corruption and informal systems allow Lebanese society to continue to function without addressing bureaucratic issues. Farajalla et al. (2017) highlight that informal systems are highly resilient, adaptable, and can provide useful examples for policy makers. Prime examples are Lebanon's informal electricity grids and transportation system, which make up for areas where official systems have failed to provide adequate services. It is worth noting that not all informal systems are illegal or corrupt, but they are intrinsically linked to the underlying factors of corruption and inefficient legitimate governance. As it stands, there are many entrenched informal systems between society and business that maintain functionality of the water, energy, and food sectors. While these systems are imperfect, they provide examples of possible resilient resource management initiatives.

One example of decentralization in practice is Electricité de Zahlé (EDZ) in the city of Zahle, Bekaa Governorate. Zahle faced long power outages after the local power plant was destroyed in the civil war. Rather than continuing to wait for the EDL to address shortages, EDZ built its own power plant in 2015 (Naylor, 2016) and now provides 24-hour electricity to Zahle and the surrounding municipalities at about 40% of the cost compared to other areas of Lebanon (Euronews, 2018). Several factors contributed to the success of the EDZ power grid. On a bureaucratic level, Zahle is unique in Lebanon: local power companies are authorized to distribute, but not generate, electricity. To overcome this issue, EDZ drew on a 1920s era law enacted before EDL existed, which permitted EDZ to generate electricity. Although other cities have applied for a similar ability to generate power, requests have thus far been refused (Euronews, 2018).

Another major hurdle was pushback from local generator owners who profited from the power outages and threatened both the authorities and customers to hinder the adoption of the new system. This hurdle was overcome by collective action and persistence. Local sector-specific initiatives, such as EDZ, also strengthen connections with other sectors in the community. One result of 24-hour electricity in Zahle is that farmers are now able to pump water consistently, thereby improving their crop production (Naylor, 2016). The EDZ also took advantage of solar power to provide electricity at a much lower cost than alternative providers.

Another instructive example of small-scale resilience is provided by Water Users' Associations (WUAs) in Lebanon. Tegoni et al. (2016) analyzed five of these WUAs and determined that the WUAs, which work to collectively manage local water resources, are not particularly resilient (Tegoni et al., 2016). WUAs are not official legal entities under the MoEW, although the MoEW has an unimplemented plan in place to involve WUAs in decision making. Instead, the WUAs rely on the MoA to recognize them as agricultural cooperatives, which are also not well supported, and keeps the role of WUAs in Lebanon informal. However, despite the lack of institutional recognition, many of the WUAs successfully distribute water resources and foster cooperation among farmers in their communities. In particular, the WUAs analyzed by Tegoni et al. (2016) succeed in governing and maintaining water infrastructure such as wells and irrigation networks. Additionally, these organizations can tailor water management to their constituents by choosing how to distribute and charge for water usage. Replicating the success of informal WUAs across Lebanon would require giving them legal recognition, authority to enforce regulations, and decision-making power at higher levels. This arrangement is already used in other MENA countries, where WUAs and private water companies are formally recognized, regulated, and supported (Farajalla et al., 2017).

The Role of External Actors

A third relevant theme of this review is the significant role outside actors play in Lebanon. The patron-client syndrome described by Bordenkircher (2020) reflects Lebanon's historic political and social reliance on outside benefactors. Similarly, BdL's reliance on foreign reserves and the general national reliance on remittances demonstrate the same trends in the financial sector. Lebanon's import-dependence has only become as critical as it is because of Lebanon's historic dependence on other countries for fuel and food; it's reliance on Turkish energy generating ships is one such example. The prevalence of external actors to support infrastructure at the local level for WUAs highlights the continuation of this underlying trend: four out of five WUAs analyzed by Tegoni et al. (2016) manage infrastructure built with the help of international donors or organizations, a local example of Lebanon's historic reliance on external support.

Lebanon's cooperation with outside actors is not an innately negative factor, rather, the balance between national sovereignty and international cooperation represents an important policy consideration for Lebanon. Becoming more resilient to geographic tensions and shocks such as the financial crisis would require shifting toward national ownership of local solutions and seeking out opportunities that do not require external support. At the same time, external collaboration is a source of necessary stability during a time of turbulence. One clear representation of the value of international cooperation is Lebanon's position with food: by choosing to produce valuable fruits and vegetables, Lebanon selects to heavily rely on imported cereals. Lebanon's position as a country that will likely always rely to some extent on international cooperation highlights a complex theme that warrants further research and clear, intentional policy.

Recommendations: Opportunities in Systems Thinking and Empowering Decentralized Initiatives

The high level of interconnectivity between water, energy, and food systems and the impact of multiple underlying factors, shocks, and outcomes points to the need for a systems approach. In addition to the many triggering events and natural challenges, poor governance has exacerbated resource scarcity and failed to address complex resource security issues. In practice, systems-thinking can facilitate the understanding and quantification of these interconnections to better support evidence-based decision making and integrative resource governance. The developed recommendations, following analysis of the complex situations described above, include a broad, long-term shift in the governance approach. The first focuses on creating a system-thinking approach to water, energy, and food systems management. This approach utilizes a cross-sectoral platform to encourage dialogue and analyze policy that reflects the entirety of the interconnected resource systems. The second recommendation is to further decentralized management and empower communities to manage their own resources in accordance with local needs. Systems-thinking can incorporate the connections between sectors while considering the economic, political, and social circumstances affecting Lebanon at national and local levels.

A Systems-Thinking Approach to Lebanon's Resource Management

Applying systems-thinking to resource planning and governance in Lebanon would require a shift away from disconnected governance. The confessionalist system, siloed management of water, energy, and food, and unintegrated informal systems underscore the norms of fragmentation in Lebanon. Ministries and offices are often focused on their own priorities, which prevents holistic, nexus-oriented policymaking.

A platform for facilitating dialogue between different stakeholders is needed: one that is oriented toward identifying the links between sectors, evaluating policy, highlighting tradeoffs, and discovering vulnerabilities within the nexus (Mohtar and Daher, 2016). Such a platform would allow for dialogue around complex issues without necessarily making major reforms to existing ministries and departments. Additionally, the platform could facilitate cross-sectoral legislation, address overlooked issues, and integrate additional actors into decision making.

An important piece of this platform would be its ability to encourage system-level analysis. Rather than analyzing issues and solutions as they pertain to only one sector, encompassing multiple factors and sectors can produce more relevant recommendations. For example, addressing food shortages must consider the availability and quality of water, the current geopolitical climate, domestic nutritional needs, and the financial ability to provide subsidies. A solution that addresses each of these features must encompass more than only the agricultural sector. The proposed platform would use systems-thinking to develop analytics that can inform holistic policy formulation.

Additionally, this platform could create avenues for dialogue between the main actors affecting interconnected resource systems: society, business, and government. A framework for facilitating dialogue between Lebanese government, society, and businesses needs to begin with building the legitimacy of the government in the eyes of the other players and facilitating dialogue within the government. There is a lack of clear mechanisms that facilitate cross-institutional communication and cooperation, and consequently, there is little communication between actors and little opportunity for thorough discussion of possible tradeoffs. The heads of MoEW and MoA often have different priorities, and although government actors rarely work together, the system often requires consensus to approve legislation. As a result, the government's management of the links between the water, energy, and food sectors is often antiquated or outdated. Focusing on multi-stakeholder dialogue and cross-sectoral policy formulation offers many opportunities for overcoming these barriers to achieve system-oriented management.

Systems-thinking is also useful for considering effects at different levels to ensure that policy is coherent and effective across different scales. In particular, research should consider trends and resilience strategies at the local and household levels to identify effective strategies and bring more actors into the dialogue. As it stands, household-level recommendations are often tone deaf and ineffective. Last year, politicians urged Lebanese to grow their own food amidst the shortages, a recommendation that was far from a large-scale solution and came with no assistance (Yee, 2020). Although growing food at home has become more common, the effect has been slight. During the 2014 water crisis, the MoEW ran an awareness campaign to encourage residents to conserve water: the $243,000 campaign asked the public to conserve water, but did not provide education on how to do so, nor was it paired with incentives (Nash, 2014). At the same time, the MoEW announced plans to drill new wells and take control of illegal ones, but none of these actions promised long-term solutions to water shortages and the campaign was received poorly by the public (Cousins, 2014). Household-level initiatives can help mitigate resource scarcity and strengthen government legitimacy, but they must be evaluated carefully (Traboulsi and Traboulsi, 2017).

Empowering Decentralized Initiatives

In addition to suggesting broad reforms at the higher levels of government, this paper argues for decentralized solutions that empower local governance and formalize existing local water, energy, and food management systems. Decentralized initiatives are valuable opportunities because they can bypass some of the underlying challenges at the national level while tailoring solutions to local contexts. The existing national system has led to endemic corruption that further complicates effective governance. Lebanon's consensus-based government is a complex, slow, long-standing structure; supporting decentralized initiatives where research and analysis suggest effective outcomes may offer quicker, small-scale ways to take advantage of pockets of resilience.

Local management encompasses both resource allocation and resource stewardship. For example, local management of electricity could include setting up electric grids that cater fairly to all residents, and local management of water resources could include public information campaigns to address water pollution. There are already local systems in Lebanon, such as informal credit agreements between farmers and suppliers and informal electricity providers. Local initiatives have the potential to lower transportation costs, bypass corruption, and strategically maximize comparative advantages. Research supports the potential of local cooperatives to help with marketing, advise on new farming methods, and organize community support for useful infrastructure such as storage and refrigeration facilities (Maalouf and Chalak, 2019; Tawk et al., 2019). The use of digital resources also has much potential to effectively link sellers and buyers (Bahn et al., 2021). A small-scale example of this came about in late 2020, when artisan producers in South Lebanon came together through the "From the Villages" e-commerce platform to sell their goods to buyers in Beirut and other metropolitan areas. Initiatives such as this could have added effects of shifting the public mindset to favor domestic products. Local communities do not exist in a vacuum: areas that rely on imported water, energy, and food would still need to coordinate with other authorities. Nonetheless, learning from existing small-scale successes, and providing national support where success is possible, is a useful way to build resilience.

Bridging Systems-Thinking and Decentralized Initiatives

The case of Lebanon highlights the usefulness of applying a systems approach to complex challenges at different scales. Implementing such approach requires both: top-down long-term strategy toward effective governance of national resources, while empowering decentralized initiatives which can guide the scaling up of successful models at local scales.

Empowering decentralization does not imply fragmentation; rather, direction provided at the national level can guide decentralized management to prioritize actions and maximize national outcomes. According to the steps developed by Terrapon-Pfaff et al. (2018), a methodology to apply WEF Nexus thinking to a local setting must include qualitative analysis of water, energy, and food linkages; quantification of the linkages; and identification of the most critical linkages. Finally, these findings should be leveraged to "generate synergies and avoid trade-offs" (Terrapon-Pfaff et al., 2018). National-level research and policy making can be used to accomplish and publicize the first three of these steps, while the final step of leveraging results and applying findings could be implemented by local communities.

This system is especially applicable to Lebanon's current context, which faces strains at all levels. Broad, systems-based reform reflects a top-down management framework that improves resource system resilience at the national level, while decentralized initiatives improve resilience from the bottom up. In both cases, applying the WEF Nexus lens amplifies potential impacts by taking advantage of insights from critical connections between sectors.

CONCLUSIONS

Considering the case of Lebanon through a Water-Energy-Food Nexus lens is a complex undertaking that reveals many interconnections, not only between water, energy, and food systems, but also between the underlying political and economic challenges and recent shocks. Some connections, such as the one between the financial crisis and increased emigration, are obvious. Other connections can only be thoroughly understood by considering the complex relations between historic trends and contemporary issues. For example, current resource shortages, even in sectors with adequate supply to match national demand such as water, can only be fully understood by drawing connections between Lebanon's historic reliance on external actors and long-standing ineffective governance. WEF Nexus insecurity stems from a variety of underlying challenges and complicated shocks, but also from longstanding poor governance of Lebanon's natural resources.

The provided recommendations highlight the benefit of using the WEF Nexus lens at the national and local levels. Nationally, a WEF Nexus approach would benefit from a platform that facilitates systems-thinking across the water, energy, and food sectors and enables improved communication between relevant stakeholders, including society, businesses, and government. The most impactful contribution of such a platform would be the facilitation of communication between decision making actors within the Lebanese government, which frequently finds itself in political standstills and interconfessional conflicts. Additionally, analysis at the national level could provide more integrative recommendations for resource management through a systems-thinking approach.

Using a WEF Nexus lens at the community level can reveal opportunities for local initiatives that may produce more resilient results to the many national-level challenges. Furthermore, initiatives at the local level will be better able to analyze tradeoffs and select management practices tailored to the needs of their constituents, thus improving the sustainability of resources at a more refined scale.

There is also room for a WEF Nexus perspective at the household and individual levels. Understanding consumption trends at the household level can inform the recommendations and policies directed at individuals, which can lead to behavioral shifts and social awareness. These contexts are vital for implementing a timely, bottom-up approach and highlight the importance of empowering local institutions and actors to manage their own sectors. Together, these recommendations combine top-down and bottom-up approaches to improve resilience in Lebanon's WEF Nexus while accounting for the nation's unique context.

DATA AVAILABILITY STATEMENT

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author.

AUTHOR CONTRIBUTIONS

BD, SH, and KP worked on conceptualizing the paper, wrote sections of the manuscript, and supervision. BD developed the manuscript figures. JR wrote the first draft of the manuscript. All authors contributed to manuscript revision, read, and approved the submitted version.

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The Future of Water for Food

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Globally, water is a bottleneck to food security and, as such, a new approach for water for food is needed. Food insecurity is knocking at every nation's door, including those of the most developed. Moreover, the disruptions in food supply chains that result from continued reliance on a business-as-usual approach of traditional, non-sustainable food and agricultural systems make food insecurity even more vividly present. This article explores the current relationship between food production and water resources. It attempts to better understand how we might reduce the inter-dependencies between food and fresh water by exploring new and alternative sources of water, including improving the efficiencies of green and recycled water.

Keywords: water-energy-food (WEF) resources, synergy driven models, green-water management, green-water accounting, wastewater reuse, water use efficiency and precision irrigation, water productivity

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INTRODUCTION

The interconnectedness of Water, Energy, Food resources is extreme, especially as these exist in the dryland regions of the world, such as the Middle East and North Africa (MENA) region. Water in particular is key for the entire food supply chain, including production and processing (Uhlenbrook et al., 2022). This paper will focus on the production side of the food system. These resources face the threat of future supply gaps, making better understanding their complexities and reducing inter-dependencies critical to ensuring community resilience. This article highlights the challenges posed by the already existing shortfalls in water, food, and energy resources and their interconnected subsystems. These challenges will only increase over the next 20 years. Lautze (2020) discussed actionable steps that the WEF nexus community must take to move the needle forward. He recommended their actions: demonstration of impact and on the ground utility, keeping the nexus message and actions simple, and multidisciplinary engagement of all sectors of the nexus.

Managing the complex and interlinked system of systems that are WEF resources must include addressing the challenges posed by issues of equity, variability in distribution, and unsustainable consumption. Much of the scientific literature fails to highlight these important and alarming issues. The non-stationary and extreme nature of the natural processes governing WEF subsystems is worrisome: we lack the tools to address the challenges they present. The current business approach for how our food is produced and managed needs revision.

Communities currently manage water resources based on the allocation of existing resources; but with climate and land-use changes, the total available water resources at the needed time and location are also changing and becoming more severe. A revised business approach is essential and must be based on the dynamic interactions and synergies of the interlinked primary resources of water, energy, and food. An example of managing water resources is the current conflict in the Nile River Basin: the GERD dam being built by Ethiopia has implications for the water supply of downstream communities. The approach fails because it changes the water allocation to those downstream communities. Success demands that it be transformed into a synergy-driven approach that realistically valorizes the resources rather than solely allocates them. Similar observations on synergy were reported by Sadoff et al. (2020), looking into achieving Sustainable Development Goal 6 on water security.

This article explores four areas of potential new water sources that can produce a transformative approach to the future of water for food. These four areas are: green-water management and accounting, wastewater reuse, water use efficiency and precision irrigation, and approaches to increase water productivity (**Figure 1**).

ALTERNATIVE WATER

Proper management of WEF resources enables resilient, sustainable communities. Such management must not ignore the role of soils, an important focal point for water and food security that receives very little attention in many current projections, especially for water. A simple example: all our soil maps, whether the FAO Digital Soil Map of the World (DSMW), the US SSURGO Database, or others, are based on rigid, non-dynamic soil maps that rely on soil texture. Today we know that soil *texture* does not reflect soil *functionality*. Dynamic soil mapping is critical to understanding the functionality of a soil system. Such mapping would evolve with time in response to external changes such as management, climate, and evolutions of soil structure. This is important because most food production depends on non-irrigated, rain-fed agriculture. Dynamic soil mapping offers an extremely important and better understanding of the soil through dynamic characterization of the soil medium (Braudeau and Mohtar, 2009; Assi et al., 2014; Braudeau et al., 2016).

A new relationship for water for food must be considered: one in which alternative water resources and new management strategies are explored alongside discussions about water efficiency and water productivity. Green water management, wastewater reuse, and smart irrigation technologies (**Figure 1**) are all pieces of the puzzle that must be stitched together to develop a new plan for understanding the interdependencies between water and food.

Consider that 60% of global food production comes from rain-fed (green water) agriculture, while 70% of the global water withdrawals are used for irrigation. This reflects the importance of green water: cereal production relies mainly on green water, and seed production would decrease by only 20% without blue water. Irrigation (only about 5% in Africa) is globally on 20% of the arable land but produces 40% of the global food. Sustainable irrigation is key to increasing the resilience of food systems. Analysis of global consumption of green and blue water highlights that green (rain-fed) water is much more significant than blue (irrigated) water in many dryland regions. The difference between the two is that blue water is surface water found in lakes, rivers, and aquifers (it is the ground water pumped for irrigated agriculture), while soils are the storage reservoir for the green water that falls as rain or is added through irrigation from blue-water reservoirs (Sulser et al., 2009; Cosgrove and Rijsberman, 2010; Siebert and Döll, 2010). For a set of studies conducted in northern Africa, most of the water resources were estimated to be green water which, though ignored for many years, is a larger pool as compared to blue water resources. Virtual (tradable) green water must also be considered: the most tradable virtual water is green water and comprises most of the flow observed on the global map. The economic importance of green water is very significant and must not be ignored by the science community (Liu et al., 2009; Aldaya et al., 2010).

However, green water lacks a unified definition and therein lies the challenge. Simply put, green water is the water that remains in the soil after rainfall; however, this definition begs the question of whether it is storage and *total transpiration* (Gerten et al., 2004), or storage and *evapotranspiration* (Falkenmark and Rockstrom, 2006). Until we have convergence on a single definition of green water, challenges to accountability will be posed. We will return to this matter below in discussing the pedostructure concept.

Most soil maps are static. A dynamic representation of the soil medium includes mapping of the medium over three axes. The *pedology plane* is the evolution and natural morphology of the soil material; the *vertical plane* is what hydrologists attempt to quantify using parameters without physical meaning or physical connection in the pedology plane. Therein lies the disconnect. Most of us are familiar with the concept of representative elementary volume, used in many computational engineering applications. In soil science, this concept fails to determine which "volume" is referred to in soil hydrology and soil processes (Braudeau et al., 2004, 2016; Braudeau and Mohtar, 2009).

The common denominator for soil is mass that it does not change over time. The volume shrinks and swells, making volume not useful as an independent variable and basis for soil dynamics modeling such as the representative elementary volume (REV). Many of us use hydraulic conductivity parameters that are not grounded in soil pedology. Over the last many years, we have worked to bridge the gaps between the system's *functionalities,* striving to ground them in soil mapping. To this end, we introduced the *pedostructure concept* of identifying *soil hydro-structural properties* by their *behaviors.* Using the pedostructure concept, we re-derived all the constitutive equations related to soil and water. An example of such a re-derived continuity equation is water content as a kilogram of water per kilogram of soil (Braudeau and Mohtar, 2014; Braudeau et al., 2014a,b).

Pedostructure uniquely characterizes a given soil based on that soil's unique properties and using 15 parameters, each of which is measured in the lab and uniquely verified in the field. This characterization provides the shrinkage curve, or *specific volume* which is the inverse of bulk density on the y-axis (Braudeau et al., 2004). On the X axis, we see the water content (Braudeau et al., 2014a,b). Beginning at that point at which the medium is fully saturated, one continuously measures the volume change and the change in moisture content to construct what we named the *shrinkage curve.* The shrinkage curve has most of the properties needed to characterize a medium called gravitational water, which is unique from inter-pedal water. After the gravitational water drains, soil shrinkage is significant. This is the point

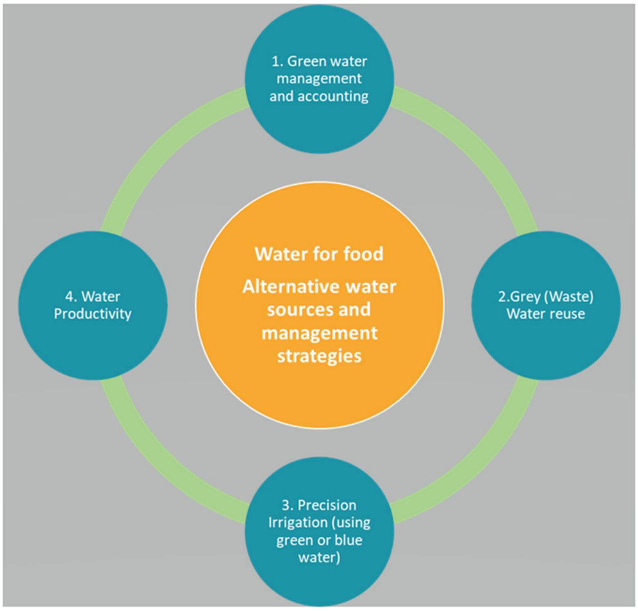

FIGURE 1 | Alternative water management approaches to support food security.

commonly known as the field capacity: the gravitational water or the moisture retained by the water matrix. Field capacity is a very useful term however, it is also a very conceptual term and until now, not physically quantified.

Using the pedostructure concept, we derive the second and third derivatives of the shrinkage curve, which allow us to precisely determine Field Capacity. Following the drying cycle, soil status reaches the permanent wilting point: that point at which all the water accessible for plant extraction is depleted and beyond which point, the plant ceases to grow. We can precisely identify and quantify this point, which has great importance for **precision irrigation** (Assi et al., 2018; Mother and Assi, 2018).

Imagine a future when, using this knowledge, we can track the soil medium from saturation to complete desiccation. At Field Capacity, the gravitational water is lost. Until now, without excess water as part of the drainage, we quantified this water and traced the shrinkage up to the permanent wilting point, that point which, from an agronomic perspective, we do not want to reach. Rather, we stop at a place above the permanent wilting point and at which the plant is not stressed. The future of irrigation lies in the way in which the most advanced knowledge of soil physics allows precision irrigation at the right time and place. Uhlenbrook et al. (2022) argue that this agricultural water use should be embedded in a larger systems approach creating the basis for policy and incentive schemes to optimize the water use for food production.

Enhancing Green Water and Improving Crop Production

"Blue Water" resources are especially limited in arid and semi-arid regions and thus, rainfed agricultural production takes on a vital role in contributing to food security. For centuries, several technologies and soil, water, and crop management practices have been used to improve "Green Water" resources. Rain harvesting technologies and conservation agriculture are known to address water shortage and increase soil fertility and crop yield. Investing in these two critical areas increases the soil water holding capacity and that portion of rainfall available for crop production. The soil's water holding capacity increases as its organic matter content increases. A one percent increase in organic content can improve soil water holding capacity by as much as 1.5% for sandy and 0.6% for silt loams or silt-clay loams (Libohova et al., 2018). Soil degradation is a serious challenge, a key limiting factor that hinders efficacy of rainfall and consequently of crop production. The cascading effects of soil degradation, including loss of soil fertility and organic matter content, lead to declining crop yields and increased human community impoverishment (Barrett and Bevis, 2015).

Since ancient times, rainfall harvesting is a common practice across the globe, especially in arid and semi-arid environments. This practice improves water harvesting and increases the efficacy of rainfall by capturing, diverting, and storing precipitation for crop production and human and animal consumption. Further, it helps minimize soil erosion and protects the environment. Thus, conservation agriculture and rainfall harvesting improve the efficiency of "green water" and enhance its contribution to food security.

Two additional, and very important, elements to consider are **wastewater reuse** and the long-term impact on soil from exposure to different types of water for irrigation. One example is a specific case study conducted in San Angelo, Texas, in which a specific block of land whose groundwater is very salty, was irrigated for 10 years with good quality wastewater. Results showed that, in this case, irrigation with wastewater is far better in terms of crop yield and soil properties than the use of groundwater would have been (Loy et al., 2018). However, this is not the situation in all locations. For example, in Jordan or Lebanon, the outcome could be quite different. While reuse is important, the long-term impact on the ecosystem in which the soil is exposed to reused irrigation water must also be considered. A project conducted in Tunisia focused on a wastewater treatment plan for water, energy, and food (WEF) (Dare et al., 2017). Though very complex due to the social issues regarding the use of wastewater on soil for food and the perception that wastewater is unsafe, the exercise addressed the feasibility at all these dimensions.

To determine the quantity of reused water available for agriculture, one must first calculate the water required for the environment, for ground water recharge, and for industrial and system losses. Agricultural demands must then be mapped: if the treatment plant is too far from the aggregated field, it may be too expensive to pump water to the field. The trade-offs are then calculated: the evaluation of the water-energy-food nexus trade-off as a function of the productive use of water. In the Tunisian case study, we were able to provide 6,200,000 m^3 of water per year that were made available by this plan for irrigation use. However, the trade-off between the abstraction pumping and trucking must also be considered: available water and available energy allow irrigation of 3.6 hectare (IRENA, 2015). The exercise must be globalized to allow real consideration of the potential reuse of wastewater (Mohtar, 2015).

This discussion began around the concept of **water productivity** and the **value of water**. Such value should be inclusive of economic, social, and cultural attributes. Currently, agriculture consumes two-thirds of global freshwater. Such consumption in the future is an unaffordable luxury: to maintain productivity, we must look at alternative water, including blue water as our first choice and alternative water sources. The business approach must be revised. Today, when a farmer is asked about water productivity, the response will be in tons per hectare or tons of produce per hectare of land. This utterly fails to consider the *value* of the water used for that production. It also fails to assign value to energy, air quality, or impact on soil. This must change—we should consider the biomass production and the nutritional value per area. We must look at the existing nexus of complexities in a new, value-based production system that considers nutritional output, water footprint, energy footprint, plant footprint, soil-health implications, air quality, water quality, etc. Though not easy, it must be done. Efficiency is necessary but insufficient where water productivity is concerned. Lebanon, for example, exports potato and other cheap produce without accounting for the loss of virtual water involved in such exports. The new agriculture business approach must properly value water, and in this context, green water cannot be ignored. Green water is a huge resource, one whose use must be maximized given what we know today about soil-water interaction and how much green water and brackish wastewater can be effectively used for agriculture production.

In the context of the Sustainable Development Goals (SDGs), alternative water is critically important. The SDGs address zero hunger and good health. Recycling looks at effective, value-based production, at clean water, sanitation, no poverty, sustainable cities, and communities. Communities are highly relevant for wastewater reuse: the trade-off between pumping and abstraction relates to whether we can build our wastewater treatment facilities close enough to production units to allow full utilization of that reuse.

CONCLUSION

We have green water and blue water: the first requires the development of a functional definition to replace existing definitions. A good definition that is quantifiable and can be generalized is presented by Assi et al. (2018). Convergence is necessary: without that definition, green water cannot be quantified. We must develop a quantitative method to account for green water. Also, we must develop effective methodologies for both field and watershed scales. Non-traditional water, including gray water, must be considered for irrigation in arid and semi-arid regions. Wastewater safety must be considered in terms of the long-term impact and scope of reuse on health and productivity. Finally, we need to understandbetter the interlinkages and trade-offs between society, environment, and water allocation strategies. The current business approach has failed—and will continue to fail. We must look at alternatives approaches that address social, economic, environmental, and cultural attributes.

AUTHOR CONTRIBUTIONS

RM and AF contributed equally in all aspects of the work and manuscript preparation. Both authors contributed to the article and approved the submitted version.

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The WEF Nexus Journey

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This paper describes the beginning of the WEF Nexus Journey in the classroom and shows how the Nexus emerged into the discipline that it is today. The paper offers definitions, shares some success stories from around the world, reflects on future opportunities, and provides a few concluding remarks.

Keywords: WEF Nexus, sustainability triangle, food security, Nexus tradeoffs, WEF analytics, WEF interlinkages, hotspots, stakeholder engagement

THE JOURNEY

In late 1990, interest in agricultural engineering was declining among students entering colleges of engineering and of agriculture. Departments across the nation changed their names to include environmental, biosystems, and other natural resource terminologies. My own department at Purdue was part of both colleges. I requested the department chair to include me in its student recruitment team for our colleges of agriculture and engineering so that, as a member of the team, I could work to recruit freshmen from both colleges into the agricultural engineering department. My recruitment strategy was focused on including non-traditional students who typically did not see agriculture as part of their future career. I introduced the department by focusing on the threatened, interconnected water, energy, and food systems; on how an agricultural engineer might contribute to this grand challenge of water, energy, and food security. My presentation introduced what I called the "sustainability triangle" (**Figure 1**). We witnessed a significant spike in interest around this grand challenge among rural and urban students of diverse ethnic backgrounds.

In 2008, as the inaugural director of Purdue's Global Engineering Program, I had the opportunity to further develop these concepts and incorporated them into the academic programs we offered. In 2009, I was invited to join the Water Security Council of the World Economic Forum and discovered that term WEF (water, energy, food) for worked well for both the Nexus and the World Economic Forum, where I further developed this systems approach to water security. The water security council included members from public and private sectors, international organizations, non-governmental organizations, and some academics. The WEF Nexus concept was adopted by the Council in January 2011 at the annual meeting of the World Economic Forum in Davos and published for the first time (Mohtar, 2011).

Thus, the Nexus took off on the global stage. What began with the water security publication of the World Economic Forum (Davos, January 2011) was followed in November with the Bonn 2011 Conference, focused on the interdependencies of water, energy, food securities and explicitly identifying the role of decision making (Hoff, 2011). In June 2012, the Rio+20 United Nations Conference on Sustainable Development recognized and highlighted the WEF linkages to nutrition, sustainable agriculture, sustainable cities, health, biodiversity, and desertification. At COP18, the United Nations Climate Change Conference of Parties in Doha, the food-water-energy nexus was presented as describing the "human face"

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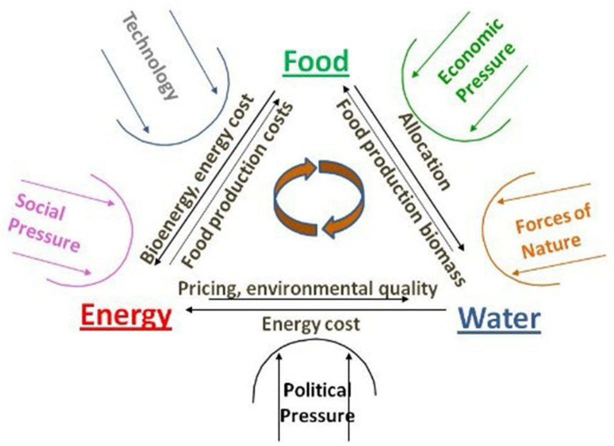

FIGURE 1 | The sustainability triangle (Mohtar, 2002).

of and solution to climate change. The conferences of the World Meteorological Organization (WMO) and the German Development Agency (GIZ) both focused on these issues. In 2014, the InterAction Council and the East-West Institute (EWI) presented the WEF nexus as a global security threat in their WEF risk report of 2012; EWI did the same in 2014. Also, in 2014, the G-20 Clean Energy Ministries launched its WEF workstream (World Economic Forum, 2012; EastWest Institute, 2014). In 2015 G-20 Clean Energy Ministries launched its WEF workstream (IISD 2015) and the 7th World Water Forum in South Korea and the SDGs Post 2015 Agenda were highlighted in Paris at the SDGs post 2015 Climate summit. The Nexus mushroomed again in Bonn, in North Carolina, and in a joint workshop in Washington DC through a Global Water System Project and grant from the Belmont Forum (Lawford and Mohtar, 2015). The World Bank launched its Thirsty Energy Initiative (Rodriguez et al., 2013) and the Department of Energy, in its 2017 Report to Congress, acknowledged that the dependence of energy on water is a risk to both water and energy security (US Department of Energy, 2017). Later that same year, the National Science Foundation (NSF) launched its INFEWS program: Innovations in Food Energy Water Systems.

Thus, was the progression and development of the Nexus. From its very early stages, the principles were those of a holistic, multiscale, multistakeholder nexus. First that the integrative view of water, energy, and food resources management must prevail at all levels and be based on inclusiveness for all sectors: governance, academic, civil society, and private. The second principle is to define and quantify the interconnectivity among the W-E-F resources, creating a basis for use in policy and planning. Third: to better engage the private sector for its role in supply chain management, mobilization of resources, conservation, and responsible investment, including research and development for enhanced business opportunities and technology development.

The early discussions focused on the Nexus approach as holistic and multiscale, involving multiple stakeholders, and the stated principles. Unlike other academic disciplines, the Nexus emerged from the need for better management of the primary resources of water, energy, and food. Policy makers and industry leaders endorsed the concept in high level discussions. We did not need to convince them of the importance of the new concept: *they got it*! However, after buying in, they needed guidance on implementation, demonstration, and they needed success stories.

WHAT IS THE NEXUS? HOW CAN WE DEFINE IT CLEARLY?

The Nexus offers a platform for a system of systems connecting the water-energy-food subsystems. It builds on, but does not replace, existing disciplines (Mohtar and Daher, 2012). The Nexus elements include the interlinkages, hotspots, and tradeoffs. Nexus builds on the water productivity concept familiar in agriculture, and on integrated water resources management, energy efficiency, and others. It connects government policy, society, and business supply chains (**Figure 2**; Mohtar and Daher, 2016).

The Nexus does not stop there, but continues beyond analytics to create a platform or framework that connects the science to the politics and to the political economy of the Nexus. It is the dialogue that moves the needle from conflict into cooperation. The two concentric circles in which the Nexus operates are the supply chain and the political economy, which comprise the defining factors of the resource availability and the portfolio of our resource nexus.

Building the WEF Nexus system using the food supply chain includes: (1) defining the components of the food supply chain, (2) establishing the water, energy, food resource portfolios, (3) quantifying the resource footprint (very important for modeling and existing data), (4) identifying the interventions that need to be studied (important crops, increasing self-sufficiency of other crops), (5) building the tool and doing the tradeoff analysis for various scenarios, (6) the sustainability index, and (7) the dialogue. Two types of dialogue are needed: one with the scientific community alone, and a second with the entire society: scientific, decision makers, and others involved in the resource nexus (Mohtar and Daher, 2016).

This brings us to the seven questions for setting up a nexus platform or solution (Daher et al., 2017). We must define the system, starting with the critical question to be answered and the scale at which this question is relevant. Not an easy task: the system must be defined so that anything beyond the boundary is excluded and everything within that boundary is included. Who are the stakeholders? What type of data is needed? What assessment tool can best asses the proposed interventions? How do we communicate with the stakeholders, involve them in the process, and assess their interaction with and acceptance of the process?

IMPLEMENTATION

The WEF Nexus Research Group at Texas A&M University has been active in many regional and international partnerships to assess different aspects of the Nexus. The research group

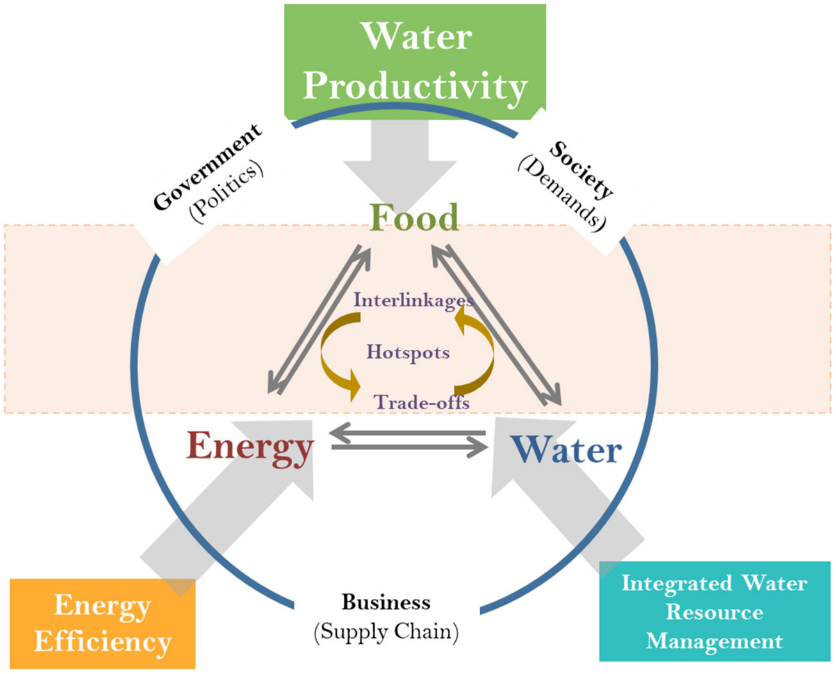

FIGURE 2 | Connectivity of the nexus elements (Mohtar and Daher, 2012).

looked at thematic and geographic applications, beginning with the launch of Qatar's National Food Security Program in 2011. When *Qatar* was struggling to find a solution to its food security challenges, our application allowed an analytical platform that considered the implications of achieving food security in Qatar (Mohtar and Daher, 2014).

In *Abu Dhabi*, the group worked with the International Renewable Energy Agency (IRENA) to help produce a comprehensive study on the steps needed for promoting renewable energy as part of the energy portfolio mix and how it interfaces with other energy sources, conditions, and limitations to this energy (International Renewable Energy Agency, 2015).

There are additional examples of energy deployment, including the sustainable energy portfolio of *Texas,* where the group worked on the projected water gap, critical when hydraulic fracturing was at its peak and the water needed for this process was taken from other sectors, mainly domestic and agriculture (Daher et al., 2019). This work focused on the tradeoffs between energy, water, and transportation. The transportation lifeline for water used in the hydraulic fracturing process are the roads, which also provide the transportation lifeline for communities and impact traffic and the safety of transport (Mohtar et al., 2019). As addressed more specifically below, the research group also considered the WEF Nexus in the San Antonio region (Mohtar, 2019), and a specific issue in Matagorda County, which neighbors Houston and has a large nuclear power plant whose need for cooling water competes with water needs of other sectors (Kulat et al., 2019).

A comprehensive study conducted in the *Gediz Basin* of Turkey looked at the tradeoffs between planting food for export, which competes for local resources in the region (Degirmencioglu et al., 2019). In Lebanon, we took a health centered approach that places health at the center of the Nexus (Bachour et al., 2020).

Morocco's phosphate industry posed a special challenge in water-scarce Morocco: phosphate production has a high-water footprint. We looked at the tradeoffs between the water used by the industry vs. the water used by other sectors, such as agriculture (Lee et al., 2020). In Morocco, we also looked at the tradeoffs between Nexus and the different sustainable development goals (SDGs) for water, energy, and food as part of the national plans for resource management (Daher and Mohtar, 2021).

In two unpublished studies, one in the Mekong Basin and the second in Nigeria, we looked at the Nexus tradeoffs between the hydropower industry (hydraulic energy), agricultural irrigation, community livelihood, and food security. Each of these case studies shares a common element of quantification of the interlinkages and the tradeoffs that exist in the analysis and validates the conclusion that the Nexus systems approach can offer economic benefits to multiple sectors.

A WEB BASED WEF NEXUS TOOL

The tool developed for implementing these concepts was first released in Qatar (Mohtar and Daher, 2012) and provided a user interface that allows entering the portfolios and questions about scenario components (food self-sufficiency, water sources and quantities, energy sources) and impact (import countries and the relative risks of importing commodities from that country). An administrative interface and a science component provide a "behind the scenes" look at local data characteristics. The Tool's output is the entire footprint of water, energy, land, carbon emission, financial constraints, and other elements. Combined, the policy and the science allowed us to produce a sustainability index, which, in turn, allowed comparison and ranking of various scenarios. Further development of the tool was later completed and published (Daher and Mohtar, 2015).

Implementation of the SDGs

The Tool allows us to look at the tradeoffs of implementing a series of interventions. The interconnected SDGs 2, 6, and 7 (zero hunger, clean water and sanitation, affordable and clean energy) represent our first attempt to create a consortium promoting the use of Nexus within the SDG community. Texas A&M led the effort in collaboration with World Wildlife Fund (WWF), International Union for Conservation of Nature (IUCN), Swedish Environmental Institute (SEI), The World Bank, International Food Policy Research Institute (IFPRI), Global Water Partnership (GWP), Deloitte, Asian Development Bank (ADB), International Water Management Institute (IWMI), and the OCP Policy Center. The take-away lessons showed that improving access to electricity can negatively impact ambient water quality, water availability, and ecosystem health. Ensuring universal access to affordable, reliable, modern energy services means substantially increasing the share of renewable energy in the global energy mix, doubling the global rate of improvement in energy efficiency, enhancing international cooperation to facilitate access to clean energy research and technology (including renewable energy, energy efficiency, and advanced, cleaner fossil-fuel technology, and promoting investment in energy infrastructure and clean energy technology). This would be done by expanding infrastructure and upgrading the technology to supply modern, sustainable energy services for all those living in developing countries, particularly the least developed countries, in accordance with their respective programs of support.

First in Morocco, we looked at the analytics of how water, energy, and food are interconnected in the national plan and then identified the associated tradeoffs. Morocco's green water plan sets targets for introducing income such as increasing production of olive, citrus, fruits, and vegetables. The effort to generate income resulted in reducing cereals production by 20% and moves from a self-sufficiency model into an economic model for agriculture. Morocco's 2030 water strategy includes desalination and treated wastewater (TWW); its energy strategy includes increasing renewable energy by up to 42%. After quantifying the interlinkages, we realized that these three plans compete for the same resources, mainly those needed for capital resources. Thus, if one looks at food, the tradeoff involves increasing the water-land-energy factor at the expense of food security. Regarding energy: reduced emissions come at the expense of finance, land, and water. Increasing the quantity of renewable energy means changing the allocation of land and water from agricultural production into energy production. Additionally, while water security is improved with added water and TWW, so are both energy demand and the financial burden. In conclusion, the tradeoffs that we identified and quantified must be considered before making the appropriate decisions presented in these national plans. The Nexus framework and Tool allow identification of these issues and is essential for such analysis to be accomplished.

The second version of the Tool, released to assess food security in Qatar (Mohtar and Daher, 2012, 2014; Daher and Mohtar, 2015), allows users to create scenarios for a given location by defining the inputs of the water, the food, and the energy portfolios. Users create scenarios and the Tool generates the sustainability index for each and quantifies the tradeoffs. This index is a measure of how sustainable the scenario is based on water, energy, land, environmental footprint and considering user preferences. For example, Qatar does not have sufficient land to independently ensure complete food security, so solutions requiring extensive land resources will not rank high on the sustainability index. The WET Tool (water-energy-transportation) used scenarios related to oil price, natural gas, and lateral drill length. We quantified tradeoff analysis for the scenarios and determined which is most site-specific and appropriate scenarios (Daher et al., 2019).

The San Antonio case studies focused on Region L of the Texas Water Plan (Mohtar, 2019) and used a system of systems approach. Thematic teams (Energy for Water, Water for Food, and Water for Energy) worked with stakeholders to collect data for modeling, governance, financing, and tradeoff analysis. A circular approach that circled some data back to stakeholders improved decision making. The goal was to better understand the Texas water gap projected over the next 20 years. By focusing on three subregions, each representing a distinct hotspot, we used a holistic systems approach to identify ways to bridge the projected 40% water gap for Texas.

We discovered that solutions are different for each zone or hotspot. In the Lubbock area, which has a declining water table due to over pumping by farmland, we encouraged dryland farming: different sources of water and fresh investment in the sector were needed for agriculture. In San Antonio, a growing area with high demand for municipal water, solutions included implementation of low impact development solutions, which requires investment and could carry potential for both ground water recharge and urban agriculture. The Eagle Ford shale region produces a lot of energy and developing shale production increases ground water consumption. One unique aspect of shale gas production is its very intense consumption of water, in both space and time. The wells are very localized and require a lot of water at certain peaks, which presents a particular challenge that must be addressed in terms of total quantity of water needed and in terms of the spatial location and time so as not to coincide with other peak demand times for water, whether for agriculture or municipal.

IMPACT OF WEF NEXUS SOLUTIONS

Three tools can highlight the impact of WEF Nexus solutions. The Water-Energy-Transportation (WET) Tool, designed to quantify the relations and tradeoffs between the water, energy, and transportation sectors for different scenarios, using factors like increased oil and gas production, market prices, lateral lengths of wells, and input amounts of water. The tool allows us to look at the scenarios and promote the best options as we move forward (Daher et al., 2019; Mohtar et al., 2019).

The Matagorda County Tool shows that annual income could increase by as much as $32 million dollars above the current “business as usual” scenario, mainly in the agriculture sector that is currently suffering from a lack of water (Kulat et al., 2019). The Energy Portfolio Assessment Tool (EPAT) allows options for the energy portfolio and shows that some energy policies can mitigate carbon emissions, even after capacity increase, by decreasing water withdrawal volume by almost 10% and, that CPP technology policy increases water consumption by 5%, land use by 143%, and cost by 18% (Mroue et al., 2019).

Tradeoffs of Wastewater Reuse in Agriculture

The benefits of wastewater reuse in agriculture are clearly translated into economic growth, coastal and riparian protection, reduction of climate variability and risk, and food security (Dare et al., 2013, 2017). Trade-offs carry some negative aspects: farmer and consumer perceptions, carbon emissions, treatment and conveyance costs, public, and environmental health risks. The tradeoffs need to be facilitated through supportive public policy, good governance, and viable economic models. The potential of water reuse for agriculture must consider all the principles identified in a water-energy-food nexus approach and then simulate these to begin assessing the different scenarios and their tradeoffs.

AUB Success Stories

In Lebanon, The American University of Beirut (AUB) launched The Water-Energy-Food-Health Nexus Renewable Resources Initiative (WEFRAH) in 2018. The WEFRAH community is one of the largest in the region working on the interconnectedness of resources. WEFRAH encompasses over 100 members and 60 researchers spread over 9 research clusters. Community members represent policy, business, agriculture, health care, technology, physical sciences, engineering, social sciences, natural sciences, arts and design, nutrition, public health, nature, ecosystems, and more. The goals of the WEFRAH community include understanding system complexities, reducing interdependencies of primary resources, increasing community resilience, and promoting ecosystem and human health and wellbeing. Adding the health component into the Nexus places additional complexity in the system. Nine projects are being developed, which impacts include: a digital framework for detection of plant pests, an optimized air distribution system for poultry houses, anaerobic digestion to head poultry houses, data on uptake of antibiotics by plants, technology based on the movement of antibiotics in water, a prototype to identify and promote healthy sustainable diets, prototypical solutions in humanitarian engineering, and circular aquaponics systems. We are looking into various venues to publish the work.

FUTURE OPPORTUNITIES

Future opportunities begin with a sustainable business model for agricultural systems: the current food and agriculture system is not sustainable. While food production has provided real success stories in terms of producing enough food globally for the world’s population, some questions have been ignored such as nutritional value relative to water and energy use, as well as air quality and impact on soil health. In the future, we will not have the same quantity of water allocated to agriculture, thus, we need a different model. One that allows the use of multiple and different sources of water; one that considers the human and ecosystem values of this water. Here is where the Nexus can contribute.

A second future opportunity lies in the circular food and agriculture system. Inputs to such a system include renewable water, renewable energy, and nutrients. A circular system would have reduced carbon emissions, reduced chemical and biological pollutants, and reduced food wastes and loss. If we look at the tradeoffs in the outcomes of such a model, keeping in mind the human and ecosystem resource nexus, the choices for a circular food and agriculture system changes and are site specific. Making such a transition requires appropriate technologies and policies but more importantly behavioral changes.

Another future opportunity is the water-food-health nexus, where “one health” is promoted through the interconnections of water and human health. Drinking water, sewage, seas, and rivers are considered with their interconnections among water, animals, and food. This includes irrigation water, farm aquaculture, food poisoning, and especially antibiotics and antibiotic resistance. All these lead to a “one-health” system that allows real focus on the human ecosystem and animals in the food supply chain, i.e., the food system as a single unit.

CONCLUSION

We must take a step back and look beyond the tradeoffs and zero-sum resources allocation model. Today we are at a place where the projected requirements for primary resources have gaps in providing the water, energy, and food needed. We have low resilience to climate change, as is manifested through wildfires, record temperatures, and reduced agricultural productivity in many parts of the world. We have inequity and variability in distribution. We have tradeoffs among possible interventions. Looking at the tools that allow work with technologies, social, political, and economic levers and into the platform created to bring in the private sector, the public sector, and civil society, it is possible to make a leap into the future. A leap that increases the resource base by creating synergies, reducing interdependencies, improving equity and distribution, to achieve the sustainable development goals (SDGs) and improve overall resilience.

AUTHOR CONTRIBUTIONS

RM is the sole author of this manuscript and wholly accountable for its contents.

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Operationalizing the Nexus Approach: Insights From the SIM4NEXUS Project

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Over the past decades, the understanding and assessment of cross-systems interactions have gained momentum in research and policy-support. As such, scientific literature on Nexus assessment methods and applications continues to grow, followed by numerous state-of-the-art reviews. Among the flexibility and variety of Nexus approaches, comprehensive, transferable and accessible methodologies with operational potential are missing. To address this gap, we introduce the SIM4NEXUS approach, which emerged from twelve test cases. Fledged from practice, the approach is a unique output in the Nexus research field. It is informed by the development of twelve case studies, which differ in spatial scope, socioeconomic and biophysical contexts, and Nexus challenges. The studies were conducted under similar conditions (e.g., timeframe and multidisciplinary teams of experts and dialogues with practitioners from policy and business). We find that transdisciplinarity and the integration of qualitative and quantitative methods are vital elements in Nexus assessments for policy support. Additionally, we also propose steps to advance Nexus assessments: 1) integration of the policy cycle in research (including monitoring and evaluation, and offer support during the implementation process), 2) multidisciplinary collaboration with different levels of engagement and financial support, 3) inclusion of ecosystems and other relevant dimensions (e.g., health) in the Nexus. Ultimately, the SIM4NEXUS approach provides practice-based guidance on conducting a Nexus assessment, and we recommend it for future Nexus assessments by the research community, institutions, and private actors.

Keywords: nexus, nexus approach, nexus assessment framework, resource management, sustainability, resource efficiency

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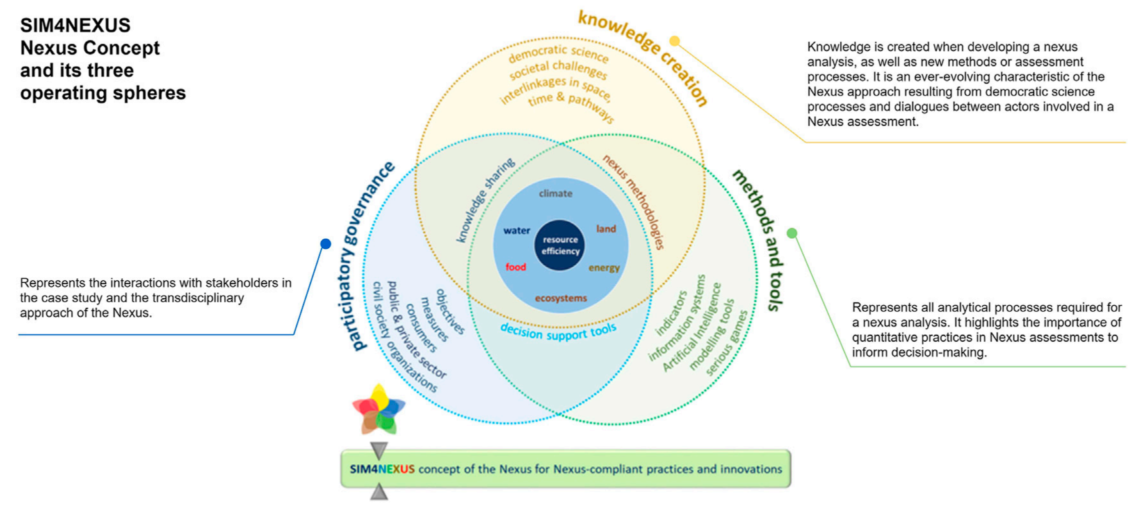
1 INTRODUCTION

Natural resources, including materials or substances occurring naturally in the environment, are not always used sustainably. The intensification of human activities and increasing demands, driven by population growth and economic development, add pressure to these reserves, raising questions regarding the environmental impacts and the feasibility of maintaining current resource management practices. This motivates the need to understand better how resources can be more efficiently managed without compromising the environment and the life of future generations. Since resources are used across systems, an integrated multi-systems perspective is needed in planning processes.


SIM4NEXUS Nexus Concept and its three operating spheres

Knowledge is created when developing a nexus analysis, as well as new methods or assessment processes. It is an ever-evolving characteristic of the Nexus approach resulting from democratic science processes and dialogues between actors involved in a Nexus assessment.

Represents the interactions with stakeholders in the case study and the transdisciplinary approach of the Nexus.

Represents all analytical processes required for a nexus analysis. It highlights the importance of quantitative practices in Nexus assessments to inform decision-making.

FIGURE 1 | Illustration of the Nexus concept from SIM4NEXUS Nexus (adapted from Ramos et al. (2020)).

The term "Nexus" relates to the identification of interactions between different entities (Liu et al., 2018) and the understanding of cross-sectoral dynamics (i.e., multi-systems thinking), whereas the "Nexus Approach" represents the effort of assessing it. In its application to the analysis of resource systems, it gained momentum with the Bonn Nexus Conference (Hoff, 2011), although the importance of assessing cross-sectoral challenges was highlighted in the Global Risks Report 2011 (World Economic Forum, 2011), and the importance of the quantitative analysis by Bazilian et al. (2011) and IAEA (2009). The Nexus approach seeks knowledge and understanding of systems interactions, what factors influence them, how to recognize and assess trade-offs and synergies, and, in this way, reconcile the interests of the different sectors which are part of the domains (i.e. systems) that constitute the Nexus context. A Nexus analysis is a multi-objective approach, which means that it does not seek for optimization in one of the interlinked systems solely, rather than a balanced combination of good solutions in all involved systems upon a Pareto-like front (Wicaksono et al., 2019).

In this paper, we summarize and derive insights from work conducted in SIM4NEXUS, a project funded by the European Commission under the Horizon 2020 programme that investigated the Water-Energy-Food-Land and Climate (WEFLC) Nexus and which was operationalized in twelve Case Studies. The research and innovation project searched for new scientific evidence on sustainable and integrated management of resources in Europe and elsewhere and adopted the Nexus concept in testing pathways for a resource-efficient and low-carbon Europe (Brouwer et al., 2020a).

The Nexus approach is embedded in the investigation of interlinkages between the Nexus systems of water, energy, food, land and climate, and aimed to create synergies and reduce trade-offs, as motivated by the sustainable and integrated management of natural resources. The latter is not possible with the current lack of policy integration and coherence; thus governance is a pivotal component in the Nexus approach (Howells et al., 2013; de Strasser et al., 2016; White et al., 2017; UNECE, 2018). A new vision for the Nexus concept emerged from this work (**Figure 1**). The WEFLC dimensions are at the center of the concept, representing the Nexus approach where all spheres overlap, with its focus on resource efficiency. The overall intersection results in innovations (social, policy, technical, business), and Nexus compliant practices. Ecosystems are added, as this dimension is considered crucial from the case study work. Hence, we recommend Nexus practitioners to also consider "Ecosystems" be part of the Nexus concept. Climate change is implicit in the climate dimension. Other than the operating spheres of Knowledge Creation, Methods and Tools and Participatory Governance (**Figure 1**), we highlight the importance of their intersections. These indicate the spheres are mutually dependent and do not operate in isolation.

The cross-overs between Knowledge Creation and Participatory Governance refer to knowledge sharing through stakeholder participation activities, as well as bilateral consultations. They are aimed to empower stakeholders empowerment, and to streamline Nexus knowledge to actual socio-economic contexts. The crossovers between Knowledge Creation and Methods and Tools enable the evolution of methods and tools to advance the Nexus concept. The Methods and Tools and Participatory Governance crossover reveals stakeholder requirements on tools, and shares Nexus insights and findings to the stakeholders through simulation, quantification and finally the popularization of the Nexus assessment. This intersection can also support the design of funding mechanisms and business models.

Nexus assessment frameworks, or Nexus approaches, consist of a set of overarching steps (including methods and tools to be adopted) that guide a Nexus assessment. Several Nexus approaches are described in the literature. They primarily focus on the process of conducting an assessment, are rather flexible in their design and are not constrained by a modelling framework or tool. Aimed at the assessment of water-energy-food (WEF) interactions, the WEF approach (Flammini et al., 2014), proposed by the Food and Agriculture Organization (FAO), is structured in three distinct components: 1) context analysis, from which results a qualitative analysis which feeds on the next phase; 2) quantitative assessment, based on matrix analysis of Nexus sustainability and resource use efficiency indicators to compare implications of interventions, and 3) response options, which translate into strategic visions and governance aspects (policy, regulations, institutions). Stakeholders are foreseen to be involved in all phases. The components can be performed independently, although “response options” would benefit from a “quantitative assessment”. A key feature of the approach is the definition of Nexus indicators which can inform about the performance of Nexus interventions, under a specific context. The Climate, Land, Energy, and Water systems (CLEWs) approach (Howells et al., 2013; Ramos E. P. et al., 2021) consists of five main phases: 1) CLEW systems’ profiling, 2) pre-Nexus assessment, 3) analytical approach, 4) analysis of results, and 5) findings and recommendations. Quantitative analyses are performed in phase 3 and can be qualitative and/or quantitative. The single-model quantitative approach, using open source software, is the most commonly deployed method and applied to national-level studies. The CLEWs methodology often involves stakeholder participation, including capacity development and Nexus dialogues, although it is not considered a requirement. The Transboundary Basin Nexus Assessment (TBNA) methodology (UNECE, 2015; de Strasser et al., 2016; UNECE, 2018), considers the Nexus of water, food, energy and ecosystems in transboundary watercourses. It is split into two interacting tracks: the technical (often quantitative), and the governance analysis. The CLEWs approach is adopted for the technical component and most basins’ analyses are based on sectoral model soft-linking (UNECE, 2018). The methodological tracks converge into six main steps: 1) socioeconomic context; 2) key sectors and key actors; 3) analysis of key sectors; 4) intersectoral issues; 5) Nexus dialogue; and 6) solutions and benefits. Stakeholder participation is necessary, and essential, for the elaboration of the transboundary Nexus assessments, since the ultimate aim of the assessments is to foster collaboration and promote dialogue between countries sharing the watercourses for the integrated management of resources at the basin/aquifer system level. Another approach is the integrated Water-Energy-Food (WEF) Nexus framework, introduced by Mohtar and Daher (2016), which focuses on using Nexus analytical approaches to facilitate multi-stakeholder dialogue. It is structured on three components: 1) WEF Nexus analytical platform; 2) Supply chain dialogue, involving different types of supply chain actors; and 3) political economy dialogue. Several Nexus tools are available that can be used for stakeholder participation in the assessments. One example is the WEF Nexus 2.0 tool (Daher and Mohtar, 2015), a comprehensive yet accessible scenario-based tool with the capacity to support decision-making processes. A transdisciplinary approach is recommended for defining quantitative boundaries of the systems, importance indices, and communication purposes. On a different approach, (Giampietro et al., 2009; Giampietro, 2013), propose a multi-scale integrated analysis of societal and ecosystem metabolism (MuSIASEM) framework that explores the interrelations between societal and natural systems and how they influence one another when interpreted as a metabolism. The analytical approach is structured around three main components: a fund-flow analysis of production-consumption socio-economic processes, a multi-level production-consumption analysis (“Sudoku effect”), and impredicative loop analysis. The approach addresses the challenge of old-fashioned quantitative approaches, which require updating, by keeping the versatility for the analysis to adapt to the changing systems, and by including quantitative elements adaptable to different dimensions and scales and semantic categories. Authors’ refer to the framework as a “multi-purpose grammar” due to its boundless applicability characteristic (Giampietro et al., 2009), supported by the numerous applications found in the scientific literature.

The Nexus approaches described share similar elements. They all consider the scrutiny of systems, the identification of interactions, and the need to identify critical interlinkages. Quantification is another common characteristic necessary for comparing alternative futures of resources’ management, policy options or changes in natural systems. Stakeholders’ involvement is also deemed key, and approaches contemplate different engagement options (e.g., interviews, consultation workshops, surveys, capacity development). The approaches also differ. One noticeable difference is the Nexus dimensions considered. Some focus on services, such as energy, water, and food, while others look into systems more from the resource’s angle, which is the case in CLEWs. Another difference is the analytical approach. The FAO-WEF approach proposes an assessment based on indicators that align with the specifics of the Nexus context under study. One method suggested in the WEF Nexus framework is informed by sustainability indicators, while the CLEWs framework considers flexible quantification methods. The governance analysis and its interconnection with the technical Nexus analysis are distinctive characteristics of the TBNA methodology. The WEF Nexus framework also discusses stakeholder dynamics in more detail than other approaches. MuSIASEM follows a very different approach to the others. It applies to any combination of systems (it is not linked to a specific set of Nexus dimensions) and can be applied at any scale using the same methods.

1.1 Gaps in Nexus Assessments Frameworks

Several Nexus assessments reviews have been conducted that compare approaches under different criteria. The reviews examine not only the methods used in an assessment but also the process in itself. We select some of these reviews and try to overcome some gaps in the existing frameworks that can improve Nexus assessments. We focus on three categories referring to the general approach and to intrinsic and extrinsic elements.

Regarding general gaps, Albrecht et al. (2018) find that quantitative approaches are often preferred in Nexus assessments. Few combine qualitative methods, while Endo et al. (2017) state that the Nexus approach is yet to be formally recognized and its complexity requires clarification. The thin interface between policy and science, and the challenging incorporation in decision-making processes, is also frequently mentioned (McGrane et al., 2018; Wiegleb and Bruns, 2018; Dargin et al., 2019). The coverage of Nexus systems also varies, and many studies tend to focus on a reduced number of systems (Endo et al., 2017). Nexus assessments also commonly prefer techno-economic and biophysical analyses, and the consideration of social science methods and aspects is limited (Kling et al., 2017; Albrecht et al., 2018).

Other gaps in Nexus approaches refer to intrinsic elements in the approach. One such gap is the lack of standard procedures, methodologies, and models (Fernandes Torres et al., 2019; Liu et al., 2017) with the capacity to adequately identify and assess the influence of Nexus interlinkages. Understanding the systems' Nexus is vital and necessary for the approach's success, and such understanding should be shared by the actors involved (McCarl et al., 2017a; Ramos E. et al., 2021). On modelling tools, Kling et al. (2017) highlight the need for model validation, while (Liu et al., 2017; McCarl et al., 2017a) suggest the need for a unifying integrated model or procedures for multi-model integration, particularly due to the challenge of reconciling differences (temporal and spatial resolution) across sectoral models. The identification of interlinkages, access to information, and terminology are another core gap in Nexus approaches. Although some approaches inform on interlinkages more broadly (Flammini et al., 2014; Ramos E. P. et al., 2021), others are specific to applications. Liu et al. (2017) note that Nexus interactions would benefit from clarification, and (Endo et al., 2017; McCarl et al., 2017b) pinpoint that clarification on the complexity of the Nexus is needed. On terminology, another challenge relates to common semantics between actors involved in the assessment to realize effective collaboration (Kumazawa et al., 2017). On the issue of data and information gaps, Lawford (2019) suggests the development of an integrated data and information service in support of Nexus assessments. The need to realize interoperability between models and model integration is pointed out by (Liu et al., 2017). Improved interdisciplinarity and transdisciplinarity practices in Nexus assessments is necessary to address sustainability challenges (Mauser et al., 2013; Ghodsvali et al., 2019). In the perspective of Kling et al. (2017), gaps in Nexus knowledge can be overcome through multidisciplinarity[1], and (Endo et al., 2017) justify the development of disciplinary integration for reducing Nexus-wide trade-offs and synergies. Additionally, coordination between different actors can be critical in data production (Liu et al., 2017). Ontology engineering is proposed by Kumazawa et al. (2017) as an approach with the potential to support interdisciplinarity efforts. However, although considered an obvious requirement, the practicality of transdisciplinary approaches is yet to be understood. Limitations to multi-stakeholder participation may prove difficult, particularly in different geographical contexts (e.g. language) (Ghodsvali et al., 2019).

Governance, financing and funding, and approach's timeframe and vision were identified as extrinsic gaps to advance Nexus approaches. These may be more challenging to address than the intrinsic ones since they depend on external factors and conditions beyond reach to practitioners. A significant obstacle to the operationalization of the Nexus approach is its application in decision-making contexts and governance (Al-Saidi and Elagib, 2017; Dargin et al., 2019). Bridging the gap between science, and policy- and decision-making, requires approaches to incorporate options that can mitigate and respond to this issue. The inclusion of transdisciplinarity practices, e.g. multi-stakeholder involvement, is paramount. Such inclusion should clarify how natural and social systems interact and how systems are managed and governed, including understanding the nature of stakeholders' "thresholds" to decisions (Ghodsvali et al., 2019). Only then synergies can be effected via integrated governance (Liu et al., 2017). Increased collaboration between stakeholders and researchers is also pointed out by (Dargin et al., 2019), in addition to strengthening the first phases of the assessment process in terms of diagnostic, guidelines and knowledge transfer opportunities to facilitate the shared understanding of the Nexus approach. Another aspect that needs consideration is the shared risks in innovative governance mechanisms and reconciling sectoral, political, and power interests (Gallagher et al., 2016). Linked to integrated governance are the approach's timeframe and long-term implementation vision of the implementation. Its long-sighted implementation requirement (Cremades et al., 2019) not only battles with existing sectoral policy integration challenges (Venghaus et al., 2019) but navigates through asynchronous policies and strategies commonly coupled with cyclic policy mandates. On the discussion of the concept of transdisciplinarity, (Ghodsvali et al., 2019), explain that effective transdisciplinarity requires the change to remain. Decisions may have conflicting implications and effects on society and places, depending on the decision context (Romero-Lankao et al., 2017; Engström et al., 2021). Thus, for the Nexus approach to promote a governance transition, it should explicitly contemplate this aspect in its structure. Commonly, assessments close with "conclusions and recommendations", which is the step from when stakeholders may need assistance and follow up on the solutions identified. If the follow-up study of interventions, or test cases, is not possible to implement, the Nexus study could be side-lined. The previous gap can be related to the project orientation and limited funding to advance the Nexus approach. Not only do assessments require financial support for researchers and practitioners, but they may also require financing of the recommendations (Hoolohan, et al., 2018; Cremades et al., 2019). In one way, an economic and cost-benefit analysis could provide an estimate of economic implications, but may not be enough. Nexus financing, and the roles of public and private sectors, is discussed by (Markantonis et al., 2019).

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[1] Tress et al. (2005) define multidisciplinarity as the interaction between different disciplines for a common goal but with different discipline objectives.

TABLE 1 | The SIM4NEXUS case studies and indicative diversity factors (GL: Global, CO: continental, TR: transboundary, NA: national, RE: regional) (Peel et al., 2007; Brouwer and Fournier, 2017; Fick and Hijmans, 2017; Eurostat and European Commission, 2019).

CS	Scale	Geography	Climate (köppen-geiger Classification)	Main Economic Activity	Critical nexus Challenge
1. Sweden	NA	Northern Europe, North Sea, Baltic Sea	South: humid continental North: cold, without dry season and with cold summer	forest products, hydropower, forest fuels	climate change impact on water resources, forest ecosystems and interlinkages
2. Latvia	NA	Northern Europe, Baltic Sea	cold, without dry season and with cold summer	agriculture, wood products, food processing, chemicals	low-carbon development and resource-efficiency policies
3. Netherlands	NA	Western Europe, North Sea	temperate without dry season and warm summer	agriculture, food industry, industry, services, tourism	the role of biomass in the transition to a low carbon economy and impact on water, food, land, climate
4. Eastern Germany-Czech Republic-Slovakia	TR	Central Europe	West: temperate without dry season and warm summer East: humid continental without dry season and with warm summer	agriculture, industry	precipitation retention as a driving force of climate-resilient landscapes, land use antagonism between bioenergy and food production
5. Counties of Devon & Cornwall, United Kingdom	RE	Southwest of the United Kingdom, Northern Europe, Atlantic Ocean, North Sea	temperate without dry season and warm summer	tourism, agriculture	cost, environment and security in water supply
6. France- Germany	TR	Upper Rhine region, Western, Central Europe	temperate without dry season and warm summer	industry, agriculture	the consequences for aquatic ecosystems and rivers, bioenergy, energy crops, land uses, water quality and quantity
7. Andalusia in Spain	RE	south of the Iberian peninsula, Southwestern Europe	Mediterranean, Temperate with dry, hot summer	agriculture, fishing, animal husbandry, forestry, energy	water-efficient irrigation, agricultural energy
8. Sardinia in Italy	RE	west of the Italian Peninsula	Mediterranean, Temperate with dry, hot summer	tourism, mining industry	limited resources under sustained socio-economic development
9. Greece	NA	South-Eastern Europe, Mediterranean Sea	Mediterranean, Temperate with dry, hot summer	agriculture, maritime industry, tourism	cross-sectoral implications of single-sector strategies
10. Azerbaijan	NA	Eastern Europe, Western Asia, Southern Caucasus region, Caspian Sea	diverse, cold semi-arid humid continental, humid subtropical, temperate oceanic	oil and gas products, agriculture, food production	lack of diversification in energy sources, food security, dependency on TR water resources, potential role of RES
11. European	CO	Northern and mostly Eastern Hemisphere	mainly temperate, diverse	diverse, services, industry, agriculture, tourism	τhe impact of transition to a low carbon economy on the Nexus
12. Global	GL	n/a	n/a	n/a	identify and assess Nexus issues at the global scale with focus on the SDGs

1.2 Unique Characteristics and Contribution

The Nexus approach designed from the SIM4NEXUS project is a unique contribution to Nexus research. An early version of the approach was informed by the FAO-WEF and CLEWs approaches, and was throughout the 4 years of project. One case study (Greece) operated as a front-runner and showcase for the other case studies.

The SIM4NEXUS approach was designed, validated and updated from the twelve case studies implemented, considering diverse geographical, biophysical, socio-economic and political contexts, and covering different spatial scales (e.g. regional, national, transboundary, continental and global scales). Very importantly, except for the case of Azerbaijan, case studies are led by locals, giving a unique advantage in the approach, considering that a foreign team would need to surpass a series of contextual difficulties (i.e., language, cultural distance, context knowledge). An overview of case studies is presented in **Table 1**. More information on the cases is available in **Supplementary Appendixes A and B**.

In order to test robustness of the approach our focus is on different spatial scales (regional, national, transboundary, continental and global). The biophysical nature differs across scales, as well as the input and output flows from the system boundaries in place. This can be depicted in the imports and exports of food and energy in all the different scales. The scale diversification in case studies plays an equally important role, if not more, in the socio-economic and the political analyses, since it shapes differentiated stakeholder maps and policy level–EU, national, regional—frameworks, respectively. Nexus A number of additional artificial and functional differences, such as the availability in data, the stakeholder participation, the capacity and expertise in tools of the different working subgroups, the resources, etc. complete the full diversity of the case studies in place.

In this paper, we present the consolidated view of the main tasks necessary to perform a comprehensive Nexus assessment through the SIM4NEXUS approach. The approach is informed by Nexus-related research and tested against twelve Nexus

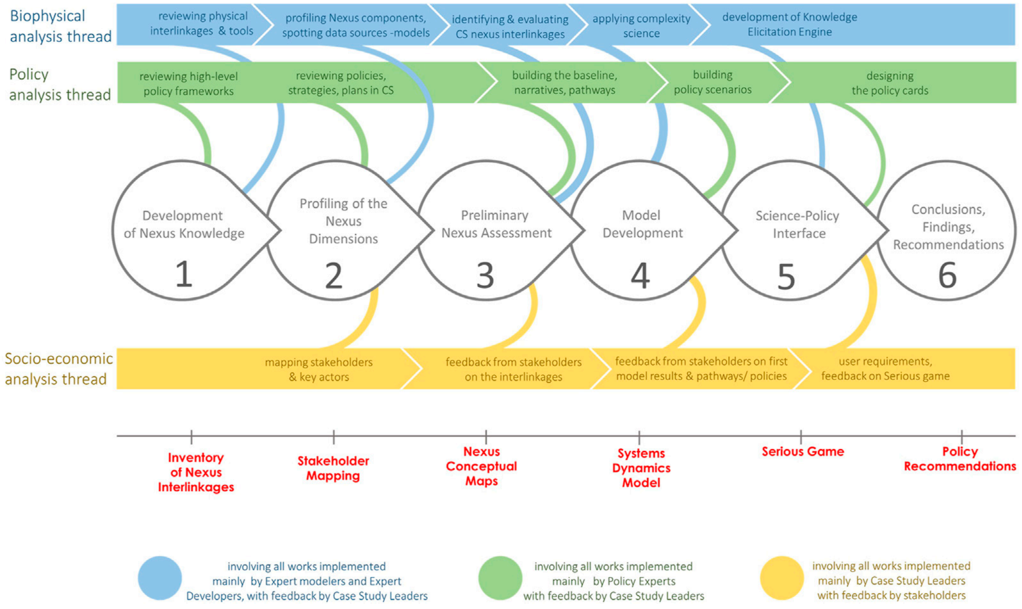

FIGURE 2 | Overview of the main steps in the SIM4NEXUS approach, including the biophysical, policy and socio-economic analyses threads, and the main outputs in a Nexus assessment.

assessments. Our ultimate aim is to release and transfer the SIM4NEXUS approach to the research, planning and policy communities[2], using the learnings and experience from the case studies. By doing so, we aim to contribute towards the operationalization of the Nexus approach, meaning its uptake and effective use in decision making.

2 MATERIALS AND METHODS

The SIM4NEXUS approach is grounded in the practice of twelve case studies that have worked under the same project showcasing geographical, social and economic diversity. They are implemented in different scales: regional, national, transboundary, European and global. This is a unique output in the Nexus approach field. To our knowledge, no other research initiatives or projects have combined so many cases, and so varied, over the same period, and involving the same and diverse teams of experts. The work in the cases was dynamically iterated within the project activities and developed in collaboration with stakeholders. Ultimately, the approach provides guidance on how to conduct a Nexus assessment and informs on the key methodological steps of the process. We recommend the approach for use in the development of future Nexus assessments by the research community, institutions, and private actors.

2.1 Description of the SIM4NEXUS Approach Steps

The SIM4NEXUS approach is presented in this section and includes three phases. It was reached following a 4 years project and completed in 2020. Initially, it was informed by existing frameworks, such as CLEWs (Howells et al., 2013; Ramos E et al., 2021) and the WEF Nexus assessment methodology by the FAO (Flammini et al., 2014), review of other approaches to the Nexus. It was then shaped according to several activities conducted in the project for the development of the Nexus assessments in each case study. A first comprehensive version was reached halfway the project. The framework was then reviewed and updated, taking stock of the continued work of the case studies until spring 2020.

The SIM4NEXUS approach is structured into six main steps: the *Development of Nexus Knowledge*, the *Profiling of the Nexus dimensions*, the *Preliminary Nexus assessment*, the *Model development*, the *Science-Policy interface*, and finally the *Conclusions, findings and recommendations.* The following description of steps and sub-steps constitutes a synthesis of the workflows in all the case studies and uses as a baseline the national case study of Greece that operated as a frontrunner. **Figure 2** depicts the six main steps, the main tasks involved in the three workflow threads: the Biophysical, Policy, and the Socio-economic analyses, as well as an abstract timeline of the main assessment outputs. A detailed description of this process follows as structured into the aforementioned six main steps and shown in **Figure 3**. Important to clarify that the framework is not an automatic process, nor is there automation in its implementation (other than inherent automatic tasks specific to the modelling tools, the SDM and the activities for the development of the

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[2] By planning communities we refer to actors which engage in planning processes within the sectors which operate in the different Nexus dimensions. Such "planning communities" can be local stakeholders responsible for a municipality, private utilities, farmer associations, etc.

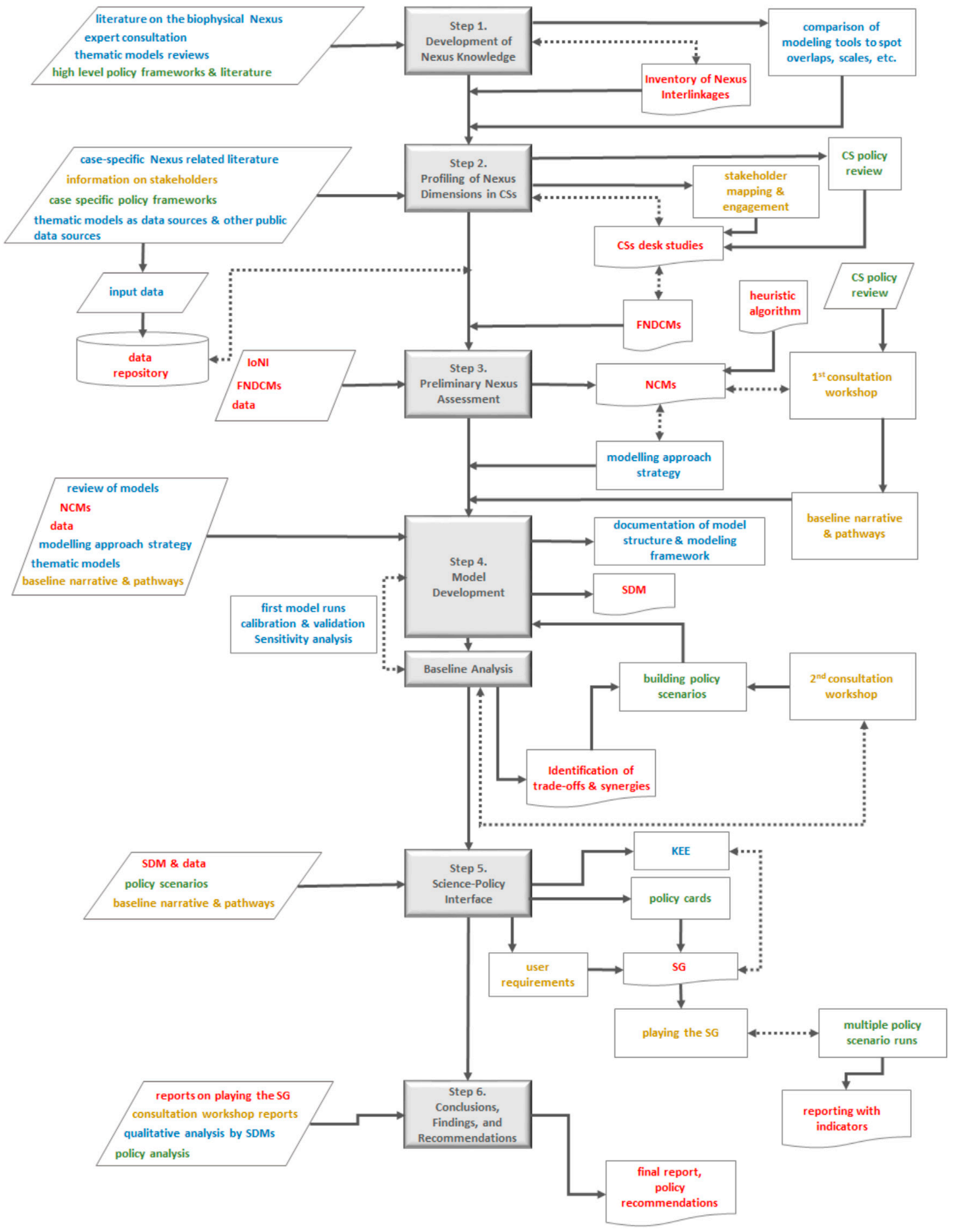

FIGURE 3 | Overview of the SIM4NEXUS approach. The workflows related to the biophysical analysis thread are noted with blue, to the policy analysis thread with green, to the socio-economic analysis with yellow, and major outputs with red. Acronyms: CM—conceptual maps; FNDCMs—Fragmented Nexus Dimensions Conceptual Maps; IoNI—Inventory of Nexus Interlinkages; NCMs—Nexus Conceptual Map; SDM—System Dynamics Model; SG—Serious Game; KEE—Knowledge Elicitation Engine.

Serious Games (SGs)). Serious Games are interactive video games that expand beyond recreational purposes and aim at skills and knowledge development by their users through problem-solving (Manero et al., 2015; Pilote and Chiniara, 2019; Sušnik and Masia, 2020).

The first step of the SIM4NEXUSapproach is the Development of Knowledge in the Science of the Nexus. This step is implemented in three sub-steps:

1) *Building the Nexus knowledge*: refers to the process of developing Nexus approach knowledge by the experts involved in the assessment. This is critical for understanding the complexity of the analysis and for clear communication with stakeholders throughout the Nexus assessment, and when communicating the assessment outcomes to different audiences.
2) *Modelling tools to assess the Nexus*: A virtual "toolbox" is set up with all relevant state-of-the-art tools and other approaches that are available for quantifying the Nexus. A comparison is performed of modelling tools regarding their capacity to cover the different Nexus dimensions, coverage of spatial and temporal scales, semantics and ontologies and overlaps in the tools are identified.
3) *Preparation of the background knowledge on the Nexus*: An Inventory of Nexus Interlinkages (IoNI), all possible systems interactions, is created (Laspidou et al., 2017), as well as a method for visualizing interlinkages in an assessment through building a Nexus tree (Laspidou et al., 2018), which can be complemented by a heuristic algorithm to quantify the relative strength of interlinkages (Laspidou et al., 2019).

Key outputs of the first SIM4NEXUS approach step are the IoNI, the review of modelling tools and integrated assessments, and a review of high-level policy frameworks and papers.

The second step is the Profiling of the Nexus Dimensions in the case study and corresponds to the assessment of Nexus systems (Water, Energy, Food, Land, and Climate), their trends, the status of sectors, and the identification of sectoral challenges. Six main tasks are included in this step:

1) *Characterization of the Nexus dimensions:* characterization of all involved Nexus dimensions systems (domains and sectors) for the case studies, using publicly available sources and expert knowledge.
2) *Policy and governance analysis, consisting of* a thorough review and understanding of policies, strategies and plans implemented or to be implemented in the near future per Nexus dimension, or across domains, at all scale levels (regional, national, continental, and global) in each case study.
3) *Collection of data and sorting:* Raw non-processed data and simulated data (assessment of available modelled data for the case study, from Step 1.ii) if necessary are collected. The data may refer to resource uses, stresses, availability, spatial and temporal distributions, etc.;
4) *Mapping of stakeholders and key actors and first stakeholders' consultations:* The key players are identified in this step, and the stakeholder engagement process initiates. At the same time, some first impression of the stakeholders on what shapes the Nexus map regarding resources, sectors and processes hotspots is recorded. The latter is done mostly via unilateral consultations.
5) *Identification of sectoral challenges:* Inputs from points i) to iv) result in the identification of sectoral challenges, which can be operational and/or at the institutional level. An example of an operational challenge would be the transition to a low-carbon economy, while an example of an institutional challenge would be the absence of inter-ministerial communication for co-designing a strategic plan for the environment, the energy, and the agricultural sectors. Challenge-implicated interactions in the systems Conceptual Maps (CM) should be identified, when possible. The DPSIR framework can be used in this step to assist in the structuring and interpretation of the information collected, from each Nexus dimension perspective.
6) *Assessment of thematic models outputs as data sources.* This is implemented to assess the potential need to obtain extra data or identify missing data to cover possible gaps in data sets. Key outputs of the second step are the sectoral assessments and Nexus systems conceptual maps, the policy analysis, the stakeholder mapping, the identification of main and/or potential data sources, and identification of the case studies hotspots regarding processes and resources.

The third step of the SIM4NEXUS approach is the Preliminary Nexus Assessment. This step develops from the outputs of Step 2, such as the desk-study and the systems conceptual maps, which are analyzed in an integrated manner following the sub-steps described below. In summary, this step includes:

1) *Scanning the systems for the identification of Nexus interlinkages:* The IoNI produced in Step 1 and the Nexus systems CMs produced in Step 2 are necessary for this step, since they are scanned to spot any interlinkage that can be considered relevant in each case study. Identifying interlinkages and assessing the complexity and extent of the interrelations among domains for the CSs leads to the drafting of Nexus CMs (NCMs) that are used later in the first consultation workshop.
2) *Preliminary estimation of the strength of the interlinkages.* The data collected are used for a first estimation of the most relevant interlinkages from the perspective of each system. The share of resources uses, and their flow from sector to sector, are quantified. This quantification may serve to filter the relevant interlinkages or reveal some important hidden interlinkages that were not perceived as critical. This preliminary Nexus quantification will also reveal the comparative spatial and temporal distributions of uses, processes and availability of resources and will help define the proper time step and granularity of the following modelling exercise according to the uniformity of the distributions. For a more systematic and standardized process of the preliminary estimation of the strength of the interlinkages, a Heuristic Algorithm for ranking the Water–Energy–Food–Land Use–Climate Nexus

Interlinkages is developed by Laspidou et al. (2019). This sub-step leads to the update of the NCMs draft.
3) *Development of final NCMs:* this is a more mature version of the NCMs representing in a single diagram how the different systems depend on each other.
4) *Consolidated identification of critical interlinkages:* Comparison of (outputs from Step 1, such as sectoral challenges, preliminary interlinkages, policy analysis) and sub-steps i)—iii) (assessment of the significance of interlinkages, and CMs) for a consolidated identification of critical interactions, and by doing so, of Nexus-induced challenges;
5) *First consultation workshop* for stakeholder input and opinion on the status of the systems, sectors and challenges. This sub-step implements the validation and/or identification of critical interactions (consolidated in iv)) making use of the previous resources developed (NCMs, sectoral briefs, policy analysis summary, etc.). Details on the stakeholder and expert consultation processes can be found in Laspidou et al. (2019). In this step, the final NCMs are also validated by stakeholders;
6) *Formulation of the baseline narrative and identification of pathways that could be of interest to analyze:* This task involves the formulation of a "raw" narrative that characterizes the baseline case (or business-as-usual) related to how stakeholders perceive the development of the different sectors following current or expected trends. This is an important step to be used as a benchmark for pathways or scenarios of interest.
7) *Definition of the modelling approach strategy (e.g. selection of thematic models):* This step builds on the previous steps (1 ii), 3 iv), and 3 vi)) and the consequent refinement of Nexus challenges and critical interactions. Thematic models and other quantification methods are identified based on their ability to cover the Nexus systems and, most importantly, to capture the cross-system dynamics related to the critical challenges identified in the case study. It will be important to assess data availability and access at this stage.

Key outputs of the third step are the NCMs, the identification of Nexus challenges, the definition of pathways, the first modelling requirements (what systems should be covered and with what level of detail), a heuristic algorithm for ranking Nexus interlinkages strengths, the preliminary selection of modelling tools, and the first version of the baseline narrative (storyline) of the case study.

The fourth step in the approach is Model Development. This step includes the use of the thematic models and System Dynamics Modelling (SDM). The latter is a complexity science approach that enables the quantification analysis of the qualitative information gathered in the previous steps (Laspidou et al., 2019; Sušnik and Masia, 2020). Such information is used in the SDM to mathematically characterise flows, stocks, tables and other simple features of the systems under investigation. The analysis helps capture complex and non-linear systems dynamics, allowing for performing scenario and uncertainty analyses (Keyhanpour, et al., 2021). The main sub-steps in this phase are:

1) *Analysis of the information available for quantification:* In this step, analysts compare inputs from the previous tasks, particularly related to the Nexus interactions, pathways and NCMs.
2) *Implementation and development of the modelling approach strategy.* The selection of modelling tools, suggested in Steps 1 ii) and 3 vii), is evaluated and (re)defined (and decided upon). The choice of thematic models is also based on data availability and formulation gaps within the SDM. Inputs and outputs of models are compared, and harmonization of input data is performed to the extent possible.
3) *Literature review regarding the overall and in-parts model structure:* The whole modelling approach involves thematic models where needed, applies them for the baseline, and links them with all relevant variables through commonly accepted formulations. The final outcome is kept as simple as possible.
4) *Characterisation of the baseline in quantitative terms:* Drivers and narrative elements are analyzed for their representation in the models, and to guide the definition of assumptions coherent with the baseline and across modelling tools. Since the thematic models will unlikely cover all Nexus systems with an equivalent level of detail, it will be important that the detailed narrative produced as a starting point covers plausibly the evolution of the Nexus systems so that "baseline" dynamics across systems are well understood (step 3.f). This is an important step prior to the definition of scenarios.
5) *Data requirements are assessed and data availability evaluated*, in order to prepare baseline models for the CS. Modelling teams clarify the type of interactions and components of the narrative they could inform about. An important step in the modelling work is the analysis of the baseline results, represented separately in the diagram. Nexus trade-offs are identified as well as potential synergies across sectors and systems. Once the baseline is prepared, scenario development and implementation can follow.
6) *Data preparation and model development:* Data is collected and prepared to be used in the thematic models. The baseline of the models is prepared. Model runs are conducted and results analyzed. Depending on results, models may require to be improved to ensure the adequate representation of the functioning of the dynamics they represent.
7) *Building the policy scenarios.* Preliminary policy work is done here, with defining policy objectives and instruments. Policy scenarios are built according to the policy papers review and stakeholder participation.
8) *Preparation of the SDM structure (complexity science tools):* Once the CMs are revised, based on activities in 3. a—f, the structure of the SDM is prepared. Data requirements of the SDM are mapped against models inputs and outputs and other relevant data available. The policy scenarios and the narratives shape the SDM structure and flow from inputs to outputs.

9) *Iterative model calibration and validation:* The runs will be used for calibration and validation. An iterative process between the SDM building (including thematic models) and the SDM runs lead to its structural improvement.
10) *Uncertainty analysis:* The dimensions of uncertainty, namely the location, the level and the nature, are identified by the involved modellers after defining all the modelling assumptions. The assumptions are labelled as contextual, structural, or parametric uncertainties (which are the locations of uncertainty). A series of sensitivity runs of the model is conducted to quantify the parametric uncertainties (Knobloch et al., 2019).
11) *The second stakeholder workshop* aims at informing stakeholders of the modelling outputs and discussing the first results. This may require updates or other iterations of the models. The workshop also initiates discussions on pathways and scenarios. The latter is done based on the selection of policies to be studied in combination with stakeholder input and feedback. SDM visualization tools are employed to show stakeholders what the potential of the tool is.

The key outcomes of the fourth step are the sectoral and/or multi-systems models, the repository of input and output data, the documentation of modelling assumptions concerning the characterization of the baseline, and the uncertainty analysis.

The fifth step corresponds to the Science-Policy interface. For results to be within reach of a variety of audiences (policy-makers and other actors of decision, in public and private institutions, academia, civil society, NGOs, etc.), they need to be packaged in a way that is simple and intuitive to interpret. In SIM4NEXUS, this is achieved with the Knowledge Elicitation Engine (KEE) in the format of an SG, which combines all efforts from the previous steps. The SG bridges the domains of science and policy-making, making the analysis accessible to a wider audience. In this way, users of the game are not required to have particular expertise or knowledge in any of the main components of the studies but will acquire knowledge on the Nexus by playing the SG. Tasks related to the development of the game include:

1) *Development of the Knowledge Elicitation Engine (KEE)*: This is the inference engine of an expert system (the SG in SIM4NEXUS).
2) *Conceptualization of the SG:* This task involves the development of Use Cases for the Serious Game, the design of the game structure, the moves that a player can implement, the rounds of the game, how a player wins, the tokens, etc. Special focus is given on the design of the policy cards, which constitute the players' option in the game that simulate in the visual environment actual resources management choices. This task also involves the creation of the Semantic repository.
3) *Definition of indicators:* In this task, established Key Performance Indicators (KPIs) are employed, and others are created from scratch to illustrate the Nexus systems' performance displayed in the game. These are designed to facilitate the understanding of the Nexus systems responses and the evaluation of the policies regarding the SDGs and Nexus coherency.

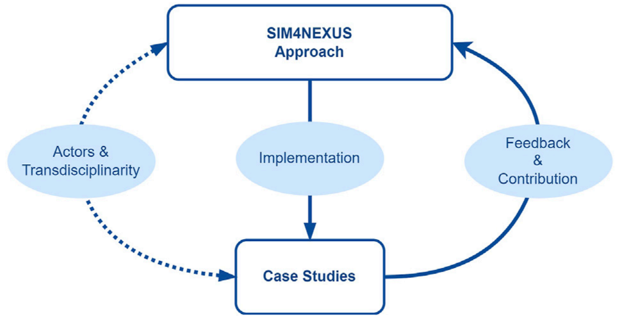

FIGURE 4 | Process for analysing the case studies in the perspective of the development of the SIM4NEXUS approach.

4) *Development of the visualization interface*: This task involves a lot of iterations among partners to provide for usability, commonly accepted aesthetics, etc.
5) Instructions of how to play the game: Instructions use popularized wording and are translated to all languages of case studies' stakeholders.
6) *The* third consultation workshopaims at presenting the game to the stakeholder group for feedback.

Key outputs of the step are the KEE, the SG, and the Nexus KPIs.

The final step naturally involves the formulation of Conclusions, Findings and Recommendations, based on the objectives of the pathways and scenarios investigated in each case study. Once the players play the game, they can manipulate the systems to explore different futures and collect messages that are specific to their choices. They will be able to infer on the coherency of policies based on the quantification analysis; the role of innovations; identification of trade-offs and synergies in the different scenarios; and assess potential solutions at the sectoral and cross-sectoral levels. This step can include the presentation of the SG in additional stakeholder consultation for the final version of the game. Other game dissemination activities include its application in universities and schools.

2.2 Methodology for the Analysis of the Case Studies

The SIM4NEXUS approach described in the previous section is the consolidated and generic version of the Nexus assessments process by the case studies. Dynamically developed, the approach provides an overall picture of how work is performed in different tasks constructing the way for the Nexus assessments. To distil learnings from the application and development of the SIM4NEXUS approach, we analyzed the cases from different viewpoints, as illustrated in **Figure 4**. Firstly, in terms of the actors involved and their role in the assessment process and transdisciplinary research characteristics. Secondly, in terms of the approach implementation. Lastly, how the work in the case studies is feedbacked to the approach is also examined. Findings from this analysis are presented in the Results section of the paper.

Nexus assessments aim towards knowledge integration from different disciplines in the investigation of Nexus challenges. With the involvement of more disciplines and actor types, assessments head towards transdisciplinarity practices. In the transdisciplinarity analysis of SIM4NEXUS case studies, we aimed at understanding the diversity of actors involved in each sub-step of the framework, their level of integration, and intensity of engagement.

To validate the SIM4NEXUS approach steps and sub-steps, we examined how case studies had implemented them. An example of the case study analysis is presented in **Supplementary Appendix C**. The analysis enabled revising the steps suggested in an intermediate project deliverable (Ramos et al., 2019) and their update according to case studies' work until the spring of 2020. It is important to note that fewer inferences are made regarding Steps 5 and 6 as many deliverables were ongoing while developing the SIM4NEXUS approach. In addition, the Covid-19 pandemic induced constraints, affecting the organization of the last set of stakeholders' workshops.

Several project deliverables informed the comparative analysis, e.g., (Blanco, 2017; Brouwer and Fournier, 2017), bi-annual case study interviews carried out by Work Package 5 (Brouwer and Fournier, 2020a), and review and direct input from CSLs through the elaboration of case study tables for the approach's validation.

The comparison was conducted in two ways. Firstly, we assessed if cases had or not performed specific approach sub-steps, which informed if the step was or not relevant and if it had to be removed or updated. Secondly, we compared the descriptions provided by each case study on how sub-steps were conducted to assess. This comparison served to identify differences and particularities in the approach's implementation (e.g., an example is the fuzzy cognitive mapping for stakeholder participation developed in the case of Andalusia (Martinez et al., 2018)).

In the step and sub-step comparisons, we looked for systematic differences that informed their refinement or prompted changes to their location and, again, their relevance. An example of inference is that cases may have completed the task as planned in the project activities, but the specific task was not found to be relevant for their Nexus assessment. In the results section, we summarize the key findings of the comparison according to the categories in the Nexus concept (Brouwer et al., 2020; Ramos et al., 2020), described in the Introduction.

3 RESULTS

This section presents the results from the comparative analysis of the case studies in SIM4NEXUS. In summary, we assess actors' involvement, disciplinarity integration, and derive insights from the approach's implementation.

3.1 Actors' Involvement and Transdisciplinarity Analysis

Different actors were involved in diverse stages of the case studies and engaged with varying intensities. Based on the SIM4NEXUS experience, we identify six types of actor types: Expert Case Study Leading teams (CSL), Expert Modellers (MOD), Policy Experts (POL), Expert Developers (DEV), Stakeholder (STK), and Other (OTH). The CSL is responsible for conducting and coordinating the case study, and in the majority of the SIM4NEXUS case studies, it is part of the case context. MODs develop mathematical models representing the Nexus systems and deal with modelling data inputs and outputs in the thematic models or the SDM. MODs also develop modelling frameworks that enable scenario analysis in the CS. POLs guide and assist the CSL in the policy analysis component of the assessment, which includes the policy coherence analysis, development of policy scenarios, and definition of policy cards for the SG. The SG is developed by DEVs, who liaise with actors engaged in SG development. Stakeholders (STK) are groups or institutions of interest that operate in the Nexus context of the case studies and are interested in the findings of the analyses. Lastly, the category "Other" (OTH) refers to actors external to the assessments' workflow but who contribute with knowledge and expertise throughout the assessment process. Examples of these actors include manuscript reviewers, the executive advisory board to the SIM4NEXUS project, and the scientific community in conferences or meetings.

After identifying actors and roles, an appreciation of their participation in each assessment stage was performed in **Table 2**. This evaluation was conducted by SIM4NEXUS project partners and was informed by the experience in the cases studies. Such knowledge is also documented in several project deliverables (Fournier, 2016; Munaretto, 2018; Brouwer and Fournier, 2020a; Echeverria et al., 2020; Sušnik and Masia, 2020). In the table, the engagement intensity is indicated using a color gradation from dark to light blue, linked to a numeric scale of 1–5, indicating high to low engagement, respectively. The results do not inform on the time effort of each task, but the timing of actors' participation and their expected level of engagement.

The results reveal the critical role of the CSLs. They are present in most assessment steps and with high participation intensity since they are responsible for the assessment development and the liaison with other experts and stakeholders. Modellers (MOD) are key in the model development step 4) and data preparation and tool selection for analyzing Nexus systems. They are also engaged in developing the SDM and providing modelling outputs for the Serious Game. Policy analysts are involved in the policy coherence assessment, identifying sectoral policy goals and instruments, in the model development stage for the definition of policy scenarios, and the Serious Game via the selection of system-level policy options the players can implement. As for the DEVs are primarily engaged in the Science-Policy interface step, which takes the format of a Nexus Serious Game or results' visualization tools. Due to their transversal role, stakeholders are present throughout the assessment process. Ultimately, they also test and play the SG, and thus are involved in retrieving Nexus (or integrated) insights. The involvement of "Other" actors can also be spotted in all framework steps since there could be opportunities for the engagement of external audiences to the CS throughout the Nexus assessment. One important role "Others" can play by testing the SG, contributing to its development and improvement.

TABLE 2 | Overview of actors involved in the different steps of the SIM4NEXUS approach and the intensity of their participation. Abbreviation meaning: CSL—CS Leading team; MOD—Expert Modeller(s); POL - Policy Expert; DEV—Expert Developer(s); STK—Stakeholder(s); and, OTH—Other actor(s). The color notation "x" expresses the degree of involvement of the actor type from high (dark blue color) to low (light blue).

SIM4NEXUS Approach Step	Actors					
	CSL	MOD	POL	DEV	STK	OTH
1. Development of Nexus knowledge						
a. Building the Nexus knowledge	1	1	1	1		
b. Screening of modelling tools and quantification approaches to assess the Nexus, and methods to compare policies	2	1	1			4
c. Preparation of the background knowledge on the Nexus	1					
2. Profiling of the Nexus domains						
a. Characterization of the Nexus domains	1					
b. Policy and governance analysis	1		1		2	
c. Identification of data requirements	1	1			2	
d. Mapping of stakeholders and key actors, and first stakeholders' consultations	1				1	
e. Identification of sectoral challenges	1				1	
f. Assessment of thematic models outputs as data sources	2	1				4
3. Preliminary Nexus assessment						
a. Comparison of systems for the identification of Nexus interlinkages	1				2	4
b. Preliminary estimation of the interlinkages significance	1				2	
c. Development of the first version of the Nexus conceptual model	1					
d. Consolidated identification of critical interlinkages	2				1	
e. First consultation workshop	1				1	
f. Formulation of the baseline narrative	1		2		2	
g. Definition of the modelling approach strategy	2	1			2	4
4. Model development						
a. Analysis of the information available for quantification	2	1				
b. Implementation and development of the modelling approach strategy		1				
c. Literature review regarding the overall and in-parts model structure	2	1				5
d. Characterization of the baseline in quantitative terms	1	1				
e. Data requirements are assessed and data availability evaluated	2	1			2	
f. Data preparation and model development	1	1			3	
g. Building the policy scenarios	1		2	3	1	5
h. Preparation of the SDM structure	1			1		
i. Iterative model calibration and validation	1	1		1		
j. The 2nd stakeholder workshop	1		3		1	
5. Science-Policy interface						
a. Development of the Knowledge Elicitation Engine (KEE)		3		1		
b. The development of "Use Cases" for the game and creation of the Semantic Repository (SR) and policy cards	2		3	1		
c. Definition of indicators to illustrate the performance of the Nexus systems	1				1	4
d. Development of the visualization interface				1		3
e. Instructions on how to play the Serious Game	1			1		3
f. 3rd consultation workshop	1				1	
6. Conclusions, findings and recommendations	1		3		2	

Several types of stakeholders were engaged in the case studies through various participatory methods. These implied varying engagement intensities, from information sharing and consultation to consensus building. An overview of stakeholders involved in the case studies and participatory methods is shown in **Supplementary Appendix D**. Such information sheds light on the transdisciplinary character of the studies. Transdisciplinarity research is characterized by high disciplinary integration (i.e., interdisciplinarity) combined with high engagement of non-academic actors, who work together for solving a common problem (Tress et al., 2005; Mauser et al., 2013). However, involving a diverse group of non-academic participants does not necessarily mean that a study is transdisciplinary if this engagement is mostly for consultation purposes, and coordination between different actors types is limited.

TABLE 3 | Analysis of the application of framework steps in case studies considering the activities reported in Deliverable 5.5 (Brouwer and Fournier, 2020b).

	Framework Step	Findings
1	**Development of Nexus knowledge**	All cases completed the sub-steps in this step. The development of knowledge in the Nexus was important for all actors involved, and having a common understanding of the Nexus approach facilitated communication among the ones involved, including with stakeholders
2	**Profiling of the Nexus dimensions**	The majority of cases validated the steps. Differences here are verified in stakeholder mapping, which was more challenging for larger-scale cases (i.e., European and Global)
3	**Preliminary Nexus assessment**	• Different approaches were used to estimate interlinkages significance: quantitative (Laspidou et al., 2019) and qualitative, e.g., stakeholder consultation and conceptual maps' development • Workshops were not always conducted within the suggested work plan, suggesting these should be flagged in the framework as tentative • The cases refined the modelling strategy throughout the assessment process, specifically when certain data were not obtained from the selected thematic models. Thus, it is critical to understand modelling tools' capabilities to assess the Nexus context in the early stages of the assessment • Collaboration between actors is intensified in this stage. Better understanding by the case study team of thematic models and SG development is vital at this stage in support of stakeholder engagement activities
4	**Model development**	• The majority of the cases implemented the sub-steps described in the framework. Differences observed related to the availability of model results (some cases already had models that could be used, including SDMs, or modellers in the case study leading team). Data complementarity issues were identified in the characterization of Nexus domains by thematic models for populating the SDM developed based on the conceptual maps. Additional data collection was performed, and thematic models contribution was revised • Workshops were conducted but not always aligned with the work plan, partly due to the timing of the first workshop, different participation approaches followed, or information requirements from the cases to support ongoing tasks
5	**Science-Policy interface**	Most cases completed the tasks in this step, distilling insights from the case study and indicating policy options to tackle the Nexus challenges, fulfilling the purpose of the assessment. Learning was achieved in elaborating policy-relevant insights by case study teams Even though SGs were not developed for all cases, some could use other cases' examples in stakeholders' interactions. Some cases opted for other results visualization options (e.g., global case study). Experts' availability (modellers and developers) created a bottleneck that influenced the completion of tasks. In a single case study assessment involving a group of experts, such challenges would probably not occur
6	**Conclusions, findings and recommendations**	Conclusions and recommendations were included in several deliverables. Policy recommendations are structured regarding changes to policy outputs, policy contents, innovation, policy processes, and the policy-science interface. The corona pandemic emergency compromised the dissemination of results planned for the first half of 2020

In these circumstances, research can be considered "participatory" and "parallel", as opposed to "transdisciplinary" and "integrative", as explained by Tress et al. (2005) and Mauser et al. (2013). When research is focused on academic practitioners, the approach to disciplinary integration (e.g. cross-disciplinary, multidisciplinary or interdisciplinary) can vary, and depends on how a goal is planned to be achieved. For example, a cross-disciplinary study considers the perspective of another discipline when solving a problem within its disciplinary field. In multidisciplinary studies, different disciplines work together towards a common objective; in interdisciplinary studies, the integration of disciplines is required to answer a common question.

Reflecting on the transdisciplinary character of SIM4NEXUS case studies, we find that these can be of many types in terms of integrative approach—and not necessarily transdisciplinary. For example, larger spatial scale assessments, such as the transboundary, continental and global have a more challenging task in stakeholder engagement and closer participation due to the involvement of multiple countries, which then multiplies the stakeholders to be engaged from different management, political, and social contexts. These actors will unlikely share similar priorities, interests, values and decision-making power or influence, influencing the level of collaboration necessary for transdisciplinarity. In contrast, case studies of smaller geographical scales, e.g., sub-national and national case studies, showed characteristics of transdisciplinarity. For example, in the Greek and Latvian case studies, transdisciplinarity was achieved by engaging a diverse group of non-academic actors; and in the South West United Kingdom (UK) case study, through a tight collaboration between academic and non-academic actors. In the latter, the case study leading team was a water systems company, and the integration of the Nexus approach was ambitioned and aligned with the company's vision.

In conclusion, transdisciplinarity requires the engagement of a plural group of actors (academic and non-academic) who collaborate intensely in the investigation of Nexus questions. One way to achieve this is by planning stakeholder participatory activities that enable a higher collaboration between actors, such as the consensus-building, through the entire process of the Nexus assessment. Larger scale assessments would either benefit with more time for the assessment, or earlier engagement of actors in steps before its start. From the perspective of non-academics, the South West UK case study illustrated the advantage of collaborating with academic partners, supporting the importance of cultivating partnerships between business and private actors and Academia.

3.2 Application of the SIM4NEXUS Approach to the Case Studies

In terms of the implementation of the suggested approach steps and their relevance, we conclude that the work conducted in the cases is aligned with the approach suggested. A summary of this analysis is presented in **Table 3**. There was high accordance on the first four approach steps, and respective sub-steps. Differences exist mostly on the engagement of stakeholders and the timing of the organization of the workshops. In some cases, e.g., Global and European, the engagement proved to be more difficult than smaller scale or national case studies. In the case of Azerbaijan, since none of the partners was based in the country, subcontracting of national experts was conducted to facilitate access to national-context knowledge. All cases were able to arrive at conclusions and recommendations. **Table 3** should be analyzed in perspective with the involvement of different actors across the various steps, as presented in **Table 2**. The steps described in the assessment are very much in line with the activities developed and co-developed in several work packages. With the framework, we also aim to provide perspective on the purpose of these activities, which many times happened simultaneously but involving different types of experts.

3.3 Contribution of the Case Studies to the SIM4NEXUS Approach Development

Although cases were guided by the same approach, differences existed between the studies due to the diversity of contexts and challenges. In this comparison element, we searched for learning from the case studies practice. These contributed to the enrichment and transferability of the SIM4NEXUS approach. The findings were grouped according to the Nexus concept defining categories, described in **Figure 1**.

On Knowledge Creation, cases identified the opportunity of developing new methods to address the tasks in the different steps, depending on the resources available and the characteristics of the case. Some resulted in the application of methods to new problems (e.g., participation of stakeholders in the identification of key interlinkages in the case of Andalusia, (Martinez et al., 2018)), methods for the identification of interlinkages relevance (e.g. as in the case of Greece (Laspidou et al., 2019)), or the application of methods developed in the project (e.g., policy coherence analysis as in (Munaretto and Witmer, 2017; Papadopoulou et al., 2020). Awareness of the Nexus interlinkages can be of value in policy design, and can increase the level of engagement of stakeholders in the analysis.

In relation to Participatory Governance, the category that embeds the interactions with stakeholders in the case studies, different ways of mapping and engaging stakeholders were followed. For example, in Andalusia, fuzzy cognitive mapping was used, while in the case study of Sweden, stakeholder mapping included a power/interest analysis (Brouwer and Fournier, 2020a). Also, challenges and opportunities of cross-sectoral collaboration were found. For example, in the Greek case study, the largest cotton production corporation expressed interest in creating the appropriate bonds to the water and energy sector, aiming at improving resource efficiency in its production chain and getting certified accordingly. In the transboundary study of Germany, Slovakia and the Czech Republic, the team was engaged in a multi-country group of stakeholders for the preparation of pilot studies for landscape water retention. The cases recognized that the iterative process between local stakeholders and the research team (MOD, DEV, CSL) is key to identifying reasonable solutions to be investigated in the Nexus assessment. Thus, the clarification of roles and responsibilities, and also the timing of the communications, are important aspects which were then made more explicit in the SIM4NEXUS approach.

Methods and Tools represent the importance of quantitative practices (e.g., indicators, data, visualization tools, SGs, and modelling tools) in the SIM4NEXUS approach. These are essential to produce science-based evidence to inform sectoral planning. In SIM4NEXUS, new Methods and Tools were developed and therefore included in the approach. Examples include the application of Artificial Intelligence for the SG development, complexity science applied to the Nexus context, inter-comparison of thematic model results; and also the identification of critical data gaps in sectoral statistics. Also in this category are the creation of data repositories (i.e., cross-sectoral databases, both in terms of inputs and modelling results) and the combination of quantitative and qualitative information (e.g. incorporation of qualitative inputs from stakeholders to the quantitative analysis). The gamification of the Nexus is another important element in the approach, providing an opportunity to national stakeholders, e.g. from academia or ministries, for exploring the impacts of different sectoral policies on the Nexus. Additionally, the SGs developed can be used beyond the project timeframe in other projects or for educational purposes, and are now hosted by Watershare® (watershare, 2021).

4 DISCUSSION

In this section, insights from the analysis of SIM4NEXUS case studies are put in perspective with the Nexus approach gaps identified in the Introduction section. Additionally, we take stock of lessons learned from applying the approach across the twelve case studies and identify critical aspects for its operationalization.

4.1 The SIM4NEXUS Approach Compared to Other Frameworks

Similarities can be identified between Nexus approaches summarized in the Introduction, in particular to the FAO-WEF and CLEWs, and the TBNA regarding the policy analysis track and stakeholder participation. The SIM4NEXUS approach, similarly to the others, also defined indicators to characterize the Nexus performance, obtained from the models and used in the SG. In the latter, aggregated indicators inform on the Nexus "health". The main differences between the SIM4NEXUS approach include the dedicated effort to build Nexus knowledge, which requires time, and the integration of thematic models, other modelling tools and data collection into a single modelling framework. The SDM, detailed to the complexity level possible, is used to quantitatively describe the Nexus contexts in the case studies, following the Nexus conceptual maps.

The general Nexus approach gaps refer to the need to integrate quantitative and qualitative approaches, clarify the meaning of complexity, strengthen the science-policy interface and incorporation of the Nexus approach in policy, and the coverage of Nexus systems inclusion of social sciences. The SIM4NEXUS approach combines qualitative and quantitative methods, and it includes aspects from social sciences, policy analysis, and player behavior in gaming. Complexity is addressed through multiple iterations between the Nexus approach threads. Its transferability is evidenced by the application to multiple cases of different contexts and scales.

Intrinsic gaps relate to the lack of standard procedures, methodologies and models, the understanding of interlinkages and terminology, and the need for improving inter/transdisciplinarity. In relation to the standardization gap, the SIM4NEXUS approach contributes to addressing these gaps by introducing, applying and validating in multiple case studies the complexity science approach, developing SDMs that unified the Nexus models and complemented the representation of Nexus systems. Also, a methodology to rank the relevance of interlinkages is developed (Laspidou et al., 2019). Clarification on interlinkages and terminology is addressed through the elaboration of IoNI (Laspidou et al., 2017), the development of background information on WELFC Nexus, and the glossary of the Nexus (Ramos et al., 2019). The glossary aims at standardizing, to the extent possible, terminology which is frequently used in Nexus discussions and can facilitate communication with stakeholders and other audiences participating in an assessment. Regarding disciplinary integrative approaches, SIM4NEXUS considers a multidisciplinary team of experts with knowledge of different Nexus systems. Thematic models with a focus on different systems and with varying operating principles are used to simulate the Nexus in the case studies. Later, an SDM, which is based on the NCMs of each case study context, incorporates information from thematic models and is complemented by other information not modelled at the previous stage. Uncertainty analysis of the models is also performed (Knobloch et al., 2019). All the continued integrative approaches culminated with the development of an SG. Stakeholders are also engaged throughout the Nexus assessment, and local CSLs facilitate multi-stakeholder engagement.

Extrinsic aspects related to governance, the understanding of a Nexus approach timeframe, and funding and financing of Nexus solutions influence the application and success of the approach. Regarding governance, in SIM4NEXUS, stakeholder participation is planned in several steps and considers the engagement of public actors from different levels of decision (local, regional and national). Participatory Governance is considered a pillar element to Nexus assessments. The SIM4NEXUS multi-stakeholder engagement process also facilitates communication between different stakeholder types and the possibility of gathering and understanding different decision level perspectives. In addition, the SIM4NEXUS network of stakeholders allows participants and institutions to extend their networks, which can be of relevance for future work. In addition, policy analysis is performed to inform policy coherence, but also for the design of case-specific policy scenarios. The approach is also analyzed from how it can be integrated with the policy cycle for identifying entry-points and mapping interaction and collaboration opportunities throughout the process (**Supplementary Appendix E**). Several cases point out that the timeframe of the project influences stakeholder engagement. On the one hand, actors recognize that for the approach to have an impact on decision-making, tools need to be more mature in the first workshops. Quantitative analysis, for being meaningful and relevant to the level required for decision, need more time for development and stakeholder collaboration. However, recognizing the importance of cross-sectoral planning is already an important achievement, in particular, when many stakeholders are involved. Such findings support the importance of creating continuation projects that can foster cooperation and co-development between Nexus practitioners and stakeholders. Another aspect requiring attention is the voluntary nature of stakeholder participation and the difficulty of engaging decision-level stakeholders with limited availability. From another angle, tools and methods developed in SIM4NEXUS can continue being developed and applied. Such examples are the use of the SG in the Nexus oriented Erasmus+ SMARTENproject, the use of the SDMs in H2020 NEXOGENESIS, the adoption of the SIM4NEXUS Semantic repository by the NEXUSNETCOST Action and in general, the fact that teams that developed Nexus knowledge continue to disseminate and advance it. Thus, a long term vision needs to grow in different lines of work, so that collaborations are effectively transdisciplinary and the approach operational. In this perspective, the SG use in education or capacity development is recommended. Funding for Nexus projects, not only by research institutions, is in great part related to the challenge of operationalizing the Nexus approach. Given the effort magnitude of engaging so many experts, securing funding is challenging yet needed. From the implementation side, financing is required to test Nexus solutions and interventions and to support innovation. In the case study of Greece, where the banking sector was involved, credit solutions were discussed as a sector's contribution to making the Nexus approach operational.

4.2 Lessons Learned From the Application of the SIM4NEXUS Approach

A key step of the SIM4NEXUS approach is the understanding of the biophysical and socioeconomic Nexus context, its drivers, dynamics, and how it links to decision making. Developing this conceptual understanding is challenging and requires iterations. In SIM4NEXUS, this process was streamlined through the collaboration of different actors, but also through peer-review occasions (projects, conferences, meetings), unfolding other key steps, such as stakeholder engagement, modelling, scenario development, and participation in policy. The development of the conceptual model was a key output that translated scientific knowledge to the case studies. It also served to communicate with stakeholders involved, enabling a set of consequent activities. The exercise of elaborating policy insights from a Nexus perspective was also critical. Knowledge was gradually constructed across all project activities and did not exclusively result from the quantitative analysis. Thus, combining quantitative and qualitative approaches in Nexus assessments is crucial to ensure a wider variety of solutions.

Regarding what is essential to apply a Nexus approach, flexibility in the implementation, in particular in the use of prescribed tools and methods, is listed high. Stakeholders may not be interested in adopting an established modelling tool if in-house robust tools exist and already inform decisions. However, Nexus knowledge is important and can be taken into consideration when using existing tools. Stakeholder participatory methods also need to be flexible and adaptable to the desired type of engagement. In terms of stakeholder participation, partners with existing networks were more efficient to engage stakeholders due to historical inter-institutional collaboration. Several cases noted that more workshops were needed to keep stakeholders engaged and for feedback and consultation on intermediary outputs of the analysis. Defining the analysis scope and expectations is also an essential component, since Nexus analyses are vast. A preliminary Nexus assessment helps define the analysis scope and prioritize what to investigate. Producing such a plan would support stakeholder engagement, more clearly understand what to focus on and when, plan for tool development, conduct an assessment of expert needs, and search for future funding. In addition, having a longer-term vision of the Nexus approach would contribute to knowledge transfer and the development of capacities at many different levels in the institutions involved and plan for the engagement of higher-level stakeholders.

Another critical point is to understand which tools are suitable, what type of coverage they provide, and to what detail (temporal, spatial and operative scales). Although thematic model suitability was performed in the initial stages of the case studies development (Fazekas et al., 2017), it was only after the finalization of conceptual models that a concrete understanding of interlinkages and quantitative inputs were specifically identified. Possibly the conceptual model should be designed before the tools were screened and chosen. Additional data collection, or use of other modelling tools, was performed to ensure SDM representation was covered. The challenge of model suitability highlights the importance of assessing tools and their documentation, methods for data integration, as well as data availability and accessibility, in the early stages of the Nexus assessment.

In SIM4NEXUS, five Nexus dimensions were selected (Climate, Land, Energy, Water and Food). As the project unfolded, several cases indicated that Ecosystems could be added as an extra dimension. This exemplifies the necessity for the Nexus approach to be plural and system-agnostic. When looking at resource efficiency and a transition to a low carbon economy, it makes sense that the resource systems (land, energy, and water), food system, and climate are interactively analyzed. However, practitioners may identify other relevant systems to analyze, depending on the Nexus context. Other systems, mainly from the economic sector, could be added, such as Tourism, which is found relevant in the cases of Greece and Sardinia, "Forestry" in the cases of Latvia and Sweden, and Economic Growth or Employment, which are proven to be interlinked to the WEF Nexus in the Mediterranean (Markantonis et al., 2019). The dimension of Health is also growingly discussed as an entry to the Nexus complex. In this context, the Texas A&M Energy Institute has established the Water-Energy-Food-Health Nexus Renewable Resources Initiative(WEFRAH) in January 2020. Alternatively, the perspective could also be different and focus more on consumers' behavior and choices; or have a business perspective to identify risks and vulnerabilities. Thus, other systems and viewpoints can be discussed and incorporated in conceptual models, based on their relative importance to the contextual challenges under scrutiny.

Frameworks, in general, lack the integration with the policy cycle and also a monitoring and evaluation component that could test recommendations and specific measures and support the decision making process. Addressing this gap implies a different intensity of actors' engagement, the extension of the project timeframe, or the use of ready-made tools. Collaboration in planning activities should be better accounted for, for the Science-Policy interface to work. This could be achieved through capacity building on the tools and methods developed or establishing collaboration protocols between researchers and institutions of interest.

5 CONCLUSION

The management of resource systems, considering environmental, techno-economic and societal factors, is a multi-objective task. The Nexus approach can support sustainable development by providing an integrated systems perspective. The SIM4NEXUS approach constitutes a unique output in the Nexus research field. It results from the development of twelve case studies of different spatial scopes and socioeconomic and biophysical contexts developed within the same timeframe. It provides a solid basis for future assessments adopting a step-wise approach which considers the 1) development of Nexus knowledge, 2) profiling of the Nexus dimensions, 3) preliminary Nexus assessment, 4) model development, 5) science-policy interface and 6) conclusions, findings and recommendations.

Important gaps on Nexus assessments are addressed with the SIM4NEXUS approach, such as integrating biophysical and social aspects, combining qualitative and quantitative methods, clarifying Nexus complexity by considering different workflows in an assessment, and by demonstrating transferability in the application to multiple case studies. From the application of the cases, multiple challenges in the operationalization of the Nexus arose, such as the incorporation of the approach in the policy cycle, the understanding of the longer-term characteristics of the Nexus approach, and ensuring funding and finance mechanisms to support Nexus solutions.

The comparative analysis of the SIM4NEXUS case studies allowed for the identification of key aspects in Nexus assessments. These included the need to flexibly select Nexus systems to study and the implications of stakeholder engagement beyond the assessment process through expanding networks and disseminating Nexus knowledge across institutions. The clarification of Nexus assessment outputs, systems coverage, and level of detail, are essential when performing an assessment and can assist with preparing subsequent Nexus complementary analyses.

The operationalization of the Nexus approach will take time and it will benefit from the realization of transdisciplinarity. The SIM4NEXUS approach can contribute to it in several ways. It can serve as a basis for planning, as it can serve as a guide for practice. Practitioners can select the steps that fit their prospective project, use the different steps to perform a needs assessment, or decide which step requires more or less effort. In line with the Nexus approach, the success of an assessment may depend on the identification of synergies, either through engaging partners with consolidated and relevant networks, by using existing quantitative approaches and methods, or through interdisciplinary practices by sharing objectives across projects.

DATA AVAILABILITY STATEMENT

The original contributions presented in the study are included in the article/**Supplementary Material**, further inquiries can be directed to the corresponding authors.

AUTHOR CONTRIBUTIONS

ER, DK, FB and CL contributed to conception and design of the study. ER implemented the review of the existing nexus frameworks, the identification of gaps, the comparison of the SIM4NEXUS framework to other frameworks, and the design of the methodological approach for the comparison of CSs. DK, ER and CL constructed the sequence and links of the methodological steps. ER, DK, CS wrote sections of the manuscript. DK and ER implemented the visualization. CL and FB implemented the supervision, project administration, funding acquisition. All authors contributed to manuscript revision, read, and approved the submitted version.

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SUPPLEMENTARY MATERIAL

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Farm-scale water-energy-food-waste nexus analysis for a closed-loop dairy system

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Largely due to manure management, intensive livestock production is known to negatively impact air, water, and soil quality. Excessive manure is often applied to soil as fertilizer or stored in lagoon. However, some thermo-chemical methods, such as gasification and pyrolysis, can transform manure from waste into a valuable resource. The closed-loop dairy concept employs these methods to create biochar derived from cow manure for use as a soil amendment and a water filtration medium. This closed-loop concept has the potential to produce syngas and bio-oil for production of electricity, and to reduce excessive nutrients in liquid manure irrigation by filtering manure slurry stored in lagoons. It replaces solid manure with biochar in land applications to further reduce nutrient runoff and increase soil resilience against erosion. In this study, a Water-Energy-Food-Waste nexus-based analysis and resource allocation tool was developed to evaluate the economic, environmental, and social feasibility of the closed-loop dairy system. The tool utilizes several levers to simulate a user-specified dairy operation, such as number of livestock, acres farmed, quantity of effluent irrigation, distribution of manure and biochar products, and type of biomass conversions. Financial estimates from central Texas in 2018 were used to evaluate the profitability of these practices against the costs of a dairy and hay operation. The study showed that the closed-loop dairy system, while case dependent, could be profitable and, based on operational costs, a small dairy of approximately 200 cows could break even. Results also indicate that the benefits of biomass conversions to produce energy byproducts should increase with scale. This study can help many dairy farms that are considering the economic and environmental sustainability of the industry, which has been under scrutiny.

KEYWORDS

biochar, manure management, water energy food nexus tool, circular dairy farm system, gasification

Introduction

Agriculture is a major sector of the economy and human survival. It provides for food security and livelihood for many communities. It is, however, has a significant water and ecological footprint. The beef and dairy industry, in particular, is a major economic engine for many communities around the world. However, the circularity and the sustainability of these systems are in question (Jones et al., 2021).

The Texas beef and dairy industries represent one of the largest, fastest growing beef and dairy-sheds in the United States. These industries are significant producers of food and carry significant environmental footprints, with 4.4 million beef cows and 490,000 dairy cows (USDA NASS, 2017). According to Safferman and Wallace (2015), one cow requires 50 gallons of water daily, for drinking, cooling, milk cooling, and washing. In a study of 47 dairy farms in western France, van der Werf et al. (2009) reported an average of 338.6 kW-hours per hectare of electricity used annually on conventional farms, and reported producing an average of 946.06, 6.49, and 136.66 kg of carbon dioxide, nitrous oxide, and methane per hectare, respectively. Regarding the impact of conventional dairy farms on surface and groundwater quality, the same study reported an average yield of 305.26 and 1.07 kg of nitrate and phosphate per hectare. Dairies lie at the intersection of water, energy, food, and environmental dynamics.

Steinfeld et al. (2006) showed that manure management impacts air, water, and soil quality. Commonly, solid manure from animal production facilities is land-applied as fertilizer and exceeds crop nutrient needs. Such application occurs locally, as the weight and quantity of manure makes transport expensive. Emissions of nitrous oxide (N2O) result from nitrification and denitrification in the soil following manure application, and from livestock bedding and surface storage pits. Methane (CH4) is produced from the anaerobic decomposition of organic matter in manure and directly from livestock by enteric fermentation (Chadwick et al., 2011). Manure applied in excess can transport nitrate and phosphate to surface water bodies through runoff. Lagoons that store slurry can leach nutrients into groundwater over the long term. Excessive nutrients in surface water leads to eutrophication (Kato et al., 2009). Nitrogen and phosphorous are the main nutrients in dairy manure. According to Lorimor et al. (2004), the average value of both nitrogen and phosphorous nutrients in dairy manure ranges from 300 to 800 parts per million (ppm). Choi et al. (2019) found total nitrogen of 460–850 ppm, total phosphorus of 60–150 ppm and total (Chemical Oxygen Demand) COD of 1,000–3,000 ppm from manure pits and first and second lagoons at the dairy farm. Closed-loop dairy systems use manure-derived biochar to treat wastewater, recover nutrients, enhance biomethane production, and capture greenhouse gases through adsorption (Anzilotti, 2017; Jang et al., 2018; Choi et al., 2019). Biochar is resistant to erosion and can be used as a slow-release fertilizer (Sadeghi et al., 2020a) studies biochar impact on reducing soil erosion in Loess and Marl soils. When modified in the lab, biochar can capture antibiotics, pesticides, hormones, heavy metals, and other possible contaminants (Baronti et al., 2010; Choi and Kan 2019; Jang and Kan, 2019). Biochar is produced both from gasification and from pyrolysis, at approximately 30% and 50–60% respectively, of biomass input. It has demonstrated benefits, including carbon sequestration, increased soil fertility, increased efficiency of nutrient and water use, and reduced emissions (Baronti et al., 2010). In a study of biochar properties from different types of biomasses, Singh et al. (2010) found that biochar derived from cow manure has high electrical conductivity, relatively low carbon, moderate nitrogen, and high phosphorus. The carbon to nitrogen ratio and high phosphorus content of manure-derived biochar makes it the most available, nutrient rich source of biochar compared to plant biomass.

Pyrolysis and gasification are two thermo-chemical methods of processing manure into valuable resources. Pyrolysis heats biomass at high temperatures in the absence of oxygen (Mukhtar and Capareda, 2012), bringing about gaseous, liquid, and solid primary products in the absence of an oxidant. It produces synthesis gas (syngas), a combination of hydrogen and carbon monoxide. The liquid product is bio-oil, and the solid product is biochar, which have various agronomic benefits.

Produced syngas has various energy uses and can be processed into other fuel or burned to generate electricity. With follow-up treatment, a process that may require adjusting acid content and removing moisture and oxygenated compounds, bio-oil has several uses including transportation and electricity generation. The third component, biochar, can be used as a cost-effective adsorbent, catalyst and photocatalyst for the removal of various contaminants in water and can replace current expensive adsorbents and catalysts used for water treatment (Kim and Kan, 2016; Choi and Kan, 2019; Jang and Kan, 2019). Most syngas is formed at higher temperatures; most solid biochar is produced at lower temperatures. Liquid products are produced at moderate temperatures (400–600°C). Bio-oil yields are maximized at a shorter residence time or lower heating rate. According to Bridgwater (2012), a temperature of approximately 400°C with a residence time of hours to days, provides conditions to produce 35% biochar, 30% liquid, and 35% gaseous products, by weight.

As discussed by Fernandez-Lopez et al. (2016), an alternative to pyrolysis is gasification or the heating of biomass in a partial oxidation atmosphere to produce syngas and biochar. In gasification operations, the air to fuel (A/F) ratio is important. It is calculated by dividing the product of each element and its molecular weight in air by that of the fuel combusted. Thus, the percent elemental components of the fuel must be known. Without controlling the A/F ratio, as much as 50% of N_2 gas, which has no energy content, can be present in the produced syngas, which can be converted to liquid fuel or electricity.

Research objectives

This research explores the technological and economic sustainability of the beef and dairy industry in Texas and how it can they be transformed into a more circular food system.

A systems model of the closed-loop system will relate water, wastewater reuse, nutrient management, energy, and agricultural productivity. By valuing the consumption and production of water, energy, emissions, and soil health for a unit of crop and animal production, the model reflects the nexus implications of agricultural systems (Mohtar, 2015). For this work, a farm scale water-energy-food nexus tradeoff analysis tool was developed to reflect an average size dairy farm in Texas. The tool can indicate the benefit to farmers of implementing the closed-loop system. To illustrate the benefits and embedded costs, the nexus-based tool depicts the tradeoffs between cost and income from respective water, energy, and food resources, and local environmental impacts of the system.

The specific objectives of the study are to: 1) build a system-based tool for tradeoff analysis and resource allocation for management of farm-scale dairy waste, agricultural yield, environmental impact, and costs; 2) evaluate the circularity of the dairy farm system using the resource tradeoffs of a closed-loop dairy system at farm scale for agricultural yield, environmental impacts, and costs.

Materials and methods

WEF nexus tradeoff analysis

The concept of Water-Energy-Food (WEF) Nexus describes a framework of resource modeling that considers the interactions and tradeoffs between sectors that normally operate in siloes (Mohtar and Daher, 2012). The concept is useful for achieving sustainable solutions to complex problems on local, regional, national, and international scales. The nexus perspective provides a platform for economic and policy decisions. Animal production systems are a nexus hotspot in Texas, for which the closed-loop system presents a holistic solution. A nexus hotspot is "a vulnerable sector or region at a defined scale, facing stresses in one or more of its resource systems due to resource allocation at odds with the interconnected nature of food, energy, and water resources" (Daher et al., 2018). As described above, dairy manure management exhibits an economic and environmental tradeoff from the waste disposal resulting from dairy operations and negatively impacts the region's environment. This externality of the dairy business is a cost of producing food for the market. Additional tradeoffs for dairy food production lie in energy consumption, both electricity and liquid fuel, to run the dairy.

Model development

The research was based at a study site of the Southwest Regional Dairy Center, Stephenville, Texas ("Dairy Center"), located in the Brazos River Basin (Figure 1). The Dairy Center has approximately 400 cows and generates approximately 3.2 tons of manure and 32,500 pounds of raw milk daily. Free stalls are flushed by water in rotation as the cows are moved to milking. Manure collects in a pit system, from which solid manure is scraped every other day. A screen at the end of the pit system filters larger particles from the liquid manure slurry, which then moves into the first lagoon. Half of the effluent from the second lagoon is returned to a water tank at the free stalls for flushing and the remaining half is used to irrigate nearby fields (see also Figure 4).

This operation is representative of many medium-sized dairies in central Texas with the potential for application of the closed-loop dairy system. Figure 2 illustrates from a system perspective, the closed-loop dairy system processes. Stages of focus are designated as inputs (yellow), system processes and stages, such as lagoons within the Dairy Center (blue), and outputs (green). System "flows" are designated by Nexus type: water, energy, food, manure, or slurry. The only system input is freshwater. Two outputs (feed and electricity) are "closed-loop" and reenter the system as inputs. Outputs include dairy products, human wastewater, runoff, and infiltration. Land application of manure and biochar are considered a closed-loop input to influence the feed.

Data collection

Liquid waste

Water quality is a main factor in identifying water reuse potential. Water samples were taken from the second wastewater treatment lagoon, the final point in the manure storage system (Figure 2; Table 1). To observe the effect of wastewater treatment as the manure effluent moves through the system, water samples were taken at pits, screen, and first wastewater treatment lagoon. To observe the effect of seasonal changes in climate on effluent water quality, samples were collected on three occasions from each location: May, June, and November 2017. Samples were tested for pH, oxygen demand (OD), nitrogen, phosphorus, ammonia, and bacteria. Five water samples of 500 ml each were drawn from radially equidistant locations around the edge of the lagoons. Five samples were taken from cascading wastewater directly from the screen, prior to flowing into lagoon 1. Five samples were collected from equidistant points throughout the pit system, starting just out of the free stalls and ending just before the solid mass of manure lying in front of the screen.

Solid waste: Manure as soil amendment

The Dairy Center provided detailed records of crops grown, lagoon water levels, effluent applications, and solid manure

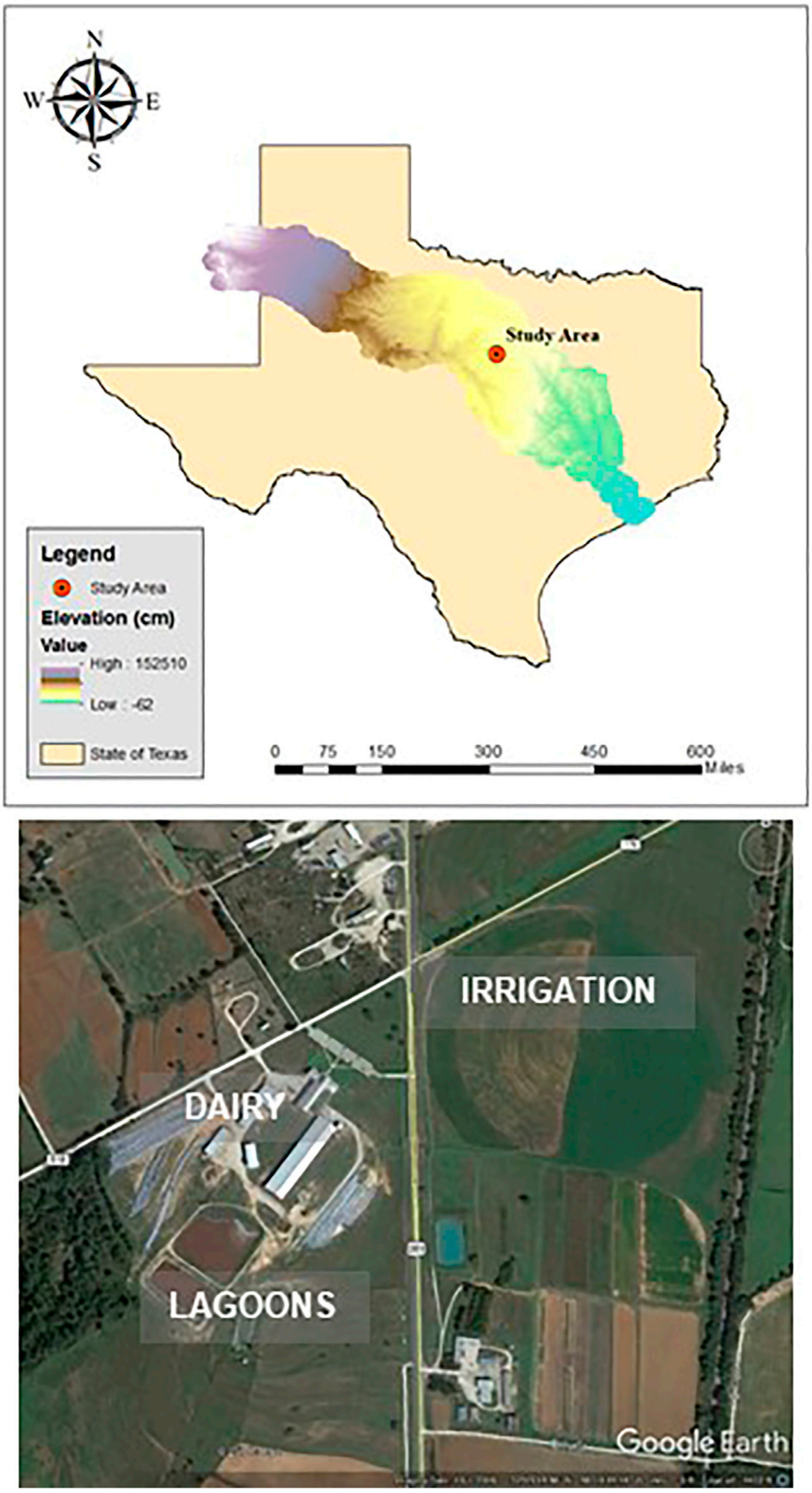

FIGURE 1
Study area: immediately north of Stephenville, Texas, in the Brazos River Basin.

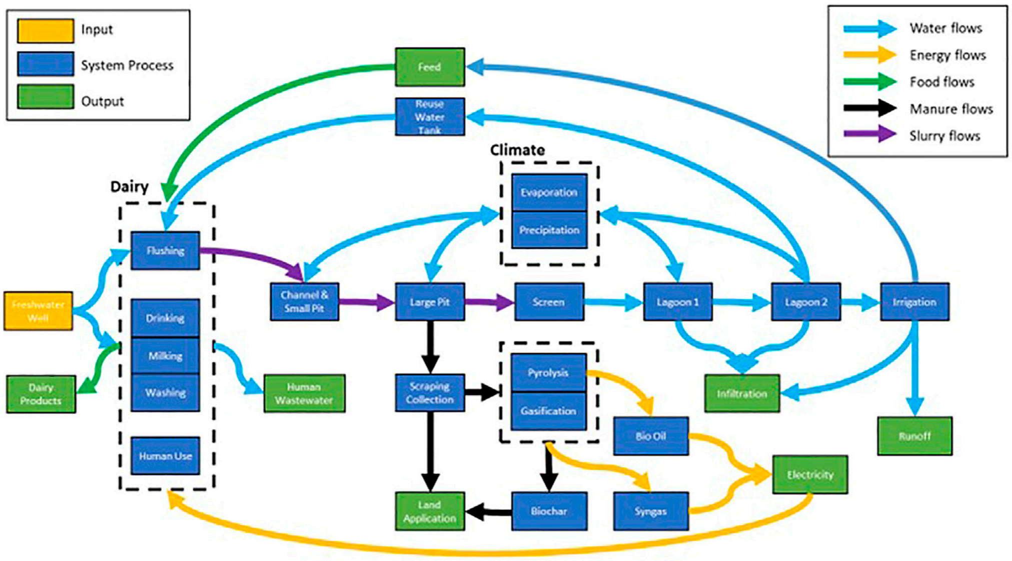

FIGURE 2
Nexus-based system schemata of the southwest regional dairy center.

TABLE 1 Water quality from the wastewater treatment lagoon.

Site	Date	pH	Oxygen demand (ppm)	Total nitrogen (ppm)	Total phosphorus (ppm)	Ammonia-nitrogen (ppm)	*E. coli* (MPN/ 100 ml)	Total coliform (MPN/ 100 ml)
Pit	May	—	—	849	154	—	—	—
	July	7.56	0.337	422	46.4	234	5.38E+07	8.80E+07
	November	7.17	—	444	39.6	299	-	-
Screen	July	6.57	0.365	478	85.0	248	6.30E+04	1.60E+05
	November	6.65	—	490	60.1	274	—	—
L1	May	-	—	622	77.1	—	—	—
	July	7.51	0.645	503	99.2	219	2.59E+07	5.12E+07
	November	7.24	—	1845	480	321	—	—
L2	May	-	—	858	56.8	-	—	—
	July	7.65	0.247	309	41.5	212	6.05E+05	1.35E+07
	November	7.44	—	337	39.4	223	—	—

applications. The Winter-2017 growing season database showed that most of the 24 fields grew different types of hay or forage, and the majority (six) grew coastal Bermuda grass, the crop selected for analysis in this study. Two fields, New Kirk East and New Kirk West, were selected to provide respectively, study application rates and intervals of effluent and manure (Figure 1). Based on records from September 2016 to July 2017, New Kirk East received effluent irrigation approximately every 3 days, with a standard deviation of 6 days. Application of manure effluent is irregular and based on the necessities of draining the lagoon and withholding irrigation due to rain. New Kirk East, approximately 85 acres, was irrigated an average of 0.37 inches per month with a standard deviation of 0.26 inches, minimum of 0.11 inches, and a maximum of 0.74 inches. Volume of effluent irrigation varies seasonally and is generally less in winter and more in summer. No supplemental freshwater irrigation is applied to New Kirk East. During the period September 2013 to August 2017, New Kirk West received solid manure application approximately every 7 days, with a standard deviation of 12 days (most of the data was from April 2016 to August 2017). According to Dairy Center records, the field received an average of 0.54 tons of manure per acre (on dry basis) with a standard deviation of 0.49 tons/acre (on dry basis). It is important to note the high deviation of values in both the application interval and rate. These amendments were applied based on farmer experience and daily climate conditions.

Solid waste: Manure as biomass energy source

Energy consumption is a major component of a dairy farm budget. The average monthly electricity use during the period June 2016 to June 2017 was provided by the Dairy Center. For this study, the amount did not include electricity for pumping water from a well reserved for the Dairy Center. Using the average local electricity rate ($0.113/kWh), the average monthly expense for the farm, and the potential savings from syngas electricity generation were calculated using local diesel prices from Stephenville in June 2020 ($1.80/gal) and potential savings from bio-oil production were estimated. The local operating costs for growing hay were obtained from Texas A&M AgriLife Extension (2018) District eight Crop and Livestock Budget Sheets, on a per-acre basis. The cost and income of milk production for the state of Texas in 2016 on a per-hundredweight (cwt) basis was taken from USDA ERS (2016). Overhead and fixed costs were ignored: while significant for a dairy farm budget, it is largely dependent on the financial conditions of the individual farm, including interest rates on loans. Focusing on the operating costs is sufficient to evaluate the closed-loop system for manure management and various outputs. The capital and operating cost of equipment needed for the closed-loop system biomass conversions were estimated from the literature.

According to Capareda (2013), the syngas yield from biochar is 2.11 m^3 per ton of manure input and its heating value is 4.19 MJ/m^3. Biochar yield from gasification was determined to be 15.0% by weight through pilot-scale research on dairy manure at Texas A&M. From pyrolysis, biochar yield was found to be 31.0% at a temperature of roughly 300°C (Cely et al., 2015). An average syngas yield of 17.6% by weight (standard deviation 5.65%) was assumed, based on literature review of a broad range of biomass (Cantrell et al., 2011; Capareda 2013; Crombie and Masek, 2014). The density of syngas (0.95 kg/m^3) was used to find the volumetric yield (Brar et al., 2013). Using the same literature as for syngas, yield of bio-oil from pyrolysis was determined to be 32.4% by weight from a broad range of biomass, with a standard deviation of 5.98%. Raw bio-oil quality as fuel is incompatible with conventional fuel because of its high oxygen content. To be used as biofuel, in place of diesel or gasoline, bio-oil must be deoxygenized and refined; many methods exist, including integrated catalytic pyrolysis, decoupled hydrotreating, zeolite vapor cracking, esterification, and gasification to syngas followed by refining (Bridgwater, 2012). Some of these processes result in a loss of yield: an upgrading efficiency of 80% was assumed for this study, based on Bridgwater (2012).

Nexus framework

Using the framework developed by Sadeghi et al., 2020b, a nexus-based tool was developed to capture the processes of the dairy farm system for purposes of the tradeoff analysis. Figure 3 portrays the tool framework and the specific calculations used. State independent variables are shown in yellow; system process calculations are in blue and using the calculation parameters listed in Table 2. Because crop yield data was unavailable, the Soil and Water Assessment Tool (SWAT) in ArcMap (ArcSWAT) was used to estimate yield and environmental impacts of the manure management (Texas A&M AgriLife Extension, 2018), as discussed below. SWAT uses water quality data to model effluent irrigation nutrient and water balance using climate and topographic data, generating estimates for both crop yield and environmental impacts. Processes performed using SWAT are shown in orange, and system outputs in green (Texas A&M AgriLife Extension, 2018). Figure 3 identifies the flows of water, energy, food, waste, and cash in the tool. The inputs were adjustable and used to create model scenarios. The tool is broken into two modules monthly: income and expenses. The income module has three submodules: crop yield, savings, and biomass conversions. The scenarios were created by adjusting the inputs and were evaluated in terms of relative financial and environmental impact.

Input and tradeoff analysis

Criteria for quantifying various levers, process parameters, and assumptions

The summary of process parameters is shown in Table 2. The input parameters include: 1) size of herd, 2) area farmed, 3) volume of effluent irrigation applied, and 4) the option of gasification or pyrolysis. Farm income is generated from crops grown on land that is irrigated with liquid manure effluent and with solid manure applied. According to the AgriLife budget sheets, a roll of hay is worth approximately $55. Fields can have some amount of biochar, produced by gasification or pyrolysis applied. Given 8.2 tons of manure produced daily by 400 cows, 0.62 tons per cow per month was used for the tool. The section on biomass conversions allows the user to choose between gasification and pyrolysis. For pyrolysis, the conditions of experimental research at Texas A&M AgriLife were used: temperature of 350°C and retention time of 3 h. The respective yield of syngas, bio-oil, and biochar factors were as discussed previously (Bridgwater, 2012). This pilot scale reactor was previously used at the Southwest Regional Dairy Center. The conditions of the Texas A&M Fluidized Bed Gasifier were assumed for gasification: the bed temperature was 762°C with an air flow of 0.42 m^3/min and fuel feed rate of 339 g/min (Capareda, 2013).

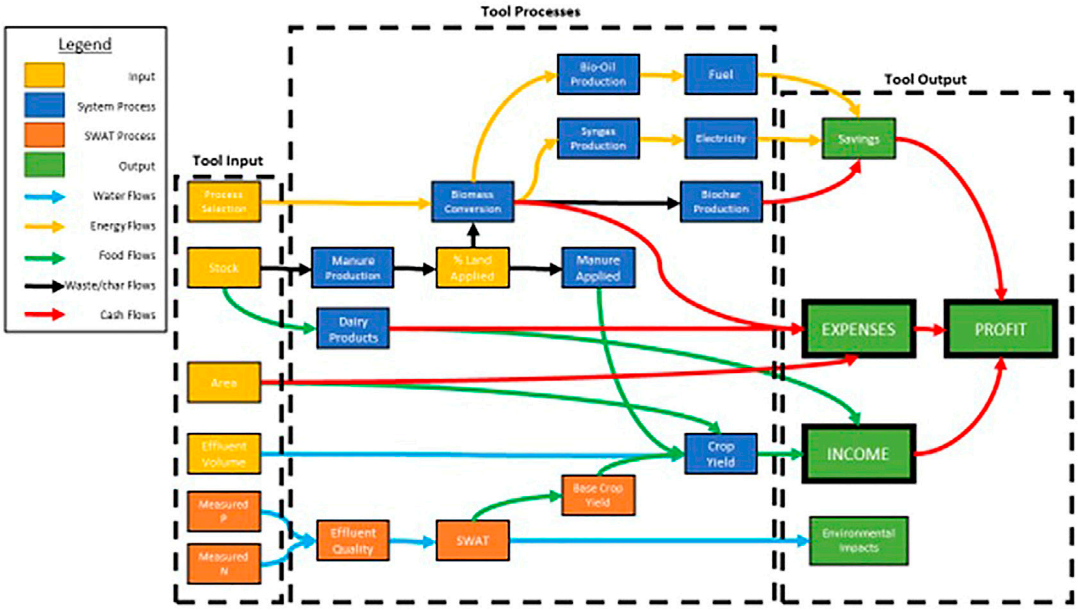

FIGURE 3
The nexus tool framework for Southwest Regional Dairy Farm. Inputs, resources flow and calculations, and outputs in the dairy system.

TABLE 2 Summary of process parameters.

Process	Parameter
Manure production	3.2 tons per 400 cows per day (0.15 ton/cow-month)
Raw milk yield	32,000 to 33,000 lbs per 400 cows per day (2,472 lbs/cow-month)
Hay value	$55 per roll, assuming half ton rolls ($110/ton-month)
Syngas yield (gasification)	2.11 m^3 per kg manure (1,914 m^3/ton-month)
Syngas yield (pyrolysis)	17.6% by weight
Syngas specific volume	0.95 m^3/kg (955 m^3/ton-month)
Syngas heating value	4.19 MJ/m^3
Bio-oil yield	32.4% by weight
Bio-oil specific volume	1,200 kg/m^3 (0.76 m^3/ton-month)
Bio-oil heating value	17 MJ/kg
Biochar yield (gasification)	15% by weight
Biochar yield (pyrolysis)	31% by weight
Value of electricity	$0.80/kWh local rate
Value of diesel	$2.60/gal local rate
Value of Biochar	$400/ton
Cost of growing hay	$14.98/ac from selected operating costs
Cost of producing dairy	$15.09/cwt from selected operating costs
Cost of biomass conversions	$10.97/ton manure processed

To determine the amount of electricity produced for the farm, an electricity conversion efficiency of 30% was estimated per Capareda (2013). The outputs of the biomass conversions submodule include electricity, fuel, and biochar production. If the user selects pyrolysis, bio-oil will also be produced. A similar process is used to estimate the savings of bio-oil refined for fuel use (Eq. 3). Calculation of manure input to biomass conversions uses Eq. 1:

$$M = N * MP * (1 - PM) \tag{1}$$

Where, M = manure input to biomass conversions (tons)

N = number of cows.

MP = manure production (ton/cow).

PM = percent of produced manure for land application (%)

Syngas can save considerable electricity consumed, the expected saving in electricity can be calculated such that:

$$ES_S = M * Y_S * HV_S * \eta_E * C_1 * EV \tag{2}$$

Where, ES_S = electricity savings from syngas ($)

Y_S = syngas yield from gasification or pyrolysis (m^3/ton).

HV_S = syngas heating value (MJ/m^3).

η_E = electricity conversion efficiency (%).

C_1 = unit conversion (0.28 kW h/MJ).

EV = electricity value ($/kWh).

Bio-oil can replace fossil fuel used in the dairy farm; the savings in fossil fuel consumption is calculated as follows:

$$FS = M * Y_{BO} * \nu_{BO} * \eta_U * C_2 \tag{3}$$

Where, FS = fuel savings ($)

Y_{BO} = bio-oil yield from pyrolysis (%).

ν_{BO} = specific volume of bio-oil (m^3/ton).

η_U = upgrade efficiency (%).

C_2 = unit conversion (264.2 gal/m^3).

Bio-oil can substitute for fuel oil in static application, including electricity generating turbines (Bridgwater, 2012). Thus, an additional user option was included to burn bio-oil for electricity instead of upgrading for biofuel. The heating value of 17 MJ/kg and the same electricity conversion efficiency as syngas were used. Notably in this study, using bio-oil produced from pyrolysis for electricity generation was always more profitable than fuel (Eq. 4).

$$ES_{BO} = M * Y_{BO} * HV_{BO} * \eta_E * C_3 * EV \tag{4}$$

Where, ES_{BO} = electricity savings from bio-oil ($)

HV_{BO} = heating value of bio-oil (MJ/kg).

C_3 = unit conversion (907.2 kg/ton).

Financial process parameters and assumptions

The module on expenses comprises dairy, hay, and biomass conversions per-unit costs. The budget sheet for dairy production was obtained from the USDA ERS (2016) and is specific to the state of Texas. From 2016, the operating costs per hundredweight included in this study were purchased feed ($10.94/cwt), labor ($2.44/cwt), and miscellaneous operating costs ($1.71/cwt) for a total of $15.09/cwt. The hay operation costs, specific to the 22-county District eight from Texas A&M AgriLife, were on a yearly basis and converted to a monthly average. The operating costs for the hay operation used for this study include insecticide ($0.56/ac), machinery labor ($1.19/ac), machinery repairs ($0.55/ac), and miscellaneous operating costs [cut and bale ($11.67/ac)] for a total of $13.97 per acre.

In this tool, the operating and maintenance (O&M) costs of Gasification and Pyrolysis facilities were included in the monthly estimate of expense. The drying and processing of dairy manure is approximately $10.71 per wet ton. In general, pyrolysis facilities require approximately 75% the O&M cost of Gasification (Thomas, 2018); therefore, the O&M cost of Pyrolysis was estimated as $8.03 per wet ton.

Environmental impact and crop production calculation: SWAT

The Soil and Water Assessment Tool (SWAT) was used to estimate crop production and environmental impact at the farm. SWAT is a physical, watershed-scale model that functions as an extension in ArcGIS; it quantifies the impact of land management in complex watersheds of various soil, land use, and management. The model delineates watersheds and streams based on topographic data and a defined outlet. SWAT uses meteorological data, (precipitation, temperature, and humidity) to perform complex hydrologic calculations to aggregate overland flow and subsurface flow from sub-basins to compute streamflow routing and discharge. This includes water balance factors, evaporation, and infiltration, determined from soils data based on permeability.

To simulate the effect of manure application in the watershed, input tables were adjusted in ArcSWAT. The digital elevation model (DEM) was obtained from the National Hydrography Dataset (NHD), version 2. The USGS gauging station (08094800) located at Hico, Texas was used to calibrate the model based on daily streamflow. The model ran from 15 April 2013 to 31 December 2017. Using this time frame, 2013 was used as model warmup, 2014–2015 for calibration, and 2016–2017 for validation. The DEM, National Land Cover Dataset (2011), and ArcSWAT STATSGO were used to delineate the model watershed and hydrologic response units. Daily precipitation and temperature data from the National Oceanic and Atmospheric Administration (NOAA) National Center for Environmental Information used by SWAT. Precipitation data was obtained from two weather stations in Stephenville, Texas, and temperature data was obtained from a combination of weather stations in Stephenville and at Proctor Reservoir, Texas.

To simulate the manure management practices in the area, the Management Input Files were adjusted in SWAT. For this stage of modeling, the study watershed was further refined to the bounds of Sub-basin 6 (Figure 4), which contains the Dairy Center and adjacent fields where manure and effluent are applied. For this watershed, a specific set of management operation parameters were imposed on all land use defined as row crop, hay, or range. The following operations were used to simulate the manure management system of the Dairy Center: Auto Irrigation, Continuous Fertilizer, Planting, and Harvest

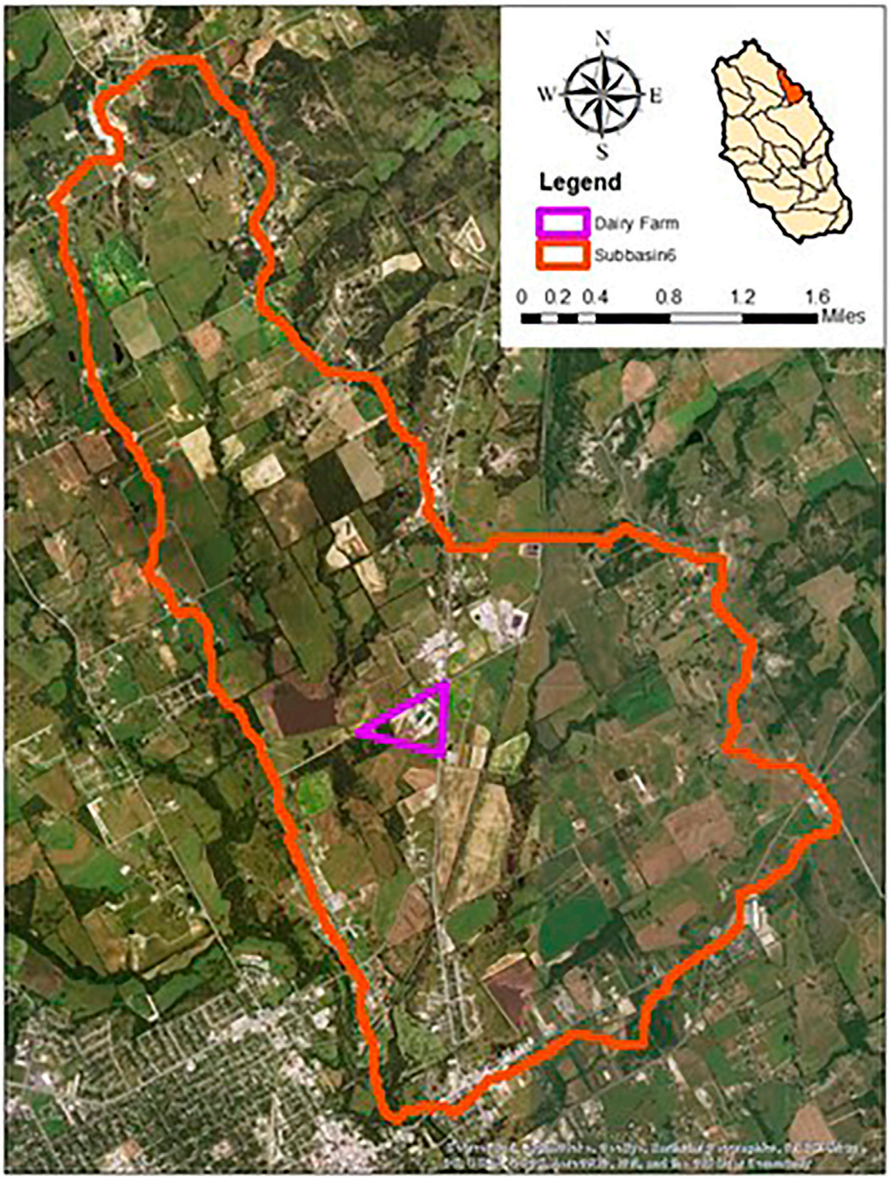

FIGURE 4
Location and satellite view of Subbasin 6, used in SWAT mode: the watershed was created by SWAT based on topography. It lies north of Stephenville and drains into the North Bosque River.

Only. The fertilizer database and general management parameters were manually edited.

A new Fertilizer type was added to the database to represent the lagoon effluent. For this, the fraction of mineral N, mineral P, organic N, and organic P was entered manually based on the measured water quality data. In addition, the fraction of mineral N applied as ammonia was entered. Because there was no distinction between mineral and organic nutrients in the lab results of water quality samples in this study, the same ratios of the dairy manure fertilizer type in SWAT were used to separate the total N and total P into mineral and organic partitions (Table 3).

The model was run following rewriting of the Management and Fertilizer input files with the edited Management parameters. The Reach output file (.rch) holds the simulated stream flow for the watershed. This dataset was compared to the observed data from the same time frame as discussed previously. The Nash-Sutcliffe Efficiency (NSE) was used to evaluate the model variance (Moriasi et al., 2007) and the NSE calculation is shown in Eq. 5. The objective of SWAT is to determine the

TABLE 3 Dairy effluent fertilizer input data for SWAT.

Parameter	Value
Total N observed	0.0590%
FMINN simulated	0.0120%
FORGN simulated	0.0480%
Total P observed	0.0040%
FMINP simulated	0.0025%
FORGP simulated	0.0015%
FNH3N simulated	0.9900%
BACTPDB simulated	6050 CFU/g fertilizer

environmental impacts of manure application in this watershed, thus calibrations were based on watershed scale and then used in the Excel tool.

$$NSE = 1 - \left[\frac{\sum_{i=1}^{n}\left(Y_i^{obs} - Y_i^{sim}\right)^2}{\sum_{i=1}^{n}\left(Y_i^{obs} - Y^{mean}\right)^2}\right] \tag{5}$$

Where, Y_i^{obs} = *i*th observation of streamflow

Y_i^{sim} = *i*th simulated value of streamflow.

Y^{mean} = mean of observed streamflow.

n = total number of observations.

To obtain an NSE greater than 0.5, the SWAT Calibration and Uncertainty Programs package (SWAT CUP) was used to link SWAT input and output files, input observed flow data, and specify parameters to iteratively change and evaluate calibration statistics. The program SUFI2 (Sequential Uncertainty Fitting) was used to alter 8 parameters within a relative range of ±30% over 500 iterations (Table 4).

To complete the calibration, the model was manually calibrated by further reducing CN2 by 10%, reducing ESCO by 20%, and increasing SOL_AWC by 10%, and increasing GWQMN (the threshold depth of water in the shallow aquifer required to return flow to occur) by 20%, the calibration obtained an NSE of 0.81. With streamflow calibrated, the SWAT model hydrology is expected to be reliable. For this study, this was deemed acceptable to use the resulting estimate of crop yield and environmental impacts.

The results of SWAT were observed from the Management (.mgt) and Water Quality (.wql) output files. The crop yield was evaluated for Subbasin six only, where Management operations were changed from the default. The average crop yield was found from each HRU, which occurred once each year with the Harvest Only operation, for 2014–2017 (ignoring the warmup period). According to SWAT, the average annual crop yield was 18.9 tons/acre (42,336 kg/ha) with a standard deviation of 2.25 tons/acre (5,053 kg/ha). To match the period of the Excel-based tool, the yield was converted to a monthly basis. It is important to note that the income modeled by the tool is not uniform by month: both income and expenses of a dairy and/or hay farming operation are concentrated and seasonal throughout the year and vary from farm to farm. The monthly estimate for crop yield was calculated at 1.57 tons per acre per month.

Based on SWAT simulations with different quantities of continuous fertilizer applied the yield was approximated as directly proportional to the amount of effluent irrigation applied. In the Excel-based tool developed for our study, a modified yield per acre is calculated as a function of the effluent irrigation and biochar applied. Based on two studies, biochar was found to increase biomass yield by 23, 8, 150, and 98 percent when 10, 10, 15, and 20 metric tons/ha were applied, respectively (Baronti et al., 2010; Uzoma et al., 2011). The average percent increase and average application rate, 70% and 13.75 metric tons/ha, were used as a ratio to alter the modified yield (Eq. 6).

$$Y_m = \frac{Y_b * EI}{EI_b} * \left(\frac{0.7 * B}{13.75 * A} + 1\right) \tag{6}$$

Where, Y_m = modified yield per acre (ton/ac)

Y_b = base hay yield per acre (1.57 ton/ac).

EI = effluent irrigation (gal).

EI_b = base effluent irrigation (1027740 gal).

B = biochar produced (metric tons).

A = area farmed (ha).

TABLE 4 SWAT CUP results, reflecting manually adjusted SWAT model parameters.

Parameter	Percent change (%)	Description
CN2	−14.79	Initial SCS runoff curve number for moisture condition 2
ALPHA_BF	14.85	Baseflow alpha factor
ESCO	−29.91	Soil evaporation compensation factor
SOL_AWC	26.67	Available water capacity of the soil layer
GW_REVAP	−22.83	Groundwater “revap” coefficient”
GW_DELAY	20.01	Groundwater delay time
SOL_K	−17.55	Saturated hydraulic conductivity
SURLAG	−24.87	Surface runoff lag coefficient

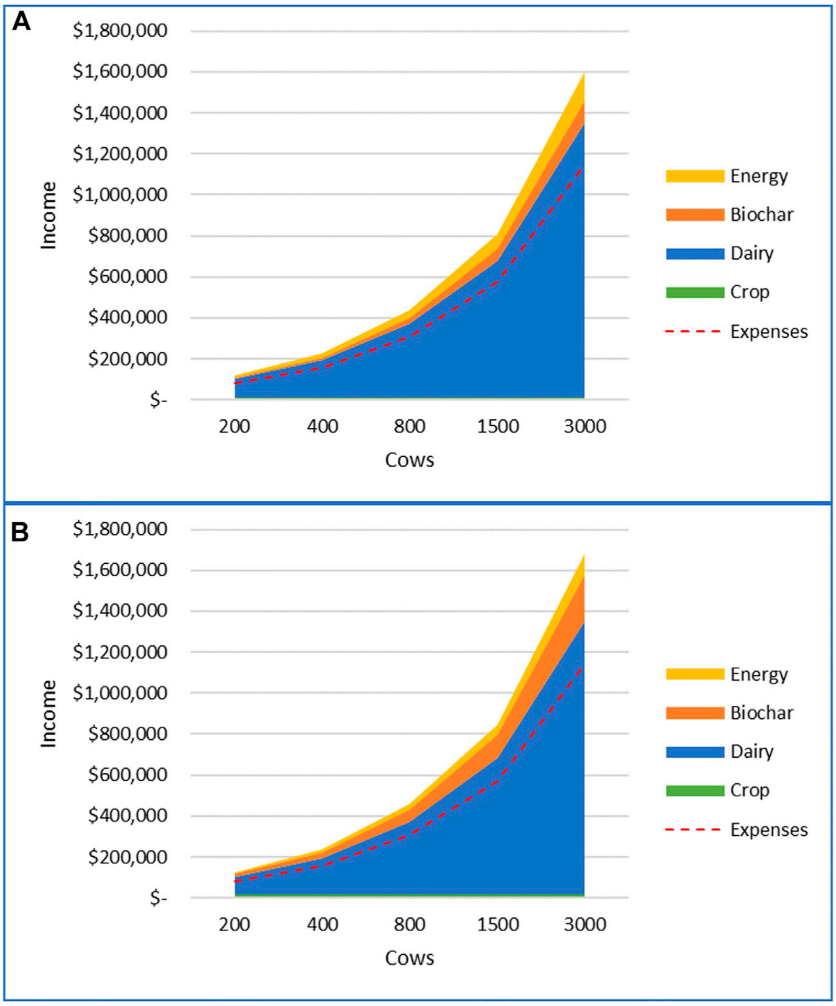

FIGURE 5
Components of monthly income using gasification **(A)** and pyrolysis **(B)**.

Several water quality parameters were tracked from SWAT output, including organic N, ammonia, nitrite, nitrate, organic P, soluble mineral P, and CBOD. These results were also evaluated for Subbasin six and analyzed as an average of 1,722 daily concentrations from 2014–2017. Comparing results with and without effluent and manure application, the model suggests that the watershed nitrate loading to surface water was approximately 149 lbs/acre, as a monthly average for the year. Furthermore, the model suggests that the watershed nitrate loading to groundwater was approximately 33 lbs/acre and the soluble phosphorus loading to surface water was approximately 173 lbs/acre as a monthly average for the year. For both nitrate and phosphorus, the nutrient loading peaks in May, then gradually falls until negligible in the winter (January through March). From Dairy Center records, the monthly volume of effluent applied is approximately 3.15 ac-ft, and 2.85 ac-ft based on individual application volume as employed in SWAT.

Assumptions used in the model include the following: all manure, effluent, and biochar are evenly applied to farmed acres; SWAT input files (including DEM, soils, and land use) are accurate and up to date; SWAT produced reliable results for crop yield and water quality by calibrating the North Bosque River watershed streamflow at the Hico USGS; the SWAT HRU definition provided sufficient hydrologic resolution for the model; hay was grown from 2013 to 2017 on all land designated by the NLCD as row crop, hay, or range within Subbasin six and that within Subbasin 6, all land designated by the NLCD as row crop, hay, or range had the same management schedule and continuously applied a consistent amount of solid manure and lagoon effluent every 8 and 4 days respectively. It was

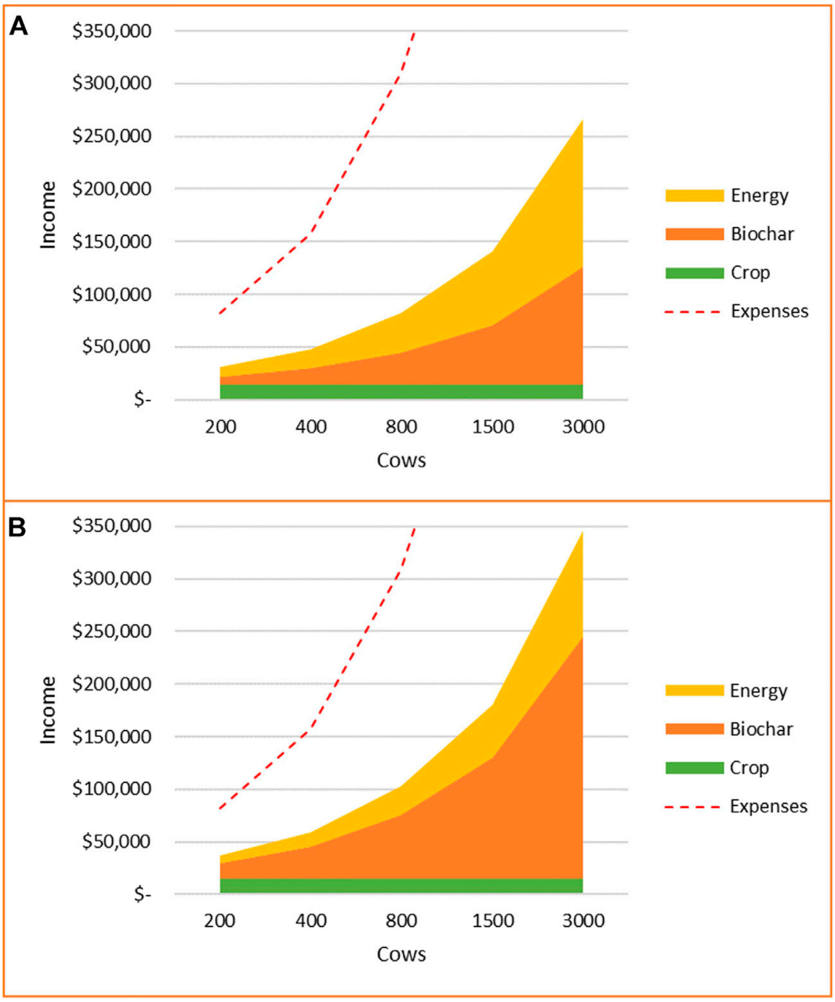

FIGURE 6
Components of Monthly Income [dairy omitted] Using Gasification **(A)** and Pyrolysis **(B)**.

further assumed that farmers did not practice contour farming; all effluent had the same water quality as measured from Lagoon two at the Dairy Center, and supply was never limited. SWAT default values for dairy manure were assumed to be the same as effluent water quality mineral and organic partitions; salinity, sodicity, pH, and organic matter were not considered. To prevent crop water stress falling below 90% in Subbasin 6, a constant volume of irrigation was occasionally applied. Irrigation efficiency was 75%, irrigation surface runoff ratio was 0.25. The harvest index override was 0.9 and hay was harvested once per year. Lastly, it was assumed that modifying the average monthly effluent irrigation volume uniformly modified the individual application volumes with the same interval; thus, the ratio between fertilizer by mass and yield by mass was used to modify estimated crop yield.

Results and discussion

Nexus tool results and evaluation

Each of the scenario levers was first altered individually around a baseline. Two biomass conversions settings were used: gasification or pyrolysis with bio-oil used for electricity. It was found that pyrolysis with bio-oil used for fuel was consistently less profitable than production of electricity, based on the offset cost of regular diesel fuel. In total, 43 scenarios were evaluated. For both gasification and pyrolysis, combinations of four levers (size of herd, acres farmed, volume of effluent irrigation, and milk price) were observed.

The financial success of the operation is a prerequisite and will be the main driver to its application. Figure 5 displays the monthly income components of a dairy with various herd size,

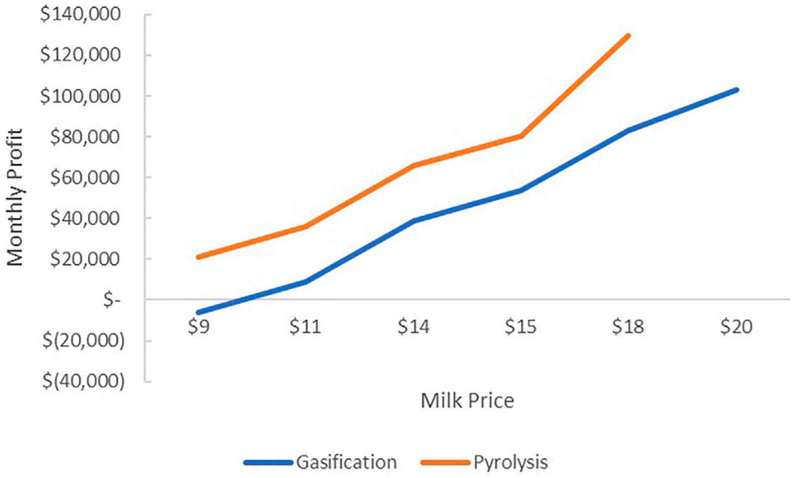

FIGURE 7
Monthly Income at varied milk price using Gasification and Pyrolysis.

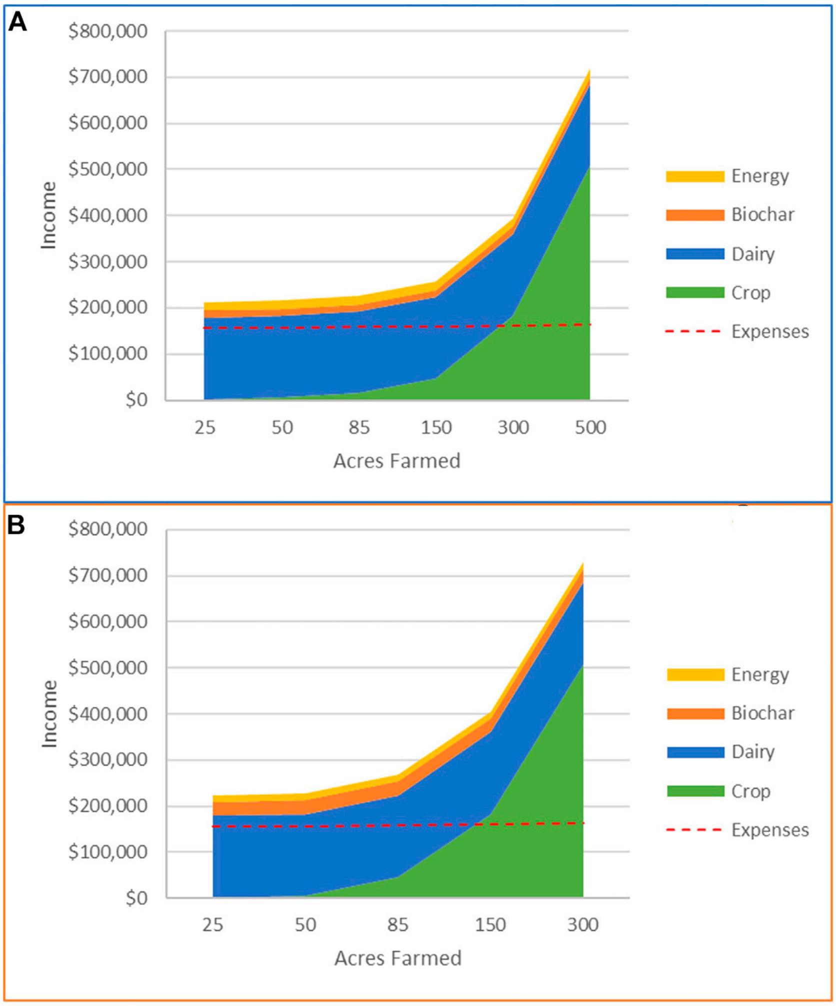

FIGURE 8
Components of Monthly Income Using Gasification, **(A)** and Pyrolysis **(B)** acres varied.

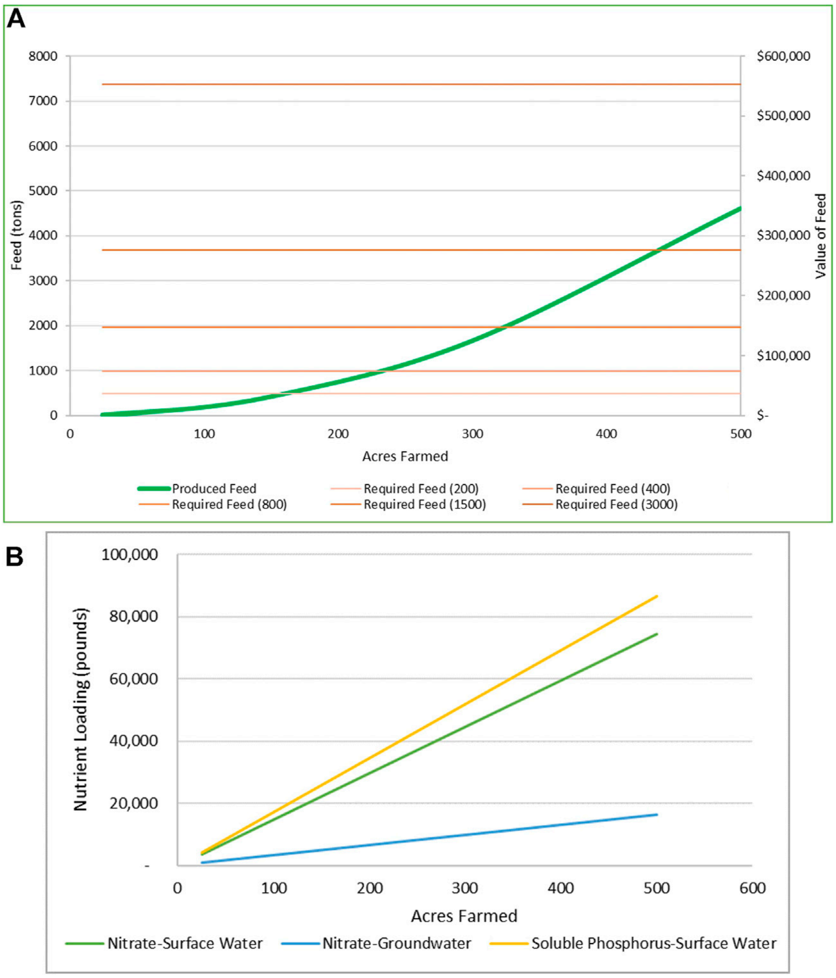

FIGURE 9
Thresholds of feed required **(A)** and nutrient loading **(B)** for dairy sizes and produced feed at various acres farmed.

overlaid by the expenses for gasification (a) and pyrolysis (b). Figure 6 displays the same data and format for gasification (a) and pyrolysis (b), omitting dairy yield to better observe the income components of energy production, crop yield, and biochar production. The expense data in Figure 6 is for the complete operation, including dairy production (as Figure 5). These data are based on a constant 85 acres farmed and 0.37 inches of effluent applied per month, both representative of the Dairy Center.

Not surprisingly, dairy production remains the dominant source of income for the farm, an average of 70 percent in these modeled scenarios. This is very sensitive to milk price, known to be volatile. Figure 7 displays the overall monthly profit for a small 400 cow dairy, such as the Dairy Center, using gasification and pyrolysis. Even with biomass conversion facilities to generate additional income, the dairy can become unprofitable if milk prices fall through the floor.

In Figures 5–7 the number of acres farmed, and the effluent applied is set at the Dairy Center values to observe the relative income components of a dairy using manure gasification or pyrolysis. Many dairies farm much more land to supplement feed while disposing of manure effluent as irrigation. In Figure 8, the income components of various acreage are displayed. Crop yield greater than what is needed for the dairy herd is sold and further increases the income. Figure 9 displays five feed thresholds in both tons and dollars and illustrates the farmed acres required to produce enough feed for various sizes of dairies (a). The outcomes of SWAT gave various constituents based on the modeled watershed. The Dairy Center fields were modeled with management practices based on continuous application of manure effluent at a rate consistent with Dairy Center records. Nutrient loading rates were determined based on the 85-acre New Kirk East field and linearly extrapolated.

Figure 9 also displays the level of nutrient loading at various acres farmed (b).

Assessment of tradeoffs among scenarios

The ten scenarios in Figures 5, 6 are all profitable as shown. While gasification can produce more (29%) energy than pyrolysis, and pyrolysis can produce more (52%) biochar. Across 21 comparative scenarios, pyrolysis generated averages of 4 percent more income and 31 percent more profit than gasification, due mainly to the greater production and value of biochar. Pyrolysis could be especially successful in periods of low milk prices. In these scenarios, income from biochar represents between 15 and 20 percent of the total income. Pyrolysis was between 40 and 128 percent more profitable than gasification (see Figure 7).

In Figures 5, 6, scenarios are represented in which the existing Dairy Center substantially increased the size of herd within the existing facilities (acres farmed, effluent applied, lagoon storage, and capacity of milk barn and free stalls). Substantial investment would be required to scale up to the herd sizes displayed, and additional effluent irrigation (whether from owned or neighboring fields) would be inevitable. To that point, one omission of this work is the increased manure effluent produced from a larger herd due to increased flushing of free stalls. This in turn would change the lagoon water balance and likely require construction of greater lagoon storage. While the increased effluent production would not necessitate the Dairy Center to farm more land, it would still need to be land applied very locally, or in significant excess. In addition, a great increase in demand for freshwater could cause the dairy to pump more groundwater, thus contributing to a regional water supply impact and increasing the dairy's electricity bill.

At the Dairy Center, solid manure is flushed from free stalls through the pit system, screened, and enters the lagoons. For this tool, all manure is considered consumed for biomass conversions. However, a portion of manure must be carried, either dissolved or in suspension, through the screen and into the lagoons where it becomes a slurry or effluent. Thus, there is an omission in the quantity of manure available for biomass conversions. Overall, possible profits from pyrolysis and gasification at dairy farms will be strongly dependent on the cost of electricity, market price of biochar, and size of dairy herds. Additionally, the environmental benefits of pyrolysis and gasification of dairy manure could also be assessed, including greenhouse gas emission, and the pollution of water and soil from land application of manure. The outcomes from this study suggest that pyrolysis and gasification of dairy manure would be viable processes to enhance environmental and agricultural sustainability at dairy farms.

Conclusion

The closed-loop dairy system is shown to be profitable, in most cases, using gasification or pyrolysis. While all dairies are sensitive to milk price, pyrolysis provides a promising buffer that could be especially useful for small dairies, such as the Dairy Center. This work is based on the struggle to survive under increasing environmental regulation and industry pressure.

In all cases, the value of electricity generated from gasification exceeded that of pyrolysis. Using bio-oil produced from pyrolysis for fuel production was not worthwhile compared to its use for electricity generation. Furthermore, upgrading the bio-oil for use as fuel would increase the capital cost and reduce yield. This study indicated that increasing size of herd, acres, or effluent irrigation will almost always increase profit, while having a clear tradeoff with environmental quality due to high nutrient loading.

To determine recommendations based on this study, it is necessary to evaluate the capital cost of biomass conversions. Capital cost was not considered in this work and will vary based on location and size of dairy. Some industry estimates suggest the cost could be minimal (around $100,000); other estimates suggest a cost several times larger. In addition to capital cost, several expense parameters, e.g., cost of feed, operating cost of biomass conversions, could vary on a case-by-case basis.

This study could be improved by considering a few dimensions. Environmental impact, an extensively complicated area, is herein extrapolated one-dimensionally, although derived using a robust, physically based model. The assessment would be made more accurate by integrating data linking the effluent irrigation to the nutrient loading at local scale with vadose zone analysis.

In this study, all biochar was considered sold (none applied to the Dairy Center acres farmed). The benefits of biochar in reducing nutrient leaching, erosion, and runoff, are discussed but not accounted for in this analysis. It is suggested that biochar may mitigate emissions, to the benefit of air quality, and improve soil nutrient and water retention. The environmental impacts could be made more robust with literature-based estimates these suggestions.

The nexus tradeoff analysis tool could also include estimation of the financial impact of environmental fines to the farm. These are administered by the Texas Commission on Environmental Quality (TCEQ) and, according to the Dairy Center, vary greatly depending on circumstances, and could be related to manure input or monitored nutrient output. Regardless, it is of interest to estimate the environmental impact in terms of nutrient load added.

The capital cost of the gasification and pyrolysis, i.e., the cost of the furnace and the heat recovery units, were not included. The operating costs, particularly energy consumption, of pyrolysis would be lower than that of gasification because of target temperature. The continuous reactors in both processes need only very short residence time (batch process needs much longer time).

We believe this study is useful to small dairy systems as it describes how these farms can transform into circular production system with lower water and energy footprint while maintaining profitability. The study is limited with several assumptions that can be considered for future studies.

Data availability statement

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

Author contributions

JM—Conceptualization, Methodology, Evaluation, Validation, Formal Analysis, Investigation, Data Curation, Writing the original draft and Review and Editing, Visualization RM—Conceptualization, Methodology, Evaluation, Validation, Resources, Data Curation, Writing, Review and Editing, Supervision, Project Administration, Funding Acquisition EK—Methodology, Evaluation, Validation, Resources, Data Curation, Writing, Review and Editing AA—Methodology, Evaluation, Validation, Data Curation, Writing, Reviewing, Editing VP—Evaluation, Validation, Data Curation, Writing, Reviewing, Editing.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

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GAN-based semi-automated augmentation online tool for agricultural pest detection: A case study on whiteflies

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Deep neural networks can be used to diagnose and detect plant diseases, helping to avoid the plant health-related crop production losses ranging from 20 to 50% annually. However, the data collection and annotation required to achieve high accuracies can be expensive and sometimes very difficult to obtain in specific use-cases. To this end, this work proposes a synthetic data generation pipeline based on generative adversarial networks (GANs), allowing users to artificially generate images to augment their small datasets through its web interface. The image-generation pipeline is tested on a home-collected dataset of whitefly pests, *Bemisia tabaci*, on different crop types. The data augmentation is shown to improve the performance of lightweight object detection models when the dataset size is increased from 140 to 560 images, seeing a jump in recall at 0.50 IoU from 54.4 to 93.2%, and an increase in the average IoU from 34.6 to 70.9%, without the use of GANs. When GANs are used to increase the number of source object masks and further diversify the dataset, there is an additional 1.4 and 2.6% increase in recall and average IoU, respectively. The authenticity of the generated data is also validated by human reviewers, who reviewed the GANs generated data and scored an average of 56% in distinguishing fake from real insects for low-resolutions sets, and 67% for high-resolution sets.

KEYWORDS

GAN, data augmentation, pest detection, whiteflies, smart agriculture

1. Introduction

Agriculture has been a central pillar in the development of humankind in the past and remains a vital driver for local and global economies. Currently, agriculture faces growing pressures with the increasing global population, which is expected to reach over 9 billion by 2050 (Leridon, 2020). With the limited availability of land resources, food security becomes a major issue. On top of that, crop production is severely handicapped by pests and diseases, reducing production by 20–50% annually, with economic losses of up 70 billion US dollars (FAO, 2019). The situation is even more dire in developing countries, where small family farms are responsible for more than 80% of agricultural production (Harvey et al., 2014). These farms often lack the expertise and technology to fight pests and diseases as effectively as industrial farms, and their losses due to these factors can surpass 50% (United Nations Environmental Programme, 2013).

The recent developments in the field of machine learning can help improve the diagnosis of plant pests and diseases through traditional visual assessment methods. Convolutional Neural Networks (CNN) have achieved superior performance in image classification and object detection tasks (Liu et al., 2022). Hughes and Salathe (2015) used the PlantVillage dataset to train a GoogLeNet convolutional network achieving a 99.34% accuracy by using transfer learning from a model pre-trained on the ImageNet dataset (Mohanty et al., 2016). Despite the high accuracy, there are no further experiments to prove the effectiveness of such classification models out in the field, due to the plant leaf images being taken in a controlled lab setting. Türkoğlu and Hanbay (2019) achieve an accuracy of 97.86% using a ResNet50 CNN and an SVM classifier, compared to only 70.90% for their best shallow-feature model, justifying the need for deep feature extractors.

In more difficult object detection tasks, Gutierrez et al. (2019) benchmark different feature extractors and detector architectures using scouting robots, to detect two tomato whitefly species in their egg and adult insect stages (four classes in total), in 54,743 images. Their RCNN model can detect the two insect stages with a 53% accuracy, but performs poorly on egg stages, with an accuracy of around 8%. Another similar study (Fuentes et al., 2017) benchmarks different architectures and feature extractors on a dataset of tomato plants, examining nine different classes of pests and diseases. Their dataset contains 5,000 images and more than 43,000 labeled objects. They compare the performance of Faster R-CNN with different feature extractors (VGG and ResNet) to that of SSD-ResNet and R-FCN-ResNet. The R-FCN-ResNet50 model achieves the highest accuracy with 86% mAP, and notably, an AP of 0.94 on the whitefly class, albeit on only 49 images with 404 insects. Selvaraj et al. (2019) use similar architectures to perform disease detection on banana crops, creating robust models with 18 disease classes in 18,000 field-captured images.

Object detection tasks are more difficult to solve, require higher computation loads, and need fine-grained annotations which are more expensive to obtain on specialized datasets. While computing power at the edge increases, the ever-present need for large amounts of data continues to be an obstacle to the development of high-performance models. Deep neural networks need a lot of data to achieve accuracy and robustness, but this comes at the cost of more computing resources spent on training (Rizk et al., 2019), and more human resources spent on data collection and labeling. Generative Adversarial Networks (GANs) have been used to help mitigate this problem of data hunger in recent years through synthetic data generation, but they come with their own sets of challenges such as the computing power needed to generate high-resolution images and the difficulty of generating fine-features at low-resolution. The medical field has made use of these architectures to overcome the data scarcity problem: Motamed et al. (2021) leverage GANs to generate synthetic data, boosting the performance of pneumonia and COVID-19 in X-rays, especially when compared to traditional augmentation techniques, such as zooming and rotating. These methods are also leveraged in the agricultural field, where Bi and Hu (2020) use a Wasserstein generative adversarial network with gradient penalty to avoid overfitting on a limited dataset, and it is shown to improve plant disease classification by around 24%.

To this end, this work proposes the use of a novel, GAN-based pseudo-automated pipeline for data augmentation, thereby leveraging synthetic data generation in order to increase dataset sizes, decrease data collection, and improve the performance of lightweight CNNs for detecting and counting large numbers of small pests on plant leaves.

This project combines the two tasks of (1) progressively building a dataset and (2) building a learning model for multiple objects types which are very small and very numerous in each image. This is what mainly sets this work apart from others. In Ramcharan et al. (2019), and most other works that target disease detection, the objects are disease symptoms which are large and less numerous in each image, making the task relatively easy. Researchers in Gutierrez et al. (2019) obtain good results on the disease-objects in their dataset, and on the single pest-object, whiteflies. However, this performance might be unreliable due to the overfitting on the small dataset of 49 images and 404 whiteflies. Our work separates itself by taking on the challenging task of detecting small objects in large numbers, and overcomes the overfitting and under-performance problems faced by limited datasets through synthetic data generation, and the hybrid use of GANs in combination with human labeling and expertise to produce authentic images. The work also uses data collected out in the field instead of a controlled lab setting, which should make the models more robust and more-readily deployable in real-world applications. Our work culminated in building an open-access tool that researchers in the field can adopt for developing their machine learning models for pest detection using a minimal set of real images.

The proposed novel augmentation pipeline is shown to improve the recall of a YOLO-based object detector for a pest-counting task by more than 38% points, by increasing a small dataset size four-fold. The data generation interface is flexible and applicable to a wide array of object detection tasks, especially improving performance when dealing with small dataset sizes. It allows users to generate synthetic data from existing images and objects, and is validated by a thorough human assessment of the authenticity of the generated data.

This novel image generation tool, which is publicly available at: https://github.com/ChristopheKar/cpb-gen, can then be used to augment small datasets, which can then be used to train accurate yet lightweight object detection models. Its annotation and generation interface is shown in Figure 1. The datasets and models can be developed, trained, and deployed by low-resource individuals on low-resource devices for a myriad of object detection tasks, and more specifically, to detect pests on plant leaves. Early and accurate detection of plant pests will allow both small and large-scale farmers to timely treat the plants, improving crop yield and production.

2. Methodology

This section will breakdown the different parts of the augmentation pipeline, from the datasets used to the different networks for image generation and object detection.

2.1. Dataset

The dataset is collected from the American University of Beirut's greenhouses, from multiple locations. The images are taken in the field so that the background and lighting variations correspond to real-world conditions, contributing to the robustness of the application. The images are captured using cell-phone cameras at different scales. The dataset contains the whitefly species *Bemicia tabaci* on five different crops: tomato, eggplant, pepper, beans, and cucumber. The dataset contains a total of 770 images with around 3,400 labeled whitefly objects. A training set of size $D_{\text{base-train}} = 560$ is chosen as the base dataset for the work, containing 2,520 whiteflies, along with a validation set $D_{\text{base-valid}} = 70$ and a test set $D_{\text{base-test}} = 140$. The validation and testing sets are fixed throughout all experiments, whereas the training set size varies to showcase the effect of data generation and augmentation.

The main task is counting the number of adult *B. tabaci* whiteflies on plant leaves. The *B. tabaci* whitefly is considered the second most widespread and economically-damaging arthropod pests, attacking an estimated range of 36 plant genera throughout 156 countries (Willis, 2017), notably affecting tomato and cotton crops, but also beans, cucurbits, peppers, cassavas, and okra (Goolsby et al., 2005). *B. tabaci* is distributed worldwide and has been rapidly spreading during the past 15 years, but is especially damaging in the tropical and subtropical regions. In addition to its feeding damage, *B. tabaci* is also a vector of more than 100 plant viruses, of which Begomoviruses cause the most damage, leading to crop yield losses ranging from 20 to 100% (Jones, 2003).

2.2. Data augmentation

Due to the extensive work that is necessary to maintain a colony of pests of different species on different crop types, collect enough images, and label each small pest with a bounding box, data augmentation is a crucial step in the pipeline toward achieving accurate detection of pests. Due to the difficulty of generating high-resolution images with fine-grained features or small objects using GANs, such as insects in our case, we have resorted to a semi-automated technique of synthetic data generation, supported by GANs and operated by humans. Noting the lack of existing augmentation tools, we have developed an image labeling and generation interface using Python, OpenCV, and Flask, accessible through a webapp, which will allow users to produce realistic pest-infested leaf images starting with a small dataset.

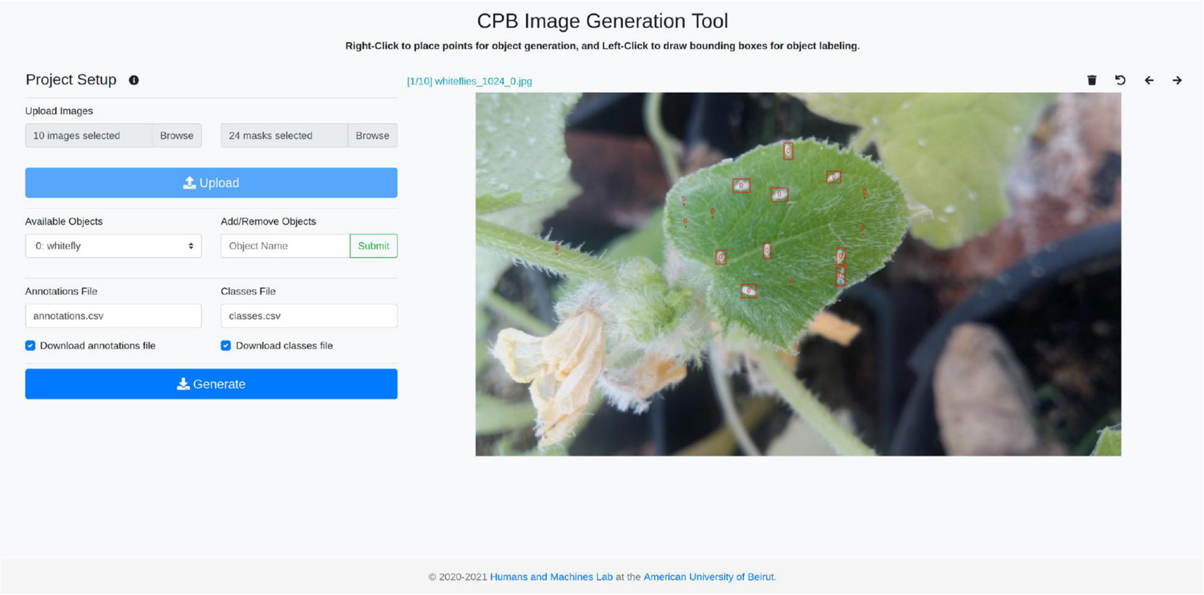
Note: In the abbreviated terms below, the first subscript refers to the image data: ***o****bjects,* ***m****asks, or whole* ***i****mages. The second subscript refers to the items'* ***i****nitial or* ***f****inal state.*

The augmentation workflow is as follows:

- Create segmentation masks for objects (pests) of interest, preferably from multiple examples for each class (species), with N_{mi} as the number of initial or source object (pest) masks.
- Optionally augment these object masks using GANs to increase the final source pool size to N_{mf} GAN-augmented object (pest) masks.
- Prepare a small dataset of background (leaf) images, with or without existing objects (pests), acting as a base/source dataset to augment, with N_{ii} initial images and N_{oi} initial objects.
- Label existing objects (pests) by drawing bounding boxes.
- Add new objects to the images by choosing one or multiple locations for each object type to be generated.

Following this workflow for our use-case, the tool will produce a final augmented dataset of N_{if} leaf images with a total of N_{of} artificially pasted pests, along with files that store the annotations and class names. The tool thus allows users to generate and label synthetic data from existing images and objects to train and develop detection models.

The result is a pipeline for generating artificial images of pest-infested leaves, as shown in Figure 2. The augmentation stage can be simplified and summarized by a three-step process: copying the source insect based on its mask, pasting it on the destination leaf image in a location chosen by a human reviewer, and blending the source insect with its destination background to maximize realism. This process will be referred to as Copy-Paste-Blend (CPB). In order to further diversify the augmented results, we introduce an additional step at the beginning of the pipeline: the initial size of the source mask pool is increased by generating new objects, thereby generating completely new insect masks not previously seen in the base dataset and diversifying the end-images. A Deep Convolutional Generative Adversarial Network (DCGAN) (Radford et al., 2015) is thus used to generate images of size



CPB Image Generation Tool

Right-Click to place points for object generation, and Left-Click to draw bounding boxes for object labeling.

Project Setup

Upload Images: 10 images selected; 24 masks selected

Available Objects: 0: whitefly

Annotations File: annotations.csv

Classes File: classes.csv

☑ Download annotations file

☑ Download classes file

[1/10] whiteflies_1024_0.jpg

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FIGURE 1
Copy-paste-blend tool for synthetic data generation.

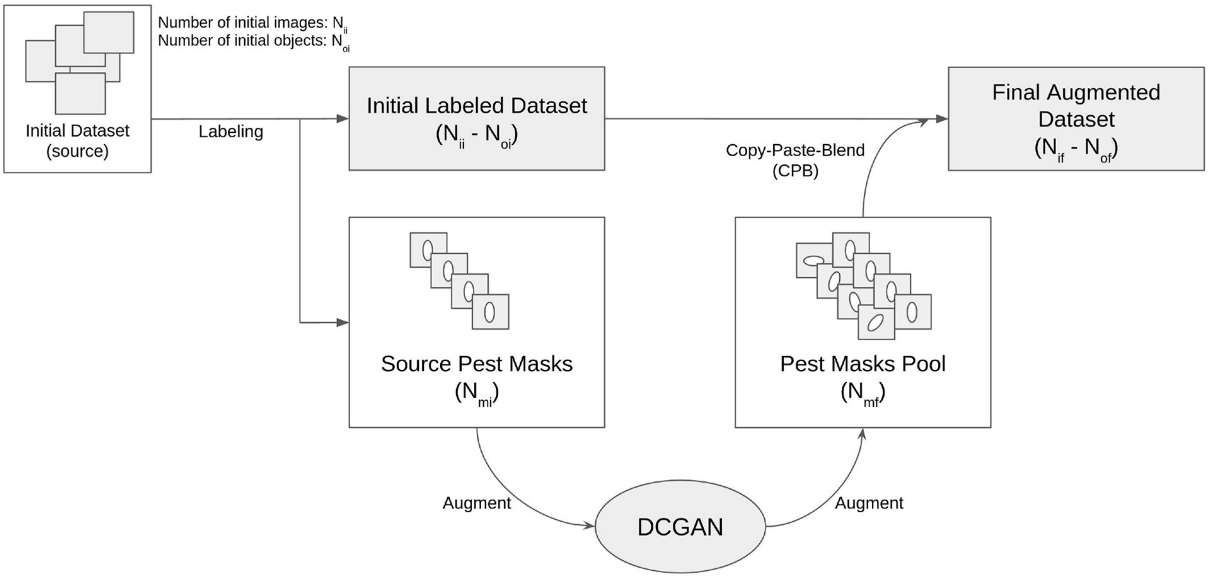

FIGURE 2
Copy-paste-blend + DCGAN augmentation pipeline (CPB+GAN).

32x32 representing individual pests of varying sizes. The entire pipeline will then be referred to as **CPB+GAN** if it includes this initial augmentation stage, and **CPB-NoGAN** if it does not generate new insect masks. A sample augmentation is shown in Figure 3.

2.2.1. Generative adversarial network

The DCGAN used for augmenting the pest masks has a generator made up of three up-sampling blocks each with an up-sampling layer, a convolution layer with ReLu activation, and a batch normalization layer, and a final convolution layer

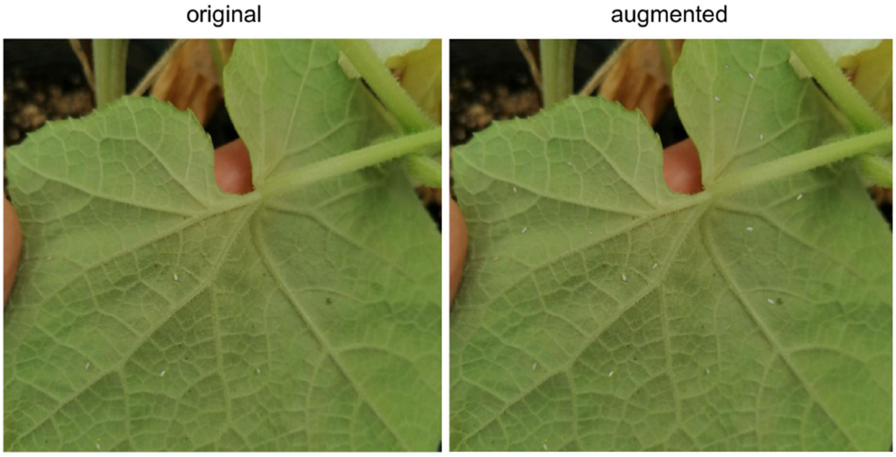

FIGURE 3
CPB+GAN output comparison.

with a hyperbolic tangent activation, outputting a 32 × 32 RGB image of a whitefly. The discriminator has three convolutional blocks using ReLu activation and dropout, as well as batch normalization on the last two blocks. The final layer is a fully-connected sigmoid activated layer. The entire network is optimized using Adam with a learning rate of 0.0002.

2.3. Object detection

For detecting pests on the leaf images, the single-stage, real-time YOLO networks are used for the experiment iterations. We consider the YOLOv3 (Redmon and Farhadi, 2018) model as well as its lightweight version, YOLOv3-tiny, in addition to a custom YOLO-based PestNet. YOLOv3 is a performant object detection model that can produce high-accuracy results while running at a high frame-rate, providing detections in real-time (>24 frames-per-second). Real-time detection is important because it allows users to receive instantaneous results in the field, and because it means that the network will still be usable even when ported to low-resource devices. The modified YOLO network, dubbed PestNet, is based off the DeepSperm network by Hidayatullah et al. (2020), whose task was to achieve a real-time bull-sperm cell detection in densely populated microscopic observation videos. The original DeepSperm network uses 29 convolutional layers, a dropout layer, and a final detection layer combined with image augmentation to prevent overfitting. It was modified through the addition six convolutional layers and a weak dropout layer with $p = 0.2$, and called PestNet. Whitefly detection and bull sperm cell detection are similar tasks due to the small size of the objects and the large numbers in which they are present in images.

2.4. Tool validation

To evaluate the realism of the generated images and the tool's effectiveness, reviewers from two different backgrounds, agricultural or image processing, were asked to visually assess real and synthetic datasets and label each image as real or artificial, but also to count the number of fake occurrences (generated pests). They provided reasons as to why certain objects were deemed unauthentic, in order to understand the shortcomings of the pipeline and the areas that need improvement.

3. Experimental results

3.1. Experimental setup

All experiments were performed on a Tesla V100 GPU with 32 GB of VRAM, using a batch size of 64 subdivided into four mini-batches of size 16, using a resolution of 512 × 512 pixels for all images. The models were trained for 3,000 batches, equivalent to about 81 full epochs. All object detection networks were trained using the Darknet framework (Redmon, 2013–2016), while the generative networks were trained using Keras and Tensorflow (version 1) (Abadi et al., 2015).

3.2. Baseline performance

The first batch of experiments aims at evaluating object detection models on the raw non-augmented dataset to provide a baseline performance which can be referenced when comparing the different augmentation techniques and experiments.

The baseline models are all validated and tested on the same sets, $D_{\text{base-valid}} = 70$ images and $D_{\text{base-test}} = 140$ images, as stated in Section 2.1. The training is done on two subsets of the base dataset, one of size 560 images ($D_{\text{base-train-560}}$) and another of size 140 images ($D_{\text{base-train-140}}$).

These baseline results are shown in Table 1. Counting the number of insects on the leaves represents the essence of this pest detection task, and as a result, recall constitutes one of the most important metrics to evaluate the performance of the models. Drawing extremely accurate bounding boxes around the pests is not as essential as detecting all the pests present on the leaf. The recall metric is thus used at two different Intersection-over-Union (IoU) thresholds, at 0.50 and 0.75 (R@.50 and R@.75). In other words, the IoU threshold defines if a detection is counted as correct (positive): if the ratio of the areas of overlap between the detected bounding box and the groundtruth bounding box is higher than the threshold fraction, the detection is counted as true. The Average Precision (AP) metric also thresholds by IoU, but combines information from both recall and precision for a more comprehensive evaluation. Finally, the model size and average training time per batch of images allow us to get an idea of the resource-consumption of the model. The YOLOv3 model exhibited the best performance when trained on $D_{\text{base-train-560}}$, followed closely by PestNet. YOLOv3 only outperforms PestNet by 1.3, 7.3, and 1.9% in R@.50, R@.75, and average IoU, respectively. On the other hand, the PestNet model size is more than 17 times smaller than YOLOv3, which will make it much easier to load on low-end devices. YOLOv3-Tiny performs badly across the board despite being comparably light to PestNet. When trained on $D_{\text{base-train-140}}$, PestNet seems to generalize better than YOLOv3 and outperforms it by a slight margin, scoring 2.6, 11.7, and 4.8% higher than it in R@.50, R@.75, and average IoU, respectively, despite being a smaller model. The performance of both models dropped by almost 50% on all metrics when the training set size dropped from 560 to 140 images.

3.3. Data augmentation

To evaluate our data generation pipeline, the different augmentation variations are tested on the PestNet model because of its superior balance between accuracy and speed. PestNet is able to offer accuracy on-par with that of YOLOv3 while being a much smaller and lighter model.

The first variation is the CPB-NoGAN version of the pipeline, augmenting the starting dataset size with the original set of pest masks of size $D_{ps} = 20$. The second variation is coupling the CPB pipeline with an initial augmentation of source pest masks using the DCGAN (CPB+GAN) to yield a usable mask pool of size $D_{pf} = 60$.

The augmentation pipeline is applied on the two sets used for the baseline training: (1) $D_{\text{base-train-140}}$ is augmented four-fold for a final size of 560 images. (2) $D_{\text{base-train-560}}$ is augmented two-fold for a final size of 1,120 images. Each of these sets is thus augmented twice, once with the original object mask pool of 20 images (CPB-NoGAN), and once with the GAN-augmented object mask pool of 60 images (CPB-NoGAN). Note that all datasets are multiples of a fundamental or base dataset size of $D_b = 140$ images. These iterations are summed up in Table 2, along with the performance results. It is interesting to examine the performance gains to each metric brought forth by each part of the pipeline: the simple increase in the number of images (CPB), and the increase in the diversity of the inserted objects (CPB+GAN). The Recall@.50 will mainly measure the number of detected pests (sensitivity), while the average IoU will mainly indicate the precision with which the bounding boxes are drawn. This comparison is shown in Figure 4 shows that augmenting the dataset size using CPB-NoGAN from 140 to 560 images brings PestNet's recall metric close to the baseline model trained on 560 images (within 1.2%), while the average IoU does not quite reach the same level as before (still 3.9% away). This may be due to the limited mask pool size, which results in the same 20 whiteflies being added to all the images. This restricted diversity in the augmented images leads to reduced performance when compared to a model trained on an original dataset equal in size to the augmented dataset: the original dataset will be more varied in terms of objects (insects) it contains. This problem is solved through the use of GANs to augment the starting mask pool from 20 to 60 masks. The increase in diversity in the final augmented dataset will lead to better generalization on the test set, contributing to the precision of the detected bounding box. The graph in Figure 4 clearly shows how the Average IoU metric is more sensitive to the dataset's diversity than the recall metric: the performance gain in average IoU from CPB-NoGAN to CPB+GAN is at 2.2% points, while the increase in recall between the two pipelines is only at +0.4% points, for the original dataset size of 560 images.

3.4. Human visual assessment

The image generation pipeline is not only validated by the performance boost of the detection model, but also by a visual assessment of the authenticity of the generated images by humans. The reviewers are 19 students (11 females and 8 males) in the same age group of 20–25, but come from two different backgrounds: computer science/vision (13) and agriculture (6). The technical background comes into play when evaluating artificial plant and pest images as the reviewers from agricultural backgrounds are better trained and equipped to recognize anomalies in the synthetic data. The reviewers assessed a total

TABLE 1 Baseline YOLO performance (no augmentation).

Network	Training size	R@.50	R@.75	Avg IoU	Model size (MB)	Train. time/Batch (s)
YOLOv3	560	**0.955**	**0.603**	**0.752**	245	6.68
YOLOv3-Tiny	560	0.528	0.135	0.472	31	**5.00**
PestNet	560	0.943	0.562	0.738	**14**	5.27
YOLOv3	140	0.532	0.214	0.330	245	6.65
YOLOv3-Tiny	140	0.196	0.042	0.101	31	**4.98**
PestNet	140	**0.544**	**0.239**	**0.346**	**14**	5.31

Best metrics are shown in bold.

TABLE 2 PestNet test performances for different CPB configurations.

Pipeline	Original dataset size	Augmented dataset size	Pest masks pool	Recall @.50	Average IoU
CPB-NoGAN	140 (D_s*1)	560 (D_s*4)	20	0.932	0.709
CPB+GAN	140 (D_s*1)	560 (D_s*4)	60	0.946	0.735
CPB-NoGAN	560 (D_s*4)	1120 (D_s*8)	20	0.977	0.806
CPB+GAN	560 (D_s*4)	1120 (D_s*8)	60	0.981	0.828

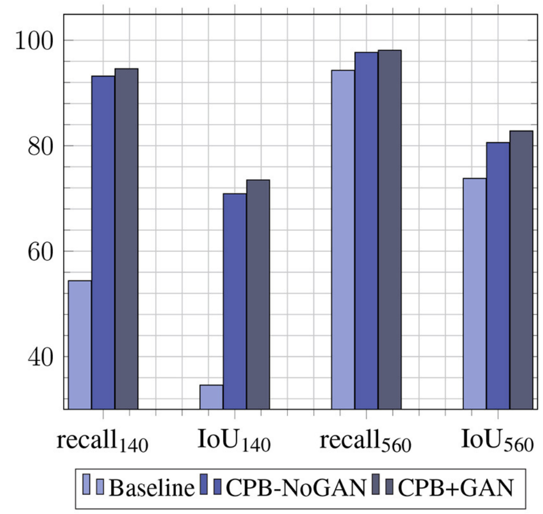

FIGURE 4
Performance gains of PestNet with CPB for Recall@.50 and Average IoU.

of three artificially-generated sets of 60 images each. The first two sets were generated using the CPB-NoGAN pipeline, from 20 original whitefly objects, at a lower-resolution of 512 × 512 pixels, and a higher-resolution of 1,024 × 1,024 pixels. The third set was generated using the CPB+GAN pipeline, from 20 original whitefly objects augmented to 60, at the resolution of 512 × 512 pixels for the images. The 512 × 512 resolution corresponds to the models' resolution for a fair comparison, but at this size the anomalies in the synthetic data are more difficult to detect for humans.

Overall, the reviewers were able to distinguish fake objects with an average accuracy of 56% at low resolution, and 67% at high resolution, as shown in Figure 5. When asked to count the numbers of fake occurrences in an image, the accuracy was 26% with an RMSE of 8.2 for low resolution, and an accuracy of 42% with an RMSE of 7.3 for high resolution, as shown in Figure 6. Clearly, the task is easier at higher resolution, but the authenticity of the generated data can be validated by low overall performance of the reviewers on these two sets. It is interesting to note the difference in performance between the vision-background students and the agriculture-background students: the top reviewer is a researcher in agriculture and can distinguish real from fake images with an accuracy of 79 and 91% for low and high resolution, respectively, and can count the number of fake occurrences with an accuracy of 42 and 72%. Compared to the average reviewer, This is an increase of around x1.4 for binary classification of real/fake, and x1.6 for counting.

3.5. Discussion

We have shown results for baseline YOLO performances, and the effect of different data augmentation pipelines on these performances. The baseline YOLO performances justify the use of PestNet, since it is a lightweight object detection model, capable of almost matching YOLOv3's performances while still being a much smaller model, which makes it more likely to be implemented in applications on low-cost devices. The merits of PestNet are further justified by the failure of YOLOv3-Tiny, another lightweight model, to produce similar results. The main focus of this work is improving these baseline performances, through the use of the data augmentation pipeline, dubbed

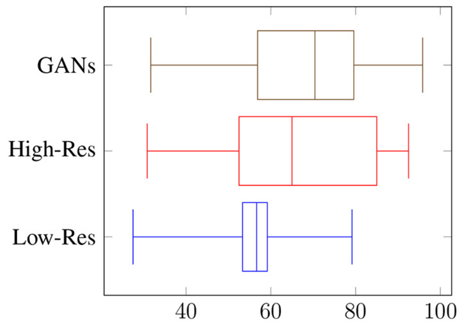

FIGURE 5
Visual assessment of generated datasets: real/fake classification accuracy (%).

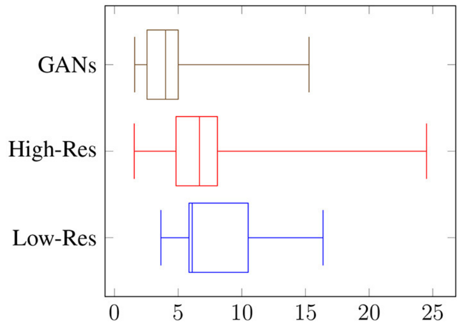

FIGURE 6
Visual assessment of generated datasets: RMSE on number of fake occurrences.

CPB. This pipeline allows us to increase the dataset sizes by reproducing the objects of interest (whitefly pests) on different plant leaves, making the model more robust by diversifying the examples it sees. As a result, augmenting the training set from 140 to 560 images using CPB-NoGAN yields a jump by 38.8% points for R@.50, almost matching the performances of a model trained on 560 original images. This highlights the need for such pipelines in scenarios where the data is limited. While CPB-NoGAN boosts both the recall and average IoU metrics, the CPB+GAN pipeline allows us to generate new pests, increasing the diversity of the objects of interest, and further boosting the resulting average IoU, which measures the precision in the bounding box detection. Therefore, starting from 140 images and applying the CPB+GAN augmentation, we can match the performance of a model trained of 560 images from the start. The augmentation pipeline has therefore fulfilled its function in decreasing the effect of data scarcity. Finally, the human reviewers serve to assess and help explain both the benefits and shortcomings of this pipeline. At the model's resolution, the reviewers can distinguish real from fake images with an accuracy of 56%, which means that the generated are realistic enough. At higher resolutions, this accuracy goes up to 67%, which means the images are still somewhat realistic, but are now easier to spot and may not be as effective in portraying real-world scenarios. The augmentation pipeline is then well-suited for training at a resolution 512 × 512, but should probably be improved before being used with higher-resolution models. However, it is important to note that most datasets do not include images at resolutions of 1,024 × 1,024, and that using lower resolutions can help with model portability and computational loads on low-end devices. The reviewers pointed out that potential areas of improvements include refining the blending process to reduce pest outline and color issues. Overall, these results justify the use of the PestNet model for this pest detection task, as well as the CPB+GAN pipeline for generating synthetic datasets. Compared to the literature, this work differs from the literature in its use of non-traditional augmentations, leveraging GANs and a semi-automated process to artificially generate new objects of interests in new configurations on different backgrounds. It also differs in its use of lightweight architectures rather than larger and slower models like the popular ResNet + Faster-RCNN for object detection, keeping portability and embeddability. Finally, it also stands out in the difficulty of the task at hand: detecting small numerous pests on a plant leaf is harder than detecting diseases whose symptoms take up a large portion of the leaves, or larger pests that are more prominent in the images, and present in fewer numbers. One shortcoming, which can also be addressed to other works in the literature, is the difficulty of comparing the detection performances of different models, due to the inherent differences in the studied crops, diseases, and pests, and the unavailability of public datasets that target similar object detection tasks.

4. Conclusion

In this work, we developed a synthetic data generation pipeline and online tool leveraging GANs, that can be used to augment small datasets in order to achieve accurate object detection with lightweight models. The publicly accessible tool allows even inexperienced users to create large datasets starting from a few real images. Developing simple tools contributes to enhanced food security by allowing all stakeholders in agriculture, whether big or small-time farmers, to optimize their pest management strategies and reduce the yield loss incurred by pest attacks.

The validity of the pipeline and accompanying tool was tested on an pest detection task for different sizes of a *B. tabaci* whiteflies dataset, collected at the American University of Beirut's greenhouses. Data generation allowed us to augment a dataset of 140–560 images, increasing the performance of a lightweight object detection model, PestNet, by 38.8% points in R@.50, and by 36.3% points in average IoU. When GANs are incorporated as a method to augment the starting object masks (pests) inserted into images, the recall and average IoU are further increased by 1.4 and 2.6% points, respectively. The

GAN variation of the pipeline especially aids in improving the precision of the detected bounding box by boosting the generalization of the model on the test set due to the increased variety in the introduced augmentations. Thus, starting from only 140 images and using data augmentation, we were able to match the performance of a model trained on 560 images.

The tool's validity is also tested through visual assessment of its image outputs, conducted by 19 student reviewers from agricultural or machine-learning backgrounds. This review serves to evaluate the authenticity of the augmented images and to identify its weaknesses for further improvement. When presented with a dataset with 512 × 512 RGB images, reviewers were only able to classify the images are real or generated with an average binary accuracy of 56%, with the best reviewer achieving 79% accuracy (agricultural background). On the more challenging task of counting the number of fake objects in each image, the binary accuracy was only 26%, with an average RMSE of 8.2. The pipeline is then well-suited for realistic data generation, but could still be improved.

The lightweight model and the small dataset size we use are both indications that this work may be beneficial for real-world applications on low-end devices. However, some shortcomings of this study include the difficulty of comparison with the literature for similar tasks due to the unavailability of data, and focus on the detection of only one pest type, the whitefly. Future work could then target the expansion of the existing dataset to include more pests, to strengthen model robustness, range of applications, and validation strength. The CPB pipeline could be improved as well by refining the blending process to reduce pest outline and color issues, marked as being the top indicators of a fake pest by reviewers. Finally, additional work could target the augmentation pipeline and tool to include additional features such as model training and deployment, further bridging the gap between model development and the end-users, which are small-time farmers interested in improving their crop health with early pest detection.

Data availability statement

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

Author contributions

CK developed the software, ran the experiments, and produced a draft of the manuscript. MA directed the research, identified the framework to be implemented and helped in the experimental setup, and revised the manuscript multiple times. YA co-directed the research, provided input on the pest cycle, and corrected final versions of the manuscript. NE collected the agriculture data, labeled it, and helped in the human annotation as well as revising the manuscript. AF collected the agriculture data, labeled it, and contributed to the manuscript write-up. All authors contributed to the article and approved the submitted version.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

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Food security under compound shocks: Can Lebanon produce its own Mediterranean food basket?

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As Lebanon faces compound challenges, a looming food security crisis is rapidly approaching, much of which could be attributed to the lack of long-term planning for sustainability in its agricultural sector. The disconnect between decision-makers within the agricultural sector, and other interconnected sectors is exacerbated by the lack of integrative national platforms and methodologies for quantifying the trade-offs associated with possible interventions. This study aims to: (1) identify and quantify the critical interconnections between water, energy, nutrition, and food systems in Lebanon; (2) develop a framework to quantify the trade-offs associated with adopting interventions within current water, energy, and agriculture portfolios and practices; (3) evaluate producers' perceptions toward their willingness to implement proposed changes in crop production, renewable energy, and water reuse. Findings show that investing in locally producing Lebanon's needs of broad beans, lentils, chickpeas, and peas, results in cost savings, increased nutritional value in the locally produced basket, and reduced reliance on foreign markets. In turn, this comes at additional water, energy, land and carbon footprints which needs to be accounted for. Given the uncertainty of future currency conversion rates, it becomes more critical to identify a strategic food basket that could be produced locally to reduce reliance on imports. Conclusions from this study can play a role in informing policymaking and planning in Lebanon, which could be adapted and replicated in other countries in the MENA Region.

KEYWORDS

water-energy-food nexus, trade-offs analysis, farmer perceptions, sustainable development, Beqaa Valley, Lebanon

1. Introduction

Water, energy, and food securities are tightly interconnected, and have direct implications on human health and wellbeing (Mohtar and Daher, 2012, 2016; Giampietro et al., 2013; Howells et al., 2013; FAO, 2014; Liu et al., 2017). Addressing the challenges facing these resource systems needs to be grounded in an understanding of their interconnections, which need to be reflected in the way they are managed (Daher and Mohtar, 2015). Trade-off analysis tools can play a critical role in catalyzing cross-sectoral dialogue between the stakeholders who regulate, manage, and consume these resource systems (Daher et al., 2019). Such dialogue enhances the processes of integrative planning, supporting the implementation of the United Nations Sustainable Development Goals.

The EAT-Lancet Commission, in its effort toward balanced nutritious diets and sustainable food systems, has proposed a list of recommendations for healthy diets. It suggests substantial dietary shifts where the global consumption of fruits, vegetables, nuts and legumes will have to almost double, and consumption of foods such as red meat and sugar will have to be reduced by more than 50% (Willett et al., 2019). The Mediterranean Diet (MD), rich in plant-based foods and with fewer animal source foods aligns with the EAT-Lancet diet recommendations, and confers both human health and environmental benefits (Naja et al., 2011, 2012, 2013, 2018; Hwalla, 2015). Naja et al. (2018), reported that one of the two main dietary patterns in Lebanon, identified as the Lebanese-Mediterranean pattern, had a lower water use and greenhouse gas emissions (GHG) associated with it compared to the "Western" pattern which is the other main dietary pattern in the country. A study by Vanham et al. (2021) compared the water footprint of the MD and the EAT-Lancet diet (Willett et al., 2019) in nine countries around the Mediterranean accounting for the food intake requirements per gender and age. They reported that the EAT-Lancet diet and the MD (MEDIT as described in Bach-Faig et al., 2011) reduce the water footprint by 17–48 and 4–35%, respectively compared to the reference, which was defined as the current dietary intake based on FAO data. An 11% reduction in GHG production was also reported by Batlle-Bayer et al. (2019) when shifting the Spanish current eating habits to the MD. Vanham et al. (2021) noted that the EAT-Lancet diet is more optimized for human health and environmental indicators that the traditional MD diet. Similar to a developing trend in the Mediterranean region, Lebanon's diet is shifting away from a concentration of pulses, vegetables and fruits toward animal products (Markantonis et al., 2019) which ultimately increases the pressure on water resources.

The impact of relying heavily on plant-based diets differs between regions, which depends on their availability of water, energy and land resources. Given the scarcity of water and arable land in arid and semi-arid regions, over which different sectors compete, our research question asks about the sustainability of producing more of the plant-based Mediterranean diet. We also ask about the ways in which alternative water and energy sources could play a role in affecting the sustainability of this diet. A gap exists in frameworks and tool that provided a system-of-systems perspective that evaluate trade-offs for decisions made across water, energy, and food sectors in Lebanon. This study used a water-energy-food system-of-systems assessment to evaluate the sustainability of such a diet in a Mediterranean country, Lebanon, with specific aims to: (1) identify and quantify the critical interconnections between water, energy, and food systems in Lebanon; (2) develop a nexus framework to assess the trade-offs associated with adopting interventions within the current water, energy, and agriculture portfolios and practices; (3) evaluate farmer perceptions and willingness to implement proposed interventions. The study outcomes will inform policy and decision makers on issues such as sustainable development of the agricultural sector, energy and water subsidy and pricing, and import/export and trade policies. The framework will play an important role in catalyzing cross-sectoral dialogue for tradeoffs evaluation among stakeholders including farmers, rural communities, consumers, industry, and market/supply chains. The developed framework allows for scaling the analysis to broader scopes or other arid and semi-arid regional geographic areas.

2. Overview of the current water, energy, and agricultural status in Lebanon

Lebanon faces serious water scarcity issues that hamper its economic and social development. Building a sustainable economic and environmental future in Lebanon requires a paradigm shift that acknowledges the nexus between the water, energy, and food systems to simultaneously address prevailing water issues, food insecurity and natural hazards. Lebanon faces various constraints such as access to water, energy, nutritious food, and health care. These gaps are expected to increase with continuing demographic and climate change. The highly interlinked resources systems carry high risks and great vulnerabilities. Ensuring food security is a national priority which should be approached through a multi-sectoral lens, which branches beyond the agricultural sector, since unilateral, thematic-based, disciplinary approaches have failed to address the deep environmental and societal issues that are currently being faced.

Lebanon is considered to be in a relatively favorable position as far as rainfall and water resources (FAO, 2008), however, Lebanon's amount of renewable water has significantly dropped from more than 1,000 cubic meters/year/person to around 700 cubic meters/year/person (Machayekhi et al., 2017). The total cultivated land area in Lebanon is about 231,000 ha (Agriculture Census, 2010); the Beqaa Valley represents 42%

of the agricultural areas in Lebanon (Machayekhi et al., 2017) where a multiplicity of grains, potatoes, stone fruits, vegetables, grapevine, and feed crops are grown (Haydamous and El Hajj, 2016). The Akkar and North Lebanon constitute 26% of the cultivated area growing cereal crops, pulses, vegetables and fruit trees including olives. South Lebanon constitutes about 22% of the agricultural area producing citrus, olives, bananas, cereals, and industrial crops such as tobacco. Mount Lebanon, covering about 9% of the cultivated area focuses on vegetable production especially under greenhouses in the coastal areas, and fruit trees in the mountains. Most farms in Lebanon are small farm holdings that do not exceed 1 hectare. The concentration of agricultural activity in the Beqaa and Akkar imposes a high demand for water, energy, and land resources. Overall, 60% of water in Lebanon is directed to agriculture; agriculture in the Beqaa consumes 86% of Beqaa's available water resources (rivers, springs, and underground aquifers), and in Akkar with over 45% of its cultivated land being irrigated, uses most of its available water resources from rivers, springs and groundwater (World Bank, 2003; MoA, 2010; El Amine et al., 2018). Despite relying on some rivers in agricultural areas such as Litani, Al-Kabir or Al-Bared rivers, and 100 s of springs, farmers rely largely (∼80%) on groundwater pumping through public and private wells. Nevertheless, water availability remains a primary challenge: the diminishing quantity and quality of water is a major stressor. Available water resources are threatened by decreasing precipitation, pollution, uncontrolled pumping, and wastewater seepage (El-Kareh et al., 2018).

As for energy, while the agriculture sector uses diesel oil for operations, such as pumping water, drying grains, supplying greenhouses and for traction vehicles, this energy use represents <9% of Lebanon's total energy demand (MoE/UNDP/GEF, 2016). The 2017 EDL (Electricité du Liban) rate of electricity generation was 15 TWh, 96% of which comes from fossil fuels, 3% from hydropower plants, and 0.35% from photovoltaic (PV) panels. Almost all the fuel for energy is imported; this places Lebanon at risk due to dependency on external primary energy resources. The energy for agricultural production is divided between diesel (70%) and gasoline (30%). Decisions related to the type of crops grown in Lebanon are the foundation for quantifying the interconnections across the resource systems considered. Current water and energy portfolios for agricultural production in Lebanon are considered.

3. Methodology

3.1. Choice of crops, water and energy options

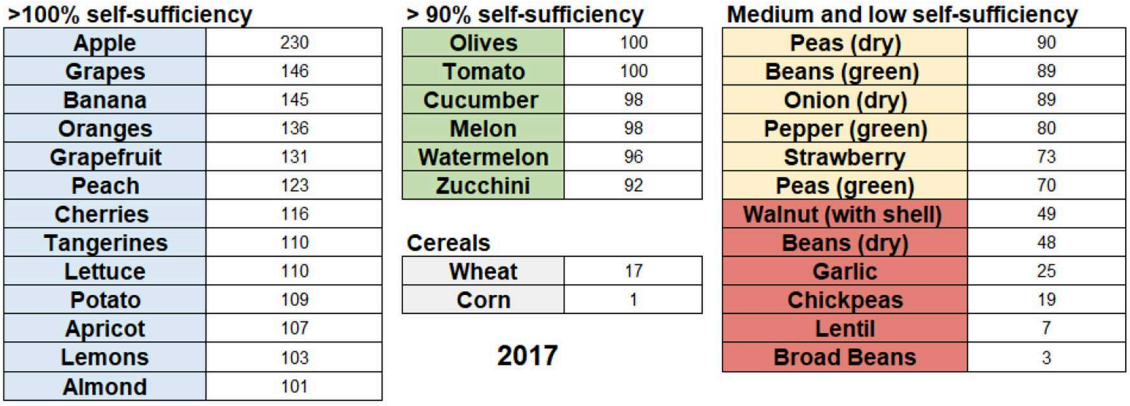
The Mediterranean diet is rich in legumes, vegetables, nuts, and fruits, many of which have beneficial health effects while having a smaller environmental footprint. The case study focuses on selected crops from the Mediterranean diet that may be produced in Lebanon. Some crops such as parsley or pine nuts, though part of the diet, were not included because their consumption and production are minor and detailed data about their production and trade is not available. A list of 33 crops including cereals (wheat and corn), vegetables (tomato, cucumber, zucchini, lettuce, potato, onion, garlic, pepper), fruits (apple, apricot, peaches, citrus fruits, banana, cherries, grapes, melon, watermelon, strawberries), nut trees (almond, walnut), olives, and pulses (peas, beans, chickpeas, lentils) that are commonly consumed in the Lebanese diet and consistent with EAT-Lancet recommendations (Willett et al., 2019) was developed for this study. The crops highlighted in red have low self-sufficiency i.e., they are being mostly imported; these crops have low irrigation requirements and high nutritional value (Figure 1). These crops, which are mostly pulses, are classified as staple Mediterranean crops that go into the making of many traditional dishes, in addition to wheat which is also considered a staple food. Figure 2 shows the crops that have low irrigation requirements, are high in protein and caloric value, and have potential to increase their acreage because they are produced on a small percentage of the agricultural land such as lentils, beans, almonds, and walnuts for example. Scatterplots for irrigation vs. calories, yield vs. protein content, and yield vs. calories showed a similar group of crops on low input-high nutritional value.

3.2. Overarching interconnections framework: Scenario inputs and outputs

A conceptual representation of the interconnections between water, energy, and food systems which are considered in this study is outlined in Figure 3. Decisions made within each of the resource systems, has an impact on others. Decisions related to the type of crops grown are the building foundation for quantifying the interconnections across the resource systems being considered. This section introduces the Water-Energy-Food (WEF) Nexus scenario evaluation structure. It outlines (1) scenario inputs and outputs, (2) a sample of the background data needs, (3) and method for evaluating stakeholder preferences.

3.2.1. Scenario inputs and outputs

The scenario inputs include the self-sufficiency ratios per crop (with 2017 ratios used as base scenario), water sources (ratios of water sources for irrigation which can be from groundwater, surface water, or treated wastewater), energy sources (ratios of energy sources including gasoline, diesel, wind and solar), currency conversion rate (ranging from official rate of 1USD = 1,500 LBP in 2017 to between 3,000 LBP and 10,000 LBP to the US Dollar). Evaluating these scenarios is done according to a list of outputs including irrigated water (m^3, representing net irrigation needs), land requirement (ha,



>100% self-sufficiency

Apple	230
Grapes	146
Banana	145
Oranges	136
Grapefruit	131
Peach	123
Cherries	116
Tangerines	110
Lettuce	110
Potato	109
Apricot	107
Lemons	103
Almond	101

> 90% self-sufficiency

Olives	100
Tomato	100
Cucumber	98
Melon	98
Watermelon	96
Zucchini	92

Cereals

Wheat	17
Corn	1

2017

Medium and low self-sufficiency

Peas (dry)	90
Beans (green)	89
Onion (dry)	89
Pepper (green)	80
Strawberry	73
Peas (green)	70
Walnut (with shell)	49
Beans (dry)	48
Garlic	25
Chickpeas	19
Lentil	7
Broad Beans	3

FIGURE 1
Lebanon's baseline (2017) self-sufficiency (SS) levels (%) for the selected crops; SS is the local production of a crop that satisfies the local Lebanese consumption (<100% means that a crop needs to be partially imported to meet market needs).

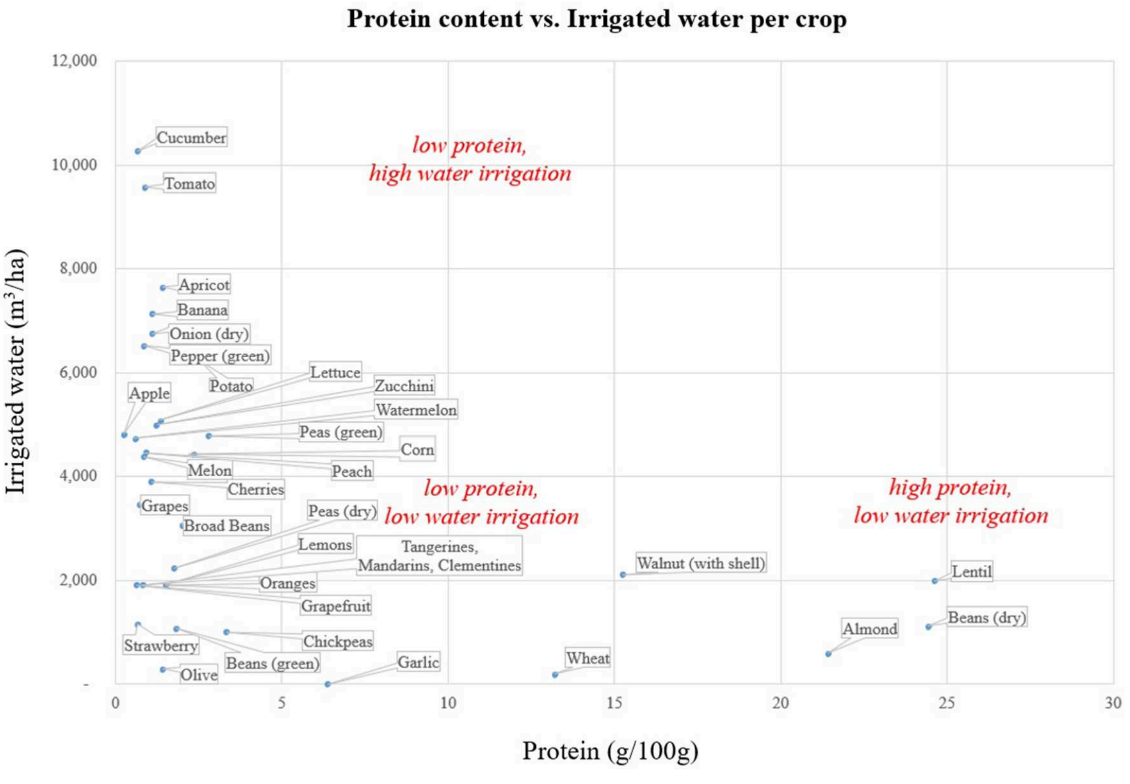


FIGURE 2
Protein content and irrigation water requirements for the different crops.

representing total land required to produce different ratios of selected crops locally), energy requirement (kJ, representing energy for pumping, treating, and conveying the different water sources E_W, in addition to energy for agricultural production including for harvesting, tillage, planting, and spraying E_a), cost (Lebanese pounds, representing the net cost of locally producing, importing, and exporting the identified list of food products), environmental impact (ton CO_2, representing the emissions associated with different scenarios based on choice of energy sources), nutrition (kcal, grams protein, fats, carbs, fiber, and sugar representing the nutritional value of the locally produced crops), and a reliance index (an indicator representing the proportion of food imports in the nationally consumed basket). A detailed description and

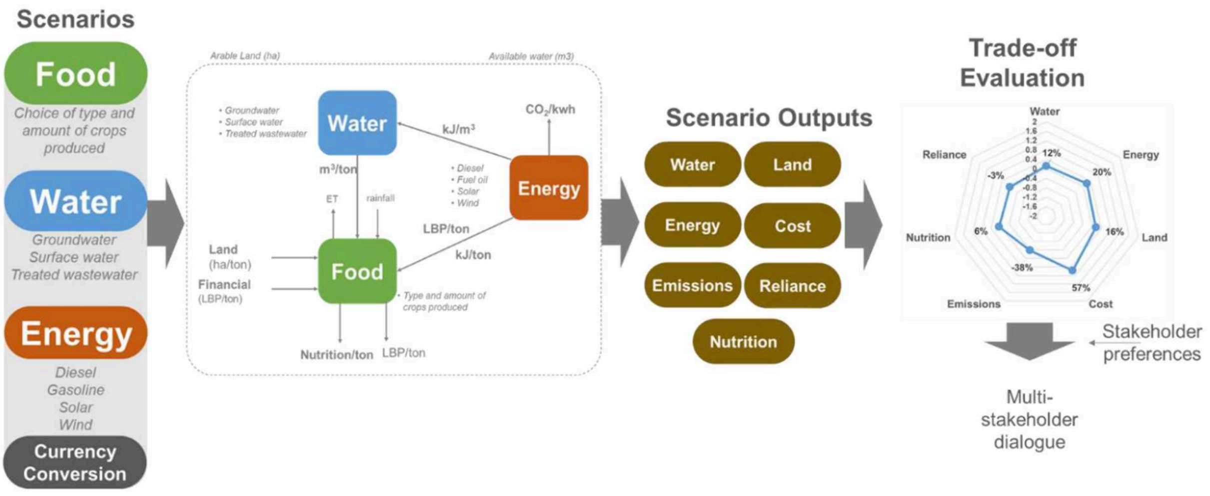


FIGURE 3
WEF framework structure.

TABLE 1 The self-sufficiency ratios (%SS), water sources, energy sources, and currency conversion in 2017.

Crops	2017 %SS	Crops	2017 %SS	Water sources	%	Energy for water	%
Wheat	17	Watermelon	96	Ground water	80	Diesel	100
Corn	1	Melon	98			Gasoline	0
Potato	109	Peach	123			Wind	0
Lettuce	110	Apricot	107			Solar	0
Tomato	100	Grapes	146	Surface water	20	Diesel	100
Zucchini	92	Beans (dry)	48			Gasoline	0
Pepper (green)	80	Beans (green)	89			Wind	0
Cucumber	98	Broad beans	3			Solar	0
Onion (dry)	89	Lentil	7	Treated WW	0	Diesel	0
Garlic	25	Chickpeas	19			Gasoline	0
Apple	230	Peas (dry)	90			Wind	0
Grapefruit	131	Peas (green)	70			Solar	0
Lemons	103	Almond	101	Energy for food		Currency conversion	
Oranges	136	Walnut (with shell)	49	Gasoline	30%	USD	1
Tangerines, mandarins, clementine	110	Cherries	116	Diesel	70%	LBP	1,500
Banana	145	Olive	100				
Strawberry	73						

equations for the outlined inputs and outputs are provided in Appendix I.

3.2.2. A sample of local data needs

FAO databases, MoA census report, USDA Food Composition Database, local weather data, local crop water requirements and others were collected from the survey questions and other published work. Examples of this data can be found in Appendix II.

3.2.3. Evaluating stakeholder preferences: Farmers' survey

In addition to the tight interconnectedness between the physical resource systems, stakeholders, with different preferences and decision-making power, also interact. As scenarios are evaluated, these preferences will be critical in driving the multi-sectoral dialogue about future trade-offs. Given the emphasis of this study on evaluating decisions and practices made at the farm level, a survey was conducted with 200 farmers in the Beqaa Valley, in an effort to

TABLE 2 Scenario outputs for base case scenario 2017.

		2017
Water	(m^3)	464,793,307
Energy	(GJ)	1,547.1
Land	(ha)	198,179
Cost	(Billion LBP)	1,538.5
Emissions	(ton CO_2)	105,743.8
Nutrition	(kcal)	1.4 E + 14
Reliance	Ratio (I/C)	0.45

learn about their willingness to shift to different crops, alternative water sources, and alternative energy sources on their farms. We were also interested to learn about farmers' priorities to minimize water, energy, land, emissions, cost, and maximize nutritional value, as they made those decisions. Insights from evaluating these preferences could be used to predict the responsiveness to different scenarios and to inform policy incentives. The survey was approved by AUB's Internal Review Board (IRB). The survey could be found in Appendix III.

According to the 2010 Agriculture census, the total farmed area in the Beqaa is about 99,274 ha and the average size of holdings is 2.9 ha resulting in an estimate of 34,085 holdings or farmers. Assuming a response rate of 80–85%, the representative sample size was calculated to be 200–245 farmers, with confidence interval of 95 and 5% margin of error. Farmers selected to participate in the survey were chosen based on contacts that the researchers have from previous projects with the American University of Beirut (AUB) and the Advancing Research Enabling Communities Center (AREC). Snowballing was used as a method to identify other farmers in the Beqaa.

4. Results

4.1. Scenario evaluation

This section includes scenarios using the developed evaluation framework. The goal is to highlight the trade-offs associated with different scenarios as the water, energy, and agricultural portfolios are changed relative to 2017 which was selected as a base year.

4.1.1. Base year scenario 2017

Table 1 shows the self-sufficiency (SS) ratios of the selected crops, water sources, energy sources, and currency conversion rate in 2017.

According to the developed evaluation framework, Table 2 outlines the outputs for the base case scenario. After establishing the different resource requirements and outputs for the base scenario, the following will explore the impact of making different interventions relative to this base year, by changing the self-sufficiency of different crops and changing water and energy sources under different currency conversion rates (Table 3).

TABLE 3 Evaluated scenarios.

Scenario A: Nutrition-centric	• **Increase** beans (green, broad, dry), lentils, chickpeas and peas (dry, green) to **100% SS** • **Water:** 80% groundwater, 20% surface water (same as 2017) • **Energy-water:** 100% Diesel (same as 2017) • **Energy-food: 70%** Diesel, 30% Gasoline (same as 2017) • **Currency conversion:** 1 USD = 1,500 LBP (same as 2017)
Scenario B1: Shifting from export to more local production	• **Increase** production of beans (green, broad, dry), lentils, chickpeas and peas (dry, green) to **100% SS** • **Decrease** production of crops with SS > 100% to SS = 100%; no export, no additional import of these products • **Water:** 80% groundwater, 20% surface water • **Energy-water:** 100% Diesel • **Energy-food:** 70% Diesel, 30% Gasoline • **Currency conversion:** 1 USD = 1,500 LBP
Scenario B2: Shifting from export to more local production under currency fluctuation	• **Increase** production of beans (green, broad, dry), lentils, chickpeas and peas (dry, green) to 100% SS • **Decrease** production of crops with SS > 100% to SS = 100%; no export, no additional import of these products • **Water:** 80% groundwater, 20% surface water • **Energy-water:** 100% Diesel • **Energy-food:** 70% Diesel, 30% Gasoline • **Currency conversion:** 1 USD = 4,000 LBP
Scenario C: Scenario A + Renewable energy + Treated water + currency fluctuation	• **Increase** beans (green, broad, dry), lentils, chickpeas and peas (dry, green) to 100% SS • **Water:** 60% groundwater, 20% surface water, 20% treated water • **Energy-water:** 50% Diesel, 50% Solar • **Energy-food:** 70% Diesel, 30% Gasoline • **Currency conversion:** 1 USD = 4,000 LBP
Scenario D: Scenario B2 + Renewable energy + Treated water + currency fluctuation	• **Increase beans** (green, broad, dry), lentils, chickpeas and peas (dry, green) to 100% SS • **Decrease** production of crops with SS > 100% to SS = 100%; no export, no additional import of these products • **Water:** 60% groundwater, 20% surface water, 20% treated water • **Energy-water:** 50% Diesel, 50% Solar • **Energy-food:** 70% Diesel, 30% Gasoline • **Currency conversion:** 1 USD = 4,000 LBP

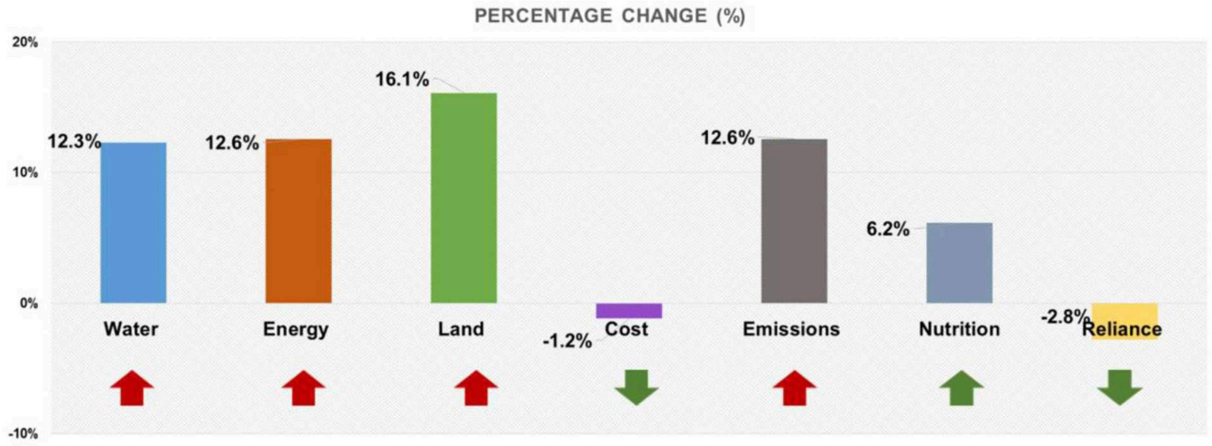


FIGURE 4
Percentage change in outputs relative to 2017 (Scenario A).

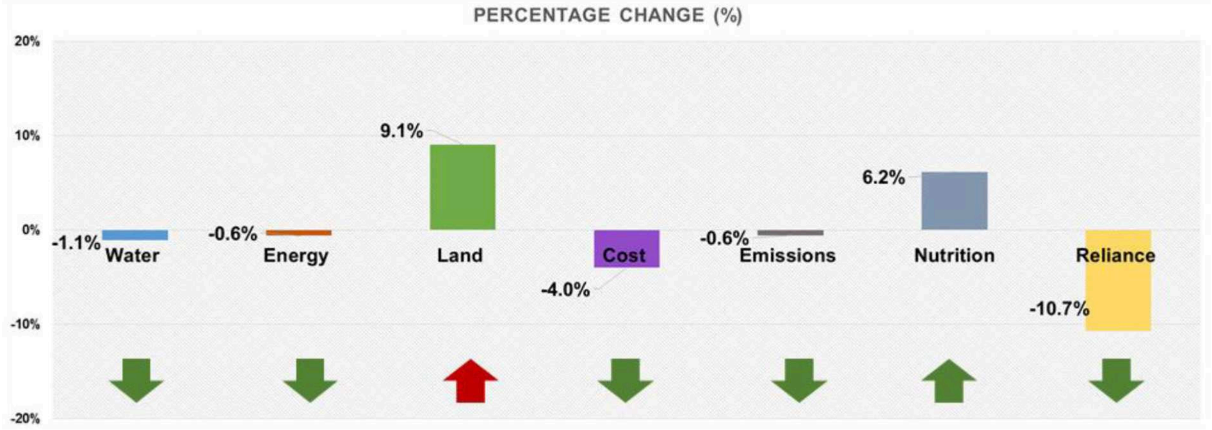


FIGURE 5
Percentage change in outputs relative to 2017 (Scenario B1).

4.1.2. Scenario A: Nutrition-centric

The current self-sufficiency of beans, chickpeas, and peas is low despite their high nutritional content and low irrigation needs. Therefore, this scenario explores the impact of increasing the self-sufficiency of these crops to 100%. The energy and water sources and ratios, as well as the currency conversion rates are kept as 2017 values. The analysis of this scenario shows that around 12% more water and energy, and 16% more land are required for achieving full self-sufficiency for beans, lentils, chickpeas, and peas (Figure 4). The arable land is estimated to be around 209,072 ha (LUC, 2017). This scenario exceeds the arable limit by 10%. This additional land requirement could be achieved by restoring degraded lands or unexploited lands, which does come at a cost that need to be further accounted for. Alternatively, improved management practices can have the potential for increasing productivity of already utilized lands and contributing to bridging this land gap. A 1.2% cost savings is noted. This is attributed to the difference in cost incurred for local production vs. import. Given that the main source of energy in the base scenario is diesel, this scenario produces 12% more emissions. Producing these crops also contributes to an increase of 6% in locally produced kcal of the overall consumed basket. Further, this also results in reducing the reliance on imports by 2.8%.

Key trade-offs: *By investing in growing our need of beans, lentils, chickpeas, and peas locally, we see cost savings, increased nutritional value in the locally produced basket, and reduced reliance on foreign markets. In return, this comes at additional water, energy, land and carbon footprint which needs to be accounted for.*

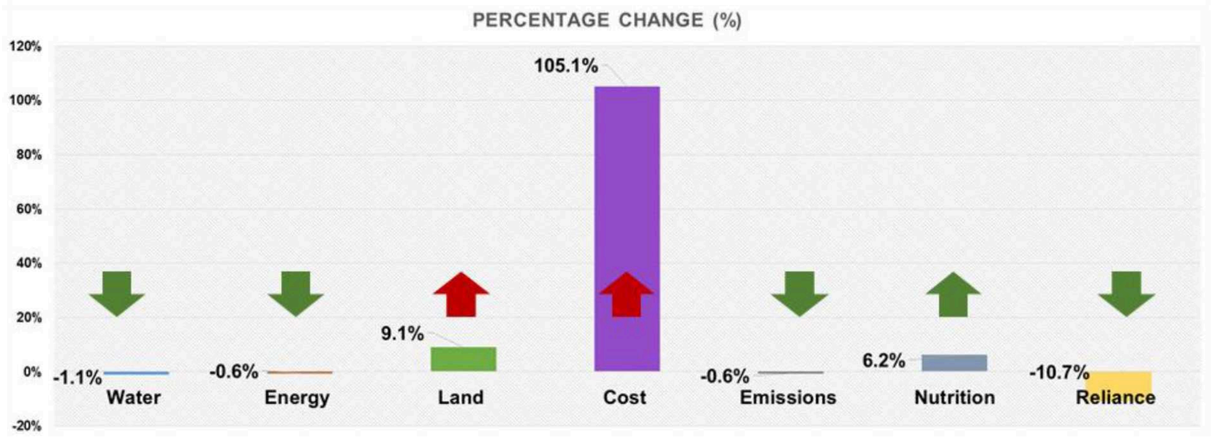


FIGURE 6
Percentage change in outputs relative to 2017 (Scenario B2).

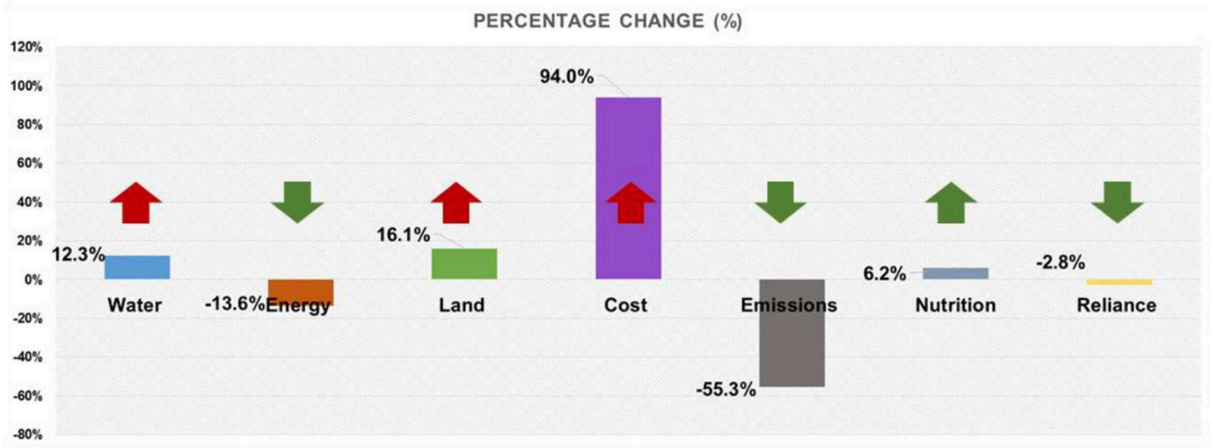


FIGURE 7
Percentage change in outputs relative to 2017 (Scenario C).

4.1.3. Scenario B1: Shifting from export to more local production

This scenario explores the possibility of reducing the local production of crops that currently exceed full self-sufficiency (SS > 100%) and are currently exported. This includes potatoes, lettuce, apple, grapefruit, citrus fruits, banana, grapes, apricots, peach, almonds, and cherries. Similar to Scenario A, Scenario B1 considers increasing the self-sufficiency of beans, lentils, chickpeas, and peas to 100%. Water and energy sources and ratios, as well as currency conversion are the same as 2017.

In this scenario, we notice a decrease in water and energy requirements, initially allocated to locally produced and exported crops in the base scenario. One of the key challenges of fully growing beans, lentils, chickpeas and peas is their low yield compared to other crops. Despite reducing the self-sufficiency of many of the currently produced and exported crops, this scenario still requires a 9.1% increase in land, compared to 2017 (Figure 5). Innovation in breeding to produce higher yielding varieties would improve these estimates. The reduction in energy requirement comes with a reduction in the carbon footprint. The increase in nutritional value is similar to that in scenario A but with a greater decrease in reliance on imports. This additional decrease compared to scenario A is attributed to limiting imports of some crops to 100% SS, which are also no longer exported according to this scenario. This analysis shows a 4% decrease in cost, this decrease is coming from replacing imported pulses by locally produced ones. This decrease in cost was slightly higher than the losses due to stop of export, hence the 4% decrease.

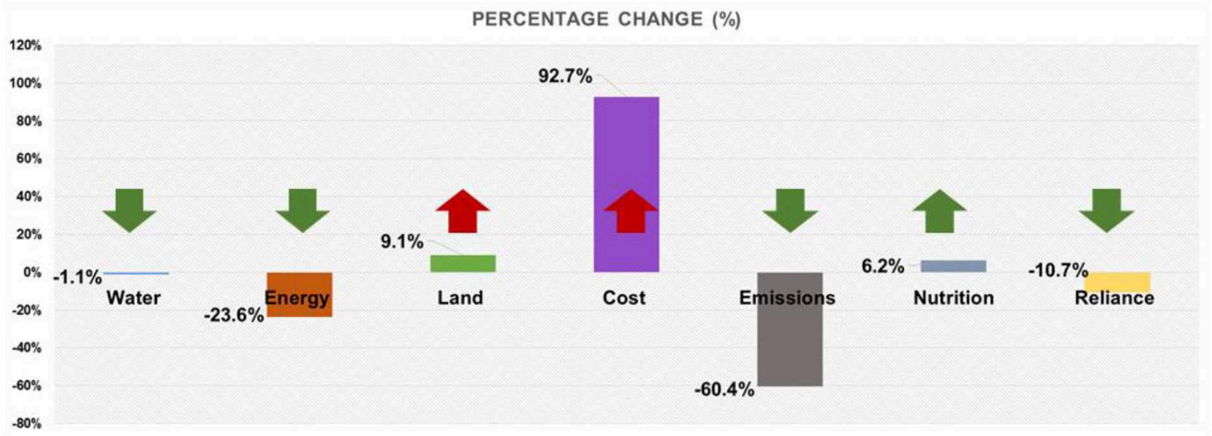


FIGURE 8
Percentage change in outputs relative to 2017 (Scenario D).

Key trade-offs: *By reallocating resources from crops currently produced above the local full self-sufficiency and exported, into producing other low self-sufficiency, high nutrition, low resource intensive crops, we can have lower reliance on foreign markets while having water, energy, cost and emission savings. Given the low yield of such crops, the other key trade-off will be more land allocation for agriculture.*

4.1.4. Scenario B2: Shifting from export to more local production under currency fluctuation

The difference between scenario B1 and B2 is in the currency conversion rate of the USD to the Lebanese Pound. This scenario explores a conversion rate of 1 USD = 4,000 LPB (compared to 1 USD = 1,500 LBP in 2017). To do this assessment, import costs and export revenues were calculated according to the new rate.

This scenario highlights the impact of the new currency conversion rate on the cost indicator. It is no surprise that given the 4,000/1,500 = 2.67-fold increase of the conversion rate there is an overall cost increase relative to 2017 (Figure 6). To do this assessment, import costs and export revenues were calculated according to the new rate. Given that many of the primary resources used on the farm are imported, it was assumed that the increase in local production costs will be equal to 50% of the increase between the 2017 and the new rate. Given the uncertainty of future currency conversion rates, it becomes more critical to identify a strategic food basket that could be produced locally, to reduce reliance on foreign markets.

Since 2019, the Lebanese Pound has lost more than 90% of its value, where 1 USD is being exchanged for 39,600 LP on the black market in 2022, compared to 1500 LP in 2019. The World Bank has described this financial crisis as one of the worst in world history (World Bank, 2022). Table 4 shows the percentage change in the demonstrated scenario cost under different LBP/USD black market conversion rates over the past years of the financial crisis. This situation makes it even more critical to develop an agricultural strategy that reduces reliance on foreign markets while improving food security and nutrition outcomes through evidence-based resource allocation.

TABLE 4 Percentage change in scenario B2 cost under different LBP/USD conversion rates.

Year	LBP/USD	%Δ Scenario cost
2017	1,500	−4
2018	1,500	−4
2019	4,000	105
2020	8,286	292.2
2021	20,000	803
2022	39,600	1,659

Key trade-offs*: The financial crises and the resulting currency fluctuation amplifies the trade-off between increasing the county's reliance on local production vs. import.*

4.1.5. Scenario C: Scenario A + renewable energy + treated water + currency fluctuation

Scenario C explores the potential of diversifying the water and energy portfolios, as it builds on the main components of Scenario A above. This scenario includes shifting from using diesel as a main energy source for pumping water on farms to solar energy. It also explores the impact of using treated wastewater as part of the irrigation portfolio.

Similar to scenario A, this scenario requires additional water and land, and provides additional nutrition and reduced reliance. Through shifting to lower energy intensive water sources (surface water and treated water) this scenario shows around 13% energy savings (Figure 7). By shifting toward a greater use of solar energy for water pumping, conveyance, and treatment, 55% of emissions are reduced. Due to the new currency conversion rate, we again see a major increase of 94% in the net cost. Given the lower $/kwh of producing energy from solar compared to diesel, producing more locally becomes more competitive, compared to import. This assessment does not currently include initial investment costs for adopting these new water and energy portfolio options. Future development of this framework would expand the cost function of the tool to include initial investment costs.

Key trade-offs: *Energy requirements, carbon emissions, and cost of local production could be reduced by shifting to less energy intensive water sources for irrigation and renewable energy, making local production more competitive compared to import.*

4.1.6. Scenario D: Scenario B2 + renewable energy + treated water + currency fluctuation

Scenario D builds on Scenario B2 while diversifying water and energy portfolios under currency conversion change. Similar to the trends in scenario C, this scenario shows greater energy savings and emissions reduction, as well as water preservation by supplementing 20% of irrigation water from treated wastewater (Figure 8).

Key trade-offs*: The key message lies in the potential of mitigating some of the negative trade-offs and improving resource savings by exploring new water and energy options for agriculture, making local production more competitive.*

4.2. Survey findings about willingness to accept

In an effort to learn about farmers' willingness to shift to different crops, alternative water sources, and alternative energy sources, we conducted an in-person survey with 200 farmers in the Beqaa Valley. We were also interested to learn about farmers' priorities to minimize water, energy, land, emissions, cost, and maximize nutritional value, as they made those decisions.

The overall results from the surveys showed that:

- The average land size of the surveyed farmers was 5.8 ha.
- 38.5% of the farmers reported their main income being from agriculture
- Land ownership: 57% owned and invested, 37% owned by farmer, 3.5% invested

The ranking related to decisions on the willingness of farmers to use alternative energy, grow different crops or use alternative irrigation sort are shown in Figure 9 and it clearly shows that these shifts would be mainly driven by the profit increase before saving on energy or water resources. The least important driver to change for the farmers was the reduction of emissions and improving nutritional value of their diets/crops.

Asked to rank options or changes that the farmers are more likely to adopt also revealed that the main incentive for change is profit which, in the Beqaa, is usually manifested in the use of alternative energy sources since energy in farming is one of the most expensive inputs. Specifically, the results of the survey revealed that farmers will most likely: (1) Use alternative energy sources as priority, (2) Grow different agricultural products as a second option, and (3) Use alternative irrigation sources (treated wastewater). Selecting treated wastewater as the least likely change to adopt shows that although farmers are somewhat willing to adopt wastewater reuse as an irrigation source, they would still be more willing to change their energy source or grow different crops than convert to using treated wastewater. Such insights are valuable in evaluating the potential adoptability of a scenario. According to the survey, farmers indicated willingness to grow different crops motivated by profit (weight = 6), energy savings (weight = 5; En), land savings (weight = 4; L), water savings (weight = 3; W), emissions reduction (weight = 2; Em), nutritional value (weight = 1; N). This could be translated to the following:

$$\begin{aligned}\text{Sustainability index (SI)} = {}&[6\%\text{Cost} + 5\%\text{En} + 4\%\text{L}\\ &+3\%\text{W} + 2\%\text{Em} - 1\%\text{N}](-1/100)\end{aligned}$$

A more favorable scenarios is one that minimize cost, energy, land, water, emissions, and maximizes nutrition which is reflected in the equation above. The higher the sustainability index, the more favorable a given scenario is for adoption, for the perspective of a specific stakeholder group.

If we take scenarios A and B1 from the farmer's perspective, for example,

$$\begin{aligned}\text{SI(A)} = {}&[6\times(-1.2) + 5\times(12.6) + 4\times(16.1) + 3\times(12.3)\\ &+(2\times12.6) - 1\times(6.2)]\times[-1/100] = -1.761\\ \text{SI(B1)} = {}&0.013\end{aligned}$$

Different stakeholder groups could have different sets of priorities and preferences which need to be accounted for. Given the developed trade-off evaluation for scenarios A and B1, combined with farmer preferences, Scenario B1 appears to be more favorable. This case might be different for a consumer vs. water provider vs. policy maker. One way of reflecting these diverse perspectives could be achieved though multi-stakeholder dialogue sessions, during which the analytics and preferences of different actors drive a dialogue about trade-offs associated with alternative pathways forward.

5. Discussions

The Mediterranean-style plant-based diet which is recommended from a nutritional and health perspective and

FIGURE 9
Overall results of farmers' willingness to adopt (WTA) changes.

shown to have a moderate environmental footprint (Naja et al., 2019), was assessed for sustainability of production in Lebanon. Resources that limit agricultural production in Lebanon are primarily water, followed by energy cost and land area. Although Lebanon produces some of the crops that constitute a Mediterranean diet, it still relies heavily on importing crops which are thought to be cheaper to import than to produce. However, the compound shocks that have face the county in the past few years, particularly its historic financial crisis, have reduced the country's ability to import food (Daher et al., 2021, 2022). That is in addition to disruptions in food supply chains resulting from the Russia-Ukraine war, two countries from which Lebanon imports 70–90% of its wheat, and secures over 25% of total calories through wheat-based products or sunflower oil (Ben Hassen and El Bilali, 2022; IFPRI, 2022). Shifting toward more local food production will have an impact on water, energy, and land resource systems (Mortada et al., 2018; Karnib and Alameh, 2020). Evaluating the impact of such decision requires a systems approach to quantify the different trade-offs and impact or resource systems that are associate with it. Building on this, we explored multiple scenarios that aim to produce more of the Mediterranean diet crops locally, which improve the nutrition of the locally produced food basket, and explore the use of alternative water and energy sources as available in Lebanon.

The framework and scenario analysis developed for this study shows that within the scope of the investigated food basket, Lebanon has the potential to be more food and nutrition secure by exploring beyond zero-sum game solutions, supported by the following three-tier approach: (1) reallocate within the existing resources pie, (2) expand the existing resources pie, and (3) create an environment that provides the necessary incentives for allowing the reallocation and expansion of the resources pie. First, by strategically reallocating resources from producing crops that exceed full self-sufficiency, to less resource intensive and nutrition rich crops with low self-sufficiency (beans, lentils, chickpeas, for example), we can have a lower reliance on foreign markets while having water, energy, cost, and emission savings. A trade-off exists between allocating resources to produce more food for local consumption vs. producing more for export. The uncertainty of future currency conversion rates amplifies the advantage of higher self-sufficiency as a key contributing factor to improved food security. Second, expanding the existing potential of resources could be done by improving efficiencies and management practices in current operations in one hand, and exploring synergies across different sectors in another. There is a need for expanding research for improving the yields and productivity of highly nutritious crops with low irrigation requirement by looking at better varieties, cropping patterns, technologies, and breeding. Intercropping or understory cropping systems could be used to minimize land use or restoration of marginal degraded land. That is in addition to improving irrigation efficiencies. This would be catalyzed by better metering and accounting for water use on farms. Investing in renewable energy expansion on farms and exploring the potential of treated water for agriculture, have the potential to improve the competitiveness of local production compared to import. Specializing in high-value cash crops for export can further play a role in expanding financial returns into the sector. Third, it is critical to create an environment with the necessary incentives for farmers to grow new crops, switch to alternative energy and water sources, invest in new more efficient technologies while accounting for their preferences and willingness to change practices on their farms. For any change to be adopted there needs to be a long-term agricultural strategy and policies set by the government, which will need to consider responding to trade risks and value chain disruptions (Al-Saidi and Hussein, 2021). Building private-public partnerships to support the investments needed could facilitate the adoption some of these solutions. It was obvious that farmers' interests and willingness to change are primarily driven by maximizing profit, followed by reduced energy use then water use. The least important driver for change from the farmers' perspective is improving environmental conditions and improving diet quality.

Questions remain about the interlinkages between agricultural production and any changes that occur therein, with other sectors that use the same resources. The feedback from farmers implies that there are avenues related to trade, import/export, markets, and general strategies that still need assessment. The framework and analytics developed in this study should be used to catalyze an evidence-based multi-stakeholder dialogue to guide policies and strategies in agriculture.

6. Conclusions

Given the uncertainty of future currency conversion rates, it becomes more critical to identify a strategic food basket that could be produced locally, to reduce reliance on foreign markets. Moving forward with WEF framework analysis, it is important to account for spatio-temporal distribution, soil suitability maps, and variability and its roles in making these trade-off decisions. This allows the development of this framework into a scalable tool that use customized WEF analytics to address questions at the country and regional levels. Using these analytics could play a role in engaging multi-stakeholders and catalyzing cross-sectoral dialogue around tradeoffs and future pathways and development strategies. This could be facilitated through engagement workshops geared at "*gamifying*" the developed analytics to drive that trade-off dialogue. Integrative agricultural strategies need to account for barriers to implementation that might results from existing farmer preferences. Understanding the preferences and perspectives of the broader group of cross-sectoral stakeholders would allow for a better evaluation of possible interventions and policy changes. On the technical side, improvement in the analytics can be made through the improvement of functions in the current evaluation including cost assessment of different scenarios which currently only look at the difference between the cost of local production and import on one hand and revenues from export on another. Further study and analysis of existing incentive structures and their impact on current farmer preferences are also needed, without omitting the urgent need for reliable country and basin level data on water accounting, water resources, agronomic practices, energy use, food consumption, and other relevant parameters.

Author's note

This study quantifies the trade-offs associated with producing more of Lebanon's food basket locally, under different food production, water, and energy scenarios in light of the country's currency devaluation. This study aims to: (1) Identify and quantify the critical interconnections between water, energy, nutrition, and food systems in Lebanon. (2) Develop a framework to quantify the trade–offs associated with adopting interventions within current water, energy, and agriculture portfolios and practices. (3) Evaluate producers' perceptions of their willingness to implement proposed changes in crop production, renewable energy, and water reuse. Findings from this study can play a role in informing policymaking and planning in Lebanon, as the country works to implement the UN Sustainable Development Goals. All authors contributed to the article and approved the submitted version.

Data availability statement

The original contributions presented in the study are included in the article/Supplementary material, further inquiries can be directed to the corresponding author.

Ethics statement

The studies involving human participants were reviewed and approved by American University of Beirut IRB protocol ID: SBS-2019-0490. Written informed consent for participation was not required for this study in accordance with the national legislation and the institutional requirements.

Author contributions

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

Supplementary material

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fsufs.2022.969248/full#supplementary-material

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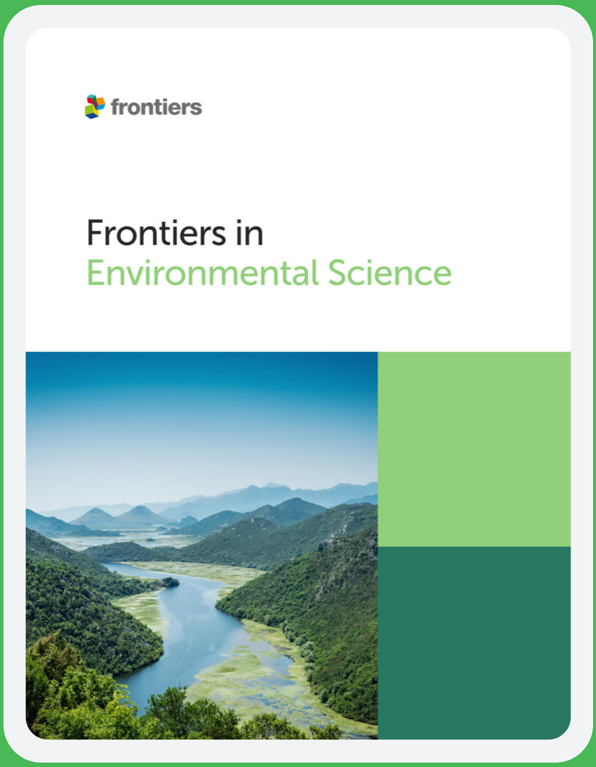

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