



# Optimization-Based Systems Modeling for the Food-Energy-Water Nexus

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## Abstract

**Purpose of Review:** Optimization-based methods for the food-energy-water nexus can assist decision-making on critical infrastructure but are limited in scope and applicability. We provide an overview of optimization-based systems modeling techniques for operations researchers and systems modelers studying the nexus.

**Recent Findings:** We find that the literature has contributed to the understanding of nexus interdependencies and has provided a framework for sustainability studies. We observe that the majority of the papers expand bottom-up models for one or two nexus components into the three, which may lead to asymmetric representation of the three sectors. Socioeconomic and political economy drivers are often exogenous to the models.

**Summary:** The vast majority of papers can be further enhanced to account for local priorities, and the underlying decision-making process of stakeholders across the supply chains and at the interdependencies. Greater regional downscaling and technological detail along with more robust data could also enhance nexus systems modeling.

**Keywords** Optimization · Food-energy-water nexus · Systems · Economic modeling

## Introduction

### Motivation

Reaping the benefits of scarce natural resources intensifies the competition between groups with conflicting interests, e.g., households and national policy-makers [1] or between countries at the international level [2]. Hoff [3] stresses the trade-off between scarcity of the food, energy, and water (FEW) resources and ensuring access to water and food for everyone. Food and energy security can be addressed through regional infrastructure investment coordination, when neighboring countries have different FEW resources in abundance [4]. Moreover, the *energy* and *agriculture, forestry, and other land use* sectors are responsible for 59%

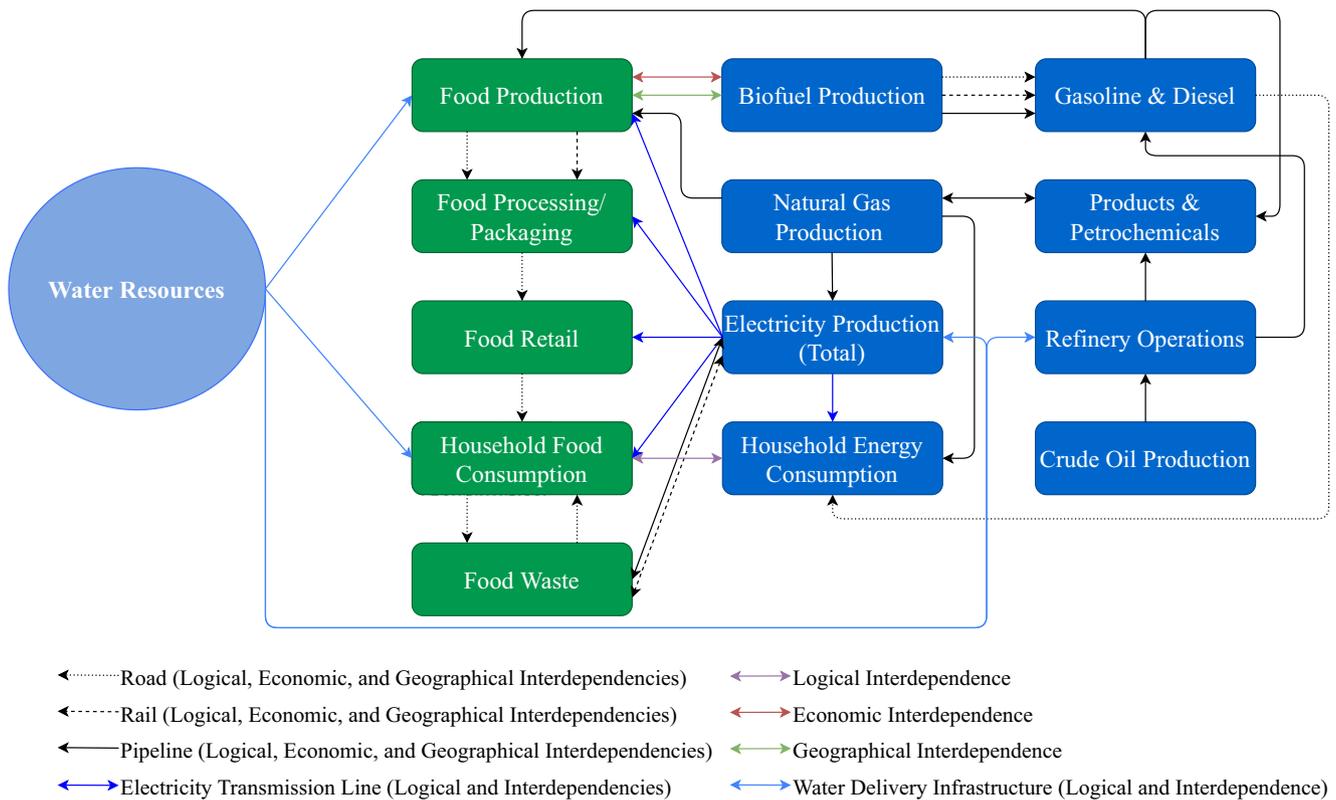
of global greenhouse gas emissions in 2018 [5]. Designing and operating the resource sectors more efficiently can alleviate the pressure to physical infrastructures but can also impact local livelihoods [6]. Although mathematical modeling—specifically optimization techniques—can address efficiency related questions, they need to be enhanced to account for the political and social factors affecting infrastructure development, including local priorities, entitlements, and power relationships between different groups. Among the resource sectors, FEW infrastructures are not only critical for human livelihood, but also strongly interconnected [7]. For example, water is the major production factor of hydropower plants and is used for irrigation in crop production (geographical interdependency, detailed in [8]). For that, the availability of water infrastructure can impact the development of energy infrastructure and agricultural land. Biofuels are used in both electricity production and for gasoline blending (physical interdependency, detailed in [9–11]), with water and other energy-intensive inputs consumed in crop production and in processing. Natural gas is purchased by gas-fired power plants (logical/economic interdependency) and is used as feedstock for

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**Fig. 1** Major interdependencies between the food, energy, and water supply chains

petrochemicals production. Petrochemicals and food production generate wastewater that pollutes the existing water resources. We summarize major FEWs interdependencies in Fig. 1.

The goal of the nexus is to minimize conflicts between and enhance synergies among the three sectors in order to improve system efficiency [6]. Beyond the physical interdependencies of the three resource sectors, Bazilian et al. [12] argue that FEW sectors are tightly connected and are similar in many aspects, including international trade, heterogeneous supply and demand, and high regulation. Thus, the three sectors need to be treated collectively. The authors also identify climate change and access to FEW services as major challenges that call for more efficient use of resources. However, optimizing technological efficiency often conceals the social and political ramifications of policy interventions [13], and can instead aggravate the vulnerability of particular groups [1]. Moreover, the development of regional water infrastructure can be affected by economic and political drivers. In the case of Sub-Saharan Africa, the lack of human, institutional, and financial capital restrains the development of irrigation infrastructure for domestic agricultural production, which impacts the dietary intake of domestic population and aggravates domestic poverty [14]. Matthews et al. [15]

argue that China’s investments on energy infrastructure of the Association of Southeast Asian Nations may not always be economically profitable, but serve international relationships or affect other macroeconomic goals that are prioritized by China’s policymakers.

Therefore, for the nexus to be a helpful tool in achieving the Sustainable Development Goals (SDGs), it needs to acknowledge the limitations of optimization frameworks and account for individual livelihoods, the environment [2], and other macroeconomic and political drivers [15]. The fact that there does not exist a single definition of the FEW-nexus<sup>1</sup> reflects the debate regarding the nature and goal of the nexus. In this paper we treat the FEW-nexus as an integrated framework that accounts for all three sectors and their interdependencies.

Individual models have been developed in the literature for the three individual resource sectors. Therefore, developing tools for the nexus overlaps with the literature on model coupling. More specifically, when interactions with another sector are critical for the development of a single sector or system, modelers can opt to expand the

<sup>1</sup>The nexus is also referred to as food-energy-water (FEW) or energy-water-food (EWF), see [16–18].

sectoral detail of existing tools. Along this line, Ringler et al. [19] and Endo et al. [20], argue that the FEW-nexus can be viewed as an extension of the Integrated Water Resource Management (IWRM) framework, introduced in the 1990s [21]. While IWRM has an explicit focus on water management, the FEW-nexus aims at understanding all three sectors in detail, along with their interdependencies.

The alternative to expanding a single model is linking existing sectoral models. In the case of the FEW-nexus, coupling bottom-up sectoral models has been employed, to the extent that hardly any new methodologies were developed specifically for the FEW-nexus [22]. Finally, the FEW-nexus has motivated the development of new tools where all three sectors are represented in a single, integrated framework.

## Objective

In this paper we focus on FEW-nexus optimization-based methods since they allow for a bottom-up representation of interactions between FEW systems. We distinguish between *top-down* and *bottom-up* approaches and discuss applications of bilevel optimization. More specifically, we aim to provide a literature review of FEW-nexus systems models and their application, identify significant trends, and discuss potential enhancements.

For the purpose of this study, we searched in Google Scholar, between June 20th and June 30th 2020, for publications in peer-reviewed journals that self-identify as “FEW-nexus” papers and employ optimization modeling to answer their research questions. Reports, book chapters, and other non-peer-reviewed articles were excluded from this review. We also excluded papers that omitted the decision-making process of all agents in the FEW-nexus. Given how broad the definition of the FEW-nexus is, we included papers that may not self-identify as “nexus” papers, but account for the interactions between any combination of the three resource sectors. We distinguish ourselves from other reviews in that we focus on optimization-based methods, point out the nuances in modeling implementation, and provide the main findings of each article. *Therefore, this review aims at providing systems modelers and the operations research community with an overview of optimization-based modeling techniques for the FEW-nexus.*<sup>2</sup> Our paper should not be treated as a systematic review of the literature, but a guide for researchers on the diversity of optimization-based methods that have been used in the FEW-nexus. Table 1 below provides a full list of citations, the type of model that was developed, and the mathematical formulation of the problem.

<sup>2</sup>Urbinnati et al. [23] report 1455 nexus-related papers.

## Overview of Optimization-Based Methods

In an optimization problem we find the minimum of a function, called the *objective function*, such that its argument satisfies a set of conditions known as *constraints*. Concisely, an optimization problem can be written as

$$\min_{x \in R^n} f(x; \theta) \text{ subject to } x \in X \quad (1)$$

where  $x$  corresponds to the decision to be taken, which is typically in the decision-maker’s control. Such a decision should belong to a *feasible set* denoted by  $X$ , and  $\theta$  correspond to the parameters of the optimization problem, i.e., everything that is exogenous or external to the optimization problem. With mild technical assumptions on  $f$  and  $X$  we can (i) model a wide variety of problems that are interesting and useful for real-life decision making, and (ii) solve them efficiently using modern computational techniques [24].

Collections of problem (1) can be used to represent decision-making of individual agents in a *non-cooperative game*. More specifically, each agent  $i$  solves their own optimization problem

$$\begin{aligned} \min_{x_1 \in X_1 \subseteq R^n} f_1(x_1; x_{-1}, \theta_1), \\ \min_{x_2 \in X_2 \subseteq R^n} f_2(x_2; x_{-2}, \theta_2), \\ \dots \min_{x_k \in X_k \subseteq R^n} f_k(x_k; x_{-k}, \theta_k) \end{aligned} \quad (2)$$

where  $x_i$  is the decision variable of agent  $i$ ,  $x_{-i}$  are the decision variables of all agents other than  $i$  whose decisions affect the objective of agent  $i$ . Similarly,  $\theta_i$  correspond to the parameters of the optimization problem of agent  $i$ . In order to solve (2) we derive the Karush-Kuhn-Tucker (KKT) conditions of each agent and solve them simultaneously. The KKT conditions of all agents form a Mixed Complementarity Problem (MCP). With mild technical assumptions on  $f_i$  and  $X_i$ , we can compute a Nash Equilibrium of (2) by solving the MCP [25].

## Bottom-up Models

Bottom-up models explicitly represent agent interactions, supply-chain interactions, and supply chain technological detail [26]. We characterize a model “*bottom-up*” when it incorporates either one or more of the above three features.

At the food-water nexus, crop yield models often incorporate water interactions, e.g., IFPRI’s<sup>3</sup> IMPACT-WATER model [27], which could explain the few mentions under FEW-nexus. Similarly, Benli and Kodal [28] enhance a crop production model with water supply constraints for

<sup>3</sup>International Food Policy Research Institute (IFPRI).

**Table 1** Summary of FEW-nexus systems models. Including food-water (FW), energy-water (EW), food-energy (FE), and FEW publications

Citation	Scope	Type of model	Optimization model
(-) Avraamidou et al. [85]	FEW	<i>Bottom-up</i> land-use allocation model, expanded to account for water and energy interactions	Non-Cooperative game solved as a Bi-Level Mixed Integer Program
(-) Fan et al. [70]	EW	<i>Computable General Equilibrium</i> model	Equilibrium Model
(-) Memarzadehet al. [87]	FEW	<i>Integrated</i> water, energy, and food interactions in a single framework	Machine Learning. Dynamic Bayesian Network
(-) Nie et al. [59]	FEW	<i>Bottom-Up</i> land-use model, enhanced for energy and water interaction	Mixed Integer Nonlinear Program
(-) Sankaranarayanan et al. [33]	FEW	<i>Integrated bottom-up</i> food, energy, and water systems in a single framework	Mixed Complementarity Problem
(-) Su et al. [73]	EW	<i>Coupling</i> a <i>Computable General Equilibrium</i> model with a <i>bottom-up</i> model of water infrastructure	Integrated framework, using a different algorithm for each component
(-) Zhou et al. [71]	EW	<i>Computable General Equilibrium</i> model	Equilibrium Model
(-)Ahmetović et al. [33]	FEW	<i>Bottom-up</i> model of corn-based ethanol production, enhanced for water and energy use	Nonlinear Program
(..) Allam and Eltahir [67]	FEW	<i>Coupled bottom-up</i> land-use model and water and energy operations model	Integrated framework, using a different algorithm for each component
(..) Bellezoni et al. [63]	FEW	<i>Input-Output</i> model enhanced to account for the economic interactions	Linear Program
(..) Da Silva et al. [81]	FEW	<i>Integrated Assessment Model</i>	Equilibrium Model
(..) Jalilovet al. [68]	FEW	<i>Integrated</i> water, energy, food models in a single framework	Nonlinear Program
(..) Karan et al. [66]	FEW	<i>Integrated</i> water, energy, food models in a single framework	Stochastic Program
(..) Karnib [82]	FEW	<i>Coupled Input-Output</i> model of energy, water, and food interactions and resources cost minimization model	Integrated framework, using a different optimization algorithm for each component
(..) Kraucunas et al. [78]	FEW	<i>Integrated Assessment Model</i>	Equilibrium model
(..) Li et al. [61]	FEW	<i>Coupled bottom-up</i> water, energy, and food models	Integrated framework, using a different optimization algorithm for each component
(..) Li et al. [62]	FEW	<i>Integrated</i> water, energy, food models in a single framework	Multi-stage process involving different optimization methods in each step
(..) Miralles-Wilhelm and Muñoz-Castillo, [80]	FEW	<i>Integrated Assessment Model</i>	Equilibrium Model
(..) Mouratiadou et al. [57•]	FEW	<i>Coupled bottom-up</i> models of water, energy, and land use	Nonlinear Program
(..) Ringleret al. [75]	FEW	<i>Coupled Computable General Equilibrium</i> with a <i>bottom-up</i> agriculture model	Integrated framework, using a different algorithm for each component
(..) Su et al. [74]	FEW	<i>Coupled Computable General Equilibrium</i> with a <i>bottom-up</i> water management model	Integrated framework, using a different algorithm for each component
(..) Tan et al. [90]	FEW	<i>Integrated</i> water, energy, food submodules in a single framework	Differential Evolution
(..) Tian et al. [65]	FEW	<i>Coupled</i> ecosystem, economic, and climate models, with <i>bottom-up</i> representation of the water, energy, and food systems	Integrated framework, using a different optimization algorithm for each component
(..) van Vuuren et al. [79••]	FEW	<i>Integrated Assessment Model</i>	Nonlinear Program
(..) Woldesellasse et al. [87]	FW	<i>Coupled</i> crop water demand model and water resources allocation model	Integrated framework, using a different algorithm for each component
(..) Yuan et al. [83]	FEW	<i>Life Cycle Assessment</i> model	Linear Program

**Table 1** (continued)

Citation	Scope	Type of model	Optimization model
(·) Zeng et al. [58]	FEW	<i>Bottom-Up</i> water reservoir system, enhanced to account for food, energy, and climate	Stochastic Program
(·) Zhou et al. [72]	FEW	<i>Computable General Equilibrium</i> model	Mixed Complementarity Problem
(·)Gao et al. [60]	FEW	<i>Bottom-Up</i> capacity expansion of food production and coal mining, processing, and conversion, enhanced for water use	Linear Program
(·) Namanyet al. [64]	FEW	<i>Integrated bottom-up</i> water, energy, and food systems in a single framework	Stochastic Linear Program
Bakker et al. [31]	FW	<i>Bottom-up</i> agricultural model that accounts for soil moisture and water retention	Mixed Complementarity Problem
Benli, and Kodal [28]	FW	<i>Bottom-Up</i> crop production model, enhanced with water supplies constraints	Nonlinear Program
Bernardi et al. [38]	EW	<i>Life Cycle Assessment</i> model of biofuel production, enhanced for its water footprint	Mixed Integer Linear Program
Bernardi et al. [35]	EW	<i>Bottom-Up</i> biofuel supply chain model, enhanced for water usage.	Linear Program
Cobuloglu and Büyüktaktakın, [50]	FE	<i>Bottom-up</i> energy and food crop model	Mixed Integer Linear Program (MILP)
Cobuloglu and Büyüktaktakın, [51]	FE	<i>Bottom-up</i> energy and food crop model	Stochastic Mixed Integer Nonlinear Program (MINLP)
Cuberos Balda et al. [54]	FE	<i>Bottom up</i> land use model coupled with a food and fuel demand model	Nonlinear Program
Dhaubanjari et al. [43]	EW	<i>Bottom-Up</i> optimal power flow model, enhanced for water interactions	Linear Program
Dubreuil et al. [42]	EW	<i>Hard-link</i> of an energy system model and a water system model	Linear Program
Fernández García et al. [41].	EW	<i>Bottom-up</i> energy production model, coupled with a water and energy use optimization model	Integrated framework, using a different optimization algorithm for each component
Garcia and Yu [36]	EW	<i>Life Cycle</i> water footprint model, enhanced with energy interactions	Mixed Integer Nonlinear Program
González-Bravo et al. [46]	EW	<i>Integrated bottom-up</i> water and power distribution models in a single framework	Mixed Integer Nonlinear Program
González-Bravo et al. [47]	EW	<i>Integrated bottom-up</i> water and power distribution models in a single framework	Mixed Integer Nonlinear Program
Govindan and Al-Ansari, [91]	FEW	Agents in all sectors are represented in an <i>integrated</i> framework	Machine Learning. Markov Decision Process
Grossman and Martín, [34]	EW	<i>Bottom-Up</i> processes design of a bioethanol production plant	Integrated framework, using a different optimization algorithm for each component
Guo et al. [52]	FE	<i>Bottom up</i> biofuel production model expanded to account for life-cycle carbon emissions and agents behavior through agent-based simulations	Integrated framework, using a different algorithm for each component
Humpenöder et al. [53]	FE	<i>Bottom-up</i> land-use model, expanded to account for bioenergy production	Nonlinear Program
(·) Karupiah et al. [49]	FEW	<i>Bottom-up</i> model of corn-based ethanol production, enhanced for water and energy use	Nonlinear Program
Khan et al. [39]	EW	<i>Hard-link</i> of a <i>bottom-up</i> energy production and capacity expansion model and a <i>bottom-up</i> water extraction, treatment, and use model	Linear Program

**Table 1** (continued)

Citation	Scope	Type of model	Optimization model
Lautenbach et al. [89]	EF	<i>Bottom-Up</i> biodiesel crop production model, enhanced for water quality	Genetic Algorithm. Non-Dominated Sorting Algorithm (NSGA-II)
López-Díaz et al. [37]	EW	<i>Coupled bottom-up</i> watershed and biofuel refining models	Mixed Integer Linear Program
Martinez and Blanco, [30]	FW	<i>Bottom-up</i> agricultural model, expanded to account for water supply	Nonlinear Program
Mekonnen et al. [55]	FE	<i>Bottom up</i> farm-level agricultural production and household biofuel use model	Optimization problem
Mortada et al. [29]	FW	<i>Bottom-Up</i> crop production and food consumption model, enhanced to account for water security	Nonlinear Program
Pereira-Cardenal et al. [40]	EW	<i>Bottom-Up</i> irrigation agriculture model, enhanced with an electricity dispatch model	Stochastic Dual Dynamic Programming
Satti, Zaitchik, and Siddiqui, [44]	EW	<i>Bottom-up</i> hydro-economic model	Nonlinear Program
Tsolas et al. [48]	EW	<i>Integrated</i> energy and water models in a single framework	Heuristic method
Wanjiru and Xia, [45]	EW	<i>Bottom-Up</i> end-user water management model, enhanced for energy consumption	Linear Program
Weng et al. [76]	FE	<i>Computable General Equilibrium</i> model, expanded to account for land allocation	Equilibrium Model
Zhang and Vesselinov, [84]	EW	<i>Integrated bottom-up</i> water and food systems in a single framework	Bilevel Program
(·) Burrow et al. [56]	FEW	<i>Integrated bottom-up</i> water, food, and electricity supply systems in a single framework	Mixed Integer Linear Program

·Papers that account for interactions between all three resources sectors

··Papers modeling all three resources sectors

Southeast Anatolia. Mortada et al. [29] build a bottom-up crop production and food consumption model, enhanced for water security and find that different definitions of water and food security can lead to different crop switching strategies. Martinez and Blanco, [30] expand the Common Agricultural Policy Regionalised Impact (CAPRI) model to account for changes in water supply. Using CAPRI, they are able to identify the cost of water and irrigation efficiency as the main drivers behind agricultural land development in the case of Andalusia, Spain. Bakker et al. [31] built the Food Distributed Extendable Complementarity Model (Food-DECO), an agricultural model for Ethiopia that incorporates stakeholders' objectives along the food supply chain and accounts for water retention and soil moisture. Using Food-DECO they simulate a crop failure scenario and assert that expansion of food distribution capacity can result in greater nutritional disruption in the regions affected the most. Finally, Sankaranarayanan et al. [32] model competing stakeholders in the FEW-nexus of Ethiopia and find that the revenues of food distributors and storage operators increase more than the revenues of crop producers when international revenues increase due to teff exports.

Many energy-water papers are centered around biofuel production. Ahmetović et al. [33] enhance a corn-based ethanol production model for water and energy use and conclude that wastewater management in industrial operations can be reduced. Along the same line, Grossman et al. [34] and Bernardi et al. [35] find that water consumption for bioethanol can drop based on the configuration of the plant model. Garcia and Yu, [36] study how the energy efficiency of water affects the lifecycle water footprint of energy-based products. López-Díaz et al. [37] expand a biorefineries operation and planning model to account for land development and the interactions with the surrounding watershed. They conclude that water consumption is lower when bio-refiner expected profit is higher in Mexico. Bernardi et al. [38] use a detailed Life Cycle Assessment (LCA) model to capture the water consumption for biorefining. They suggest that stress on water infrastructure can be high even for an attainable greenhouse gas target.

For the energy-water interactions, most papers reviewed here coupled or expanded an energy operations or planning model to account for water interactions. Khan et al. [39]

hard-link an energy production and capacity expansion model and a water extraction, treatment, and use model. Using a scenario of increased energy and water demand in Spain, they compare the results of fully integrated and non-integrated energy-water systems. They conclude that the solution to the fully integrated case is less costly and more energy efficient. Pereira-Cardenal et al. [40] conclude that in the Iberian Peninsula high irrigation marginal benefits are sub-optimal when irrigation is allocated to low productivity hydropower plants. They arrive in this result by coupling a power system operation model with a hydrological system. Fernández García et al. [41] couple an energy production model with a water and energy use model for a system in Southern Spain and derive the optimal operation of the irrigation network. Dubreuil et al. [42] use an energy system model to compute energy inputs to a water system model. They report a 60% decrease in desalinated water production in the Middle East for a water-saving scenario. For Nepal, Dhaubanjari et al. [43] find that water deficits vary depending on the season. They perform a multi-objective analysis using an optimal power flow model, coupled with a water resources model. Satti et al. [44] build a bottom-up hydro-economic model for the Sudanese section of the Blue Nile. Given the available water resources, their model computes the optimal water allocation to hydropower production and irrigation.

More nuanced energy-water applications include end-user water management, modeling of stakeholder incentives, and modeling the FEW-nexus interactions using a grid. Wanjiru and Sia [45] focus on energy consumption of end-user water management and find that water from direct municipal sources can significantly increase water savings. González-Bravo et al. [46, 47], model the objectives of different FEW-nexus stakeholders. They conclude that economic and social objectives affect the results more than environmental objectives of stakeholders in Northwestern Mexico. Tsolas et al. [48] represent energy and water resources as nodes and energy-water interactions as interconnections in a grid. Their model minimizes energy and water consumption of Spain. They also use their model to compute the total redundant energy and water in California.

The majority of the food-energy nexus papers reviewed here are also centered around biofuel production. Specifically, Karuppiyah et al. [49] use a detailed model of corn-based ethanol production, enhanced for water and energy use to provide directives for the reduction of steam consumption. Cobuloglu and Büyüktaktın [50] build a food and energy crop production model that decides the optimal allocation of crop yield to food plants or a biorefinery at Hugoton, Kansas. They find that planting switchgrass is more profitable than corn in cropland. In their 2017 study, Cobuloglu and Büyüktaktın [51] use a stochastic version of the food and energy crop production model that

incorporates uncertainty in crop yield and yield prices and compare economic and environmental benefits between the stochastic and deterministic formulation for the same case study. Guo et al. [52] couple a model of biomass cultivation, and biofuel production and distribution with a LCA model and an agent-based model. They apply the proposed framework to case studies in the Philippines, South Africa, and Thailand. The authors identify agricultural waste recovery and non-food biomass planted on marginal land as sustainable actions that contribute to food and energy security of the three countries. Humpenöder et al. [53] argue that the tradeoff between bioenergy production and SDGs heavily depends on future food demand. For their analysis, they expand the global land-use model MAgPIE<sup>4</sup> to account for bioenergy production. Cuberos Balda et al. [54] couple a land use model with a food and fuel demand model to study food and energy security in Miyagi Prefecture, Japan. They assert that establishing energy self-sufficient farms in abandoned land can contribute to increased biofuel production without compromising food security. Mekonnen et al. [55] study a representative rural household in Ethiopia that can allocate their labor to agricultural production or biomass collection for domestic energy uses. Their analysis shows that on-farm fuelwood production allows for easier fuelwood collection for households and allows households to invest more labor in crop production instead.

The majority of the bottom-up systems models in this review that account for all FEW interdependencies focus on water management and agriculture. Burrow et al. [56], build a water reservoir operation and expansion model that accounts for agriculture production, water storage, and power supply in northeastern Colorado. They find that small reservoirs can mitigate local agricultural water shortages. Mouratiadou et al. [57] couple a global vegetation and hydrology model with a land use model and a bottom-up energy model to study water demand for energy and food. They find that under climate change, irrigation of bioenergy crops leads to higher water requirements. Zeng et al. [58] couple a water reservoir system with a soil and water assessment tool and find that low water flow leads to greater discrepancies between water, energy, and food supply and demand in the Jing River basin of China. Nie et al. [59] build a crop-livestock model and compute the optimal energy, water, and land resources needed to meet different targets of total profit, food production, total energy use, total water use, and total environmental impact in Yucheng, China. Gao et al. [60] develop a capacity expansion model of food production and coal mining, processing, and conversion, enhanced for water use for China. Li et al. [61] and [62], use stochastic programming and chance-constrained

<sup>4</sup>Model of Agricultural Production and its Impact on the Environment (MAgPIE).

optimization to study FEW interactions in the agricultural sector in China. They find that crop farming generates more economic benefit and less pollution than livestock farming. Bellezoni et al. [63] use Input-Output equations to grasp FEW interactions in Brazil and derive that sugarcane expansion in the Goiás region would minimally affect water and land use. Namany et al. [64] compute the minimum energy and water cost of food production in Qatar using stochastic programming. They conclude that the additional investment in renewables and water infrastructure requires high investment with a short capital recovery time. Tian et al. [65] couple an agricultural model with a water and energy allocation model and a regional climate model to study the impact of nitrogen fertilizer reduction in China. They find that national soil N<sub>2</sub>O emissions can be cut by 50% while crop production shrinks only by 2% for a 60% decrease in fertilizer use. Karan et al. [66] study FEW interactions at the household level. In all climate-related scenarios simulated, the largest portion of household payments were for energy needs while the second largest payment was for water needs.

The literature also includes water-centric FEW models that analyze energy production and agricultural tradeoffs of hydropower dams, where new dams increase energy supply for upstream countries but can alter water supply for irrigation in downstream countries. Allam and Eltahir [67] study the optimal allocation of land and water resources considering agriculture expansion and hydropower generation in the upper Blue Nile basin. Jalilov et al. [68] build an operational model of the Rogan Dam in the Amu Darya River Basin and focus on the economic and agricultural benefits of Tajikistan and Uzbekistan.

### Top-down Models

Top-down models emphasize the interactions of a system with the macro-economy. Given our focus on optimization-based systems models, we only refer to Input-Output (IO) models and LCA models when they account for inter-sector economic interactions. We focus on the other two established top-down methods, namely Computable General Equilibrium (CGE) models and Integrated Assessment Models (IAMs).

A CGE model includes all sectors of an economy and economic transactions between them. Sectoral decisions are represented by a single agent that decides their output and inputs of production factors by maximizing their utility or minimizing their production cost [69]. Fan et al. [70] find that an increased water fee coupled with an emissions tax enhances emissions reduction and water conservation. Zhou et al. [71] and [72], couple a CGE with different bottom-up water management models of China. They find that an energy tax contributes to water preservation. Su

et al. [73] and [74], evaluate the impact of CO<sub>2</sub> mitigation strategies on water savings in China, with a focus on pollutants emission. Ringler et al. [75] couple a CGE with IFPRI's IMPACT model, an IAM focused on agricultural production. They find that food security is minimally affected by a fossil fuel tax. The impact is further alleviated if reduced emissions mitigate climate change. Weng et al. [76] focus on China's food security. They find that the projected biofuel expansion is based on energy crops planted mostly in marginal land and leads to little land reallocation of rice, forest, and grassland fields to non-grain feedstock. The study is based on a CGE that is expanded to incorporate land use management and crop switching.

Although IAMs are not necessarily optimization-based models, we have included them because they have traditionally been used along with CGEs in economic top-down analysis and have a structure that mimics optimization. IAMs are equilibrium models that are founded on assumptions that make it easier to account for interactions with the climate and the environment compared to GCEs [77]. Kraucunas et al. [78] introduced the Platform for Regional Integrated Modeling and Analysis (PRIMA) model, which extends GCAM<sup>5</sup> to include more detailed FEW and land submodules. Van Vuuren et al. [79••] use IMAGE<sup>6</sup> to study how technological change and human behavior can help in achieving the SDGs. They find that hunger eradication and energy access do not intensify climate change significantly; and in scenarios where sectors transform marginally, the SDGs are not met. Moreover, meeting the environmental objectives defined in the SDGs would require substantial improvement of energy efficiency and agricultural yield. Miralles-Wilhelm and Muñoz-Castillo [80] use GCAM and find that the primary conflict upon introducing climate policies according to the Nationally Determined Contributions in Latin America is between electricity production and crop production that compete for water resources. Da Silva et al. [81] use GCAM and find that bioenergy coupled with Carbon Capture and Storage allows for greater decarbonization in Latin America. The approach used in both studies is similar.

Finally, enhanced LCA and IO models have also been expanded and used for economic system assessment. LCA models track the environmental impact of a product across the entire life-cycle of the inputs used for the product, while IO models account for all sectoral interactions in an economy. Karnib [82] couples an IO model of energy, water, and food interactions with a resources cost minimization model and finds the cost of the additional water and energy resources used when food production is increased. Yuan et al. [83] couple a LCA model with a climate

<sup>5</sup>Global Change Assessment Model (GCAM).

<sup>6</sup>Integrated Model to Assess the Global Environment (IMAGE).

simulation model and conclude that for water conservation purposes, rice cultivation needs to be decreased across Taiwan; however demand for bioethanol production leads to an increase of rice and corn cultivation in southern Taiwan.

## Bilevel Optimization Applications

Bilevel optimization, which includes leader-follower games, has also been employed for the study of FEW-nexus problems. Zhang and Vesselinov [84] form a bilevel problem that maximizes power generation in the upper level and minimizes total system cost in the lower level, i.e., the sum of the costs of water delivery, fuel, electricity production, and the capital cost of power plants. They find that coal-fired plants barely expand compared to gas-fired plants when population increases. Avraamidou et al. [85] develop a bilevel model where the government minimizes FEW conflicts as the leader and the follower is a land developer who seeks to maximize their profit. They compute a 20.4% improvement of FEW conflict metrics when the government subsidizes renewables and crop production.

## Conclusions

### Summary

We find that there does not exist a single established FEW framework, even for the subset of optimization-based systems models, in accordance with Albrecht et al. [22]. Moreover, very few of the references categorized as bottom-up consider decision making at the farm or plant level. Two out of the three FEW sectors are modeled in 33 references, which implies that certain critical FEW-nexus interactions are omitted. The asymmetric representation of the three sectors in these cases may conceal other critical interactions that can bias the results.

In parallel to the development of nexus methodologies, machine learning applications have also been growing in the last ten years. Interestingly, the framework is not common for nexus-related questions [86].<sup>7</sup>

Optimization-based nexus models inherit some of their shortcomings from existing modeling tools. More specifically, uncertainties due to socioeconomic changes and climate change are mostly exogenous [92]. To a greater extent, nexus governance directives are neglected in the vast majority of papers along with most political economy drivers [93]. Moreover, consistent with the findings of Hoolohan et al. [94], the vast majority of papers in this review focus

on the physical interactions between the three sectors without including the competing objectives of the associated stakeholders.

## Recent Developments and Potential for Future Research

Recent developments in the literature aim at expanding the detail of existing models. FEW sectors are among the 16 sectors that are identified as critical in the Presidential Policy Directive 21 [95] for the USA. Although interactions between some critical infrastructure sectors have been studied, e.g., between FEW-nexus and Transportation Systems [96], other interdependencies have not been incorporated in FEW-nexus systems models, e.g., the FEW-nexus and Emergency Systems interdependencies. Research on these other sectors has the potential to elucidate insights through modeling.

Moreover, meaningful development of nexus methods needs to take into account that most of the FEW interactions happen at different points in the supply chains of the three sectors. In Section “[Overview of Optimization-Based Methods](#)” we detail how researchers choose to model FEW-nexus interactions at different geographical scales, from the farm level to the country level. Moreover, the representation of technological detail of the FEW-nexus supply chains varies between studies, with some studies choosing an aggregate representation of each sector [63] and others including certain features of each process [57•].

Apart from operating the FEW-nexus in a way that accounts for the FEW-nexus interdependencies, the availability of resources in one FEW sector can either limit or enable infrastructure investment on another FEW sector [14]. FEW-nexus systems models provide a framework that can be used to investigate expansion planning decisions, where interdependencies between FEW-nexus infrastructures are also considered [64]. Nevertheless, all approaches depend on data availability on all three sectors and data consistency at their interdependencies. Compiling such datasets remains a challenge [2, 97] and limits the applicability of the nexus to real-world problems. Greater regional downscaling and enhanced technological detail calls for the collection of detailed data and the development of robust data generation techniques.

The challenge of integrating the FEW-nexus sectors can be physical, economic, and political. Studying all three sectors in a single framework provides the opportunity to study the interactions between agents of all three sectors. However, the asymmetric sectoral detail in a model can lead to misrepresentation of the objectives of individual agents of the FEW-nexus. Moreover, FEW-nexus sectors are considered critical infrastructures, which implies that agents in the FEW-nexus may also consider the geopolitical

<sup>7</sup>FEW-nexus systems applications include neural networks [87], Dynamic Bayesian Networks [88], genetic algorithms [89], Differential Evolution [90], and Reinforcement Learning [91].

ramifications of FEW-nexus investments [15]. Nonetheless, the consideration of all interacting FEW-nexus stakeholders and a more precise representation of their objectives can provide further insight on the benefits, economic or other, accrued by each stakeholder in each sector. Studying the decisions of each individual agent in each sector allows us to devise strategies that can overcome economic and political challenges of sector integration.

Finally, the potential for synergies does not immediately imply incentive-compatibility of individual agents across all sectors. Apart from the economic incentives, Leck et al. [93] highlight the importance of political economy drivers, e.g., the role of power relationships, poverty, and entitlements. Ensuring incentive compatibility along all these dimensions in the three systems can facilitate translating nexus-oriented results into governance propositions and evoke public engagement toward achieving these goals [23]. Local governance, where nexus conflicts are resolved in practice beyond optimization models, are a valuable resource when it comes to understanding inter-sectoral coordination [93]. We find examples of studies that apply optimization-based tools to FEW-nexus analysis in a manner that explicitly accounts for limitations in efficiency-oriented analysis or for the needs of particularly vulnerable groups, e.g., [31, 44]. Optimization-based models would benefit by incorporating power dynamics and local priorities in FEW-nexus analysis. We argue that a FEW-nexus framework that accounts for political trade-offs and incorporates non-economic incentives into the underlying decision-making process of individual agents could also affect the results.

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