Simulation and optimization in cross-sectoral water: a review

Adrielly Nahomee Ramos Alvarez[1[+525562168795]], Idalia Flores-De la Mota[1[+525532007699]] and Francisca Irene Soler Anguiano[1[+525556223281]]

[1] National Autonomous University of Mexico, Coyoacan Mexico City, Mexico
adrynahr@gmail.com, idalia@unam.mx,
francisca.soler@ingenieria.unam.edu

Abstract. Simulation and optimization models have been of pivotal importance in bringing solutions to major problems. However, their impact is determined by the accuracy and level of detail of the conceptual models describing the systems. In water management these tools have provided valuable solutions, nonetheless, throughout the years models have simplified critical aspects that curb efforts to deliver more effective results. That is the case of cross-sectoral relationships that are often misrepresented in the models despite their relevance with the aim to reduce complexity. Cross-sectoral perspectives have taken place in recent years due to the valuable insights they deliver by addressing those commonly unseen relationships. As a result, the objective of the present article is to introduce a brief review of the cross-sectoral studies that using simulation and optimization techniques have contributed to mitigate the effects of the current and future water crisis through a change of paradigm in models' constructions.

Keywords: Cross-sectoral optimization, water simulation, water optimization, sustainability.

1 Introduction

Water is a fundamental resource in every economical sector, and its adequate management soon will constitute the difference between success and failure. Nowadays countries experience a hydric crisis exacerbated by poor regulation, lack of initiatives, insufficient strategies, inadequate technology, and the absence of accurate models and data.

This crisis is not particular of a certain sector or region, the scarcity and contamination of the resource in one affect, both directly and indirectly, the others due to the existing interactions among sectors. These interactions are not always taken into consideration while modelling the system or implementing solutions, being rather simplified in most simulations. Throughout the years several studies have focused in describing, understanding, and facing the problem in parts, by looking at the relationships inside the sectors but not necessarily among them, leaving important aspects of the system unattended. According to Lara-Rosano "One of the difficulties in focusing a problem is to think that the problem lays in the parts, when generally lays in the relationships between the parts" (Lara-Rosano, 2017). Considering these relationships has provided important findings leading to the development of more effective solutions. This is visible in water systems where cross-sectoral approaches have directed efforts towards more sustainable practices improving the hydric situation significantly.

Modelling systems from a cross-sectoral perspective has contributed to fill gaps with vital information. United Nations affirms that "water-related data and information are central to understanding and valuing the resource" and that "Further efforts and investments are required to sustain the supply chain of data … across sectors and scales." (UN Water, 2021) to have a wider vision of the problem and the situation providing more elements to complete the hydric scenario. Although "A degree of information/knowledge deficiency is generally present in any model development activity" (Birta et al., 2019) in complex issues such as water management, lacking the awareness of the relationships between sectors, can lead to an important "…misrepresentation of impacts" (Harrison et al., 2016) building considerable obstacles in developing efficient simulation models, optimization strategies and effective solutions. Consequently, water simulation models that work under the assumption and simplification that interactions with other sectors are despicable, fall short to properly describe the system.

Cross-sectoral studies are still scarce, but their results are of crucial importance. Specially in environmental matters where correct representation of relationships offers insights that otherwise would remain invisible by estimating more precisely the magnitude and behavior of the interactions and influences across sectors. Therefore, the aim of the present paper is to introduce an overview of cross-sectoral simulation and optimization investigations highlighting their contributions and opportunity areas in order to set a starting point for developing simulations that effectively describe cross-sectoral interactions to bring more impactful optimizations. Helping confront long lasting complex problems such as the ones the world faces in environmental and sustainability matters.

2 Water Context

2.1 Global Water Context

Although water is a fundamental resource for every human activity it has not been valued nor represented properly as it can be seen in the current hydric situation. Water levels have been decreasing around the world, in 1967 renewable water per capita was 13,400 cubic meters, while in 2017 it declined to 5,732 cubic meters (Oxford, 2018).

It is important to highlight that hydric challenges vary according to the region (UN-Water, 2021):

In Sub-Saharian Africa water resources are unequally distributed, despite having 9% of global fresh water, access to water is scarce, only 24% of the region's population has access to drinking water (UN-Water, 2019). Coupled with rapid population growth, inappropriate water governance, environmental degradation, deforestation, the socioeconomic situation, and unsustainable financial investments, there is a lack of infrastructure and plans adapted to the needs of the continent.

Transboundary water management in the Pan-European Region is a major challenge, countries use different approaches for its administration and the benefits of cooperation between countries are substantial; however, determining the value of water represents a substantial challenge, especially in collecting quantitative data.

The growing water stress in the Latin America and the Caribbean region has triggered conflicts between sectors that compete for scarce resources. Poor regulation, lack of initiatives and investment are factors that show the value attributed to water in the region despite its strategic value in multiple production processes or in the context of climate change.

Due to population growth, urbanization and rapid industrialization in Asia and the Pacific competition for water between sectors has become more severe, threatening agricultural production and food security as well as water quality. Unsustainable water withdrawals have in some cases exceeded half of supply availability. Wastewater remains under used and there is an urgent need to reduce aquifer pollution and promote water efficiency.

It is important to mention that a crucial part of water management is in the adequate valuation of the resource, that comes from a systemic approach and a proper representation of the relationships among the elements of the system which is obtained through the accurate collection of data and information with its correct analysis. Despite the usefulness of hydrological data for the generation of solutions, the levels of reported public data have decreased significantly with respect to the 20th century, for 2010 the number of stations reporting data decreased by 31% with respect to the reports of the decade of 1980 (UN-Water, 2021). Proper data collection and analysis specially among sectors, basins and frontiers is crucial to find and understand the existing relationships that are affecting the system in different levels. This is crucial for developing strategies and solutions.

Simulation and optimization models potential

One of the hardest things to accomplish is to determine the interactions among the elements of the system. It is through simulation that those cross-sectoral interactions can be addressed, quantified, and explored. While optimization techniques provide significant value for a sustainable use of the resources.

2.2 Sectorial Water Context

Global water use has increased substantially in recent years, and it is projected to grow more while aquifer levels decrease. Even though the exact amount of required water is not certain, additional volumes of water will be necessary since food demand is expected to grow in 50% by 2050 relative to 2012 levels (UN Water, 2022), industry and domestic demands are also expected to raise. Just in 2016 an estimated of four billion people lived in areas that suffered critical water scarcity (Mekonnen and Hoekstra, 2016) and due to demographic growth, this scarcity will become more critical.

The use of groundwater in agriculture accounts for 59% of the areas equipped for irrigation in North America and 57% in South Asia. Water is rarely quantified in food

production despite of its high value and the amount of water that is needed to guarantee its security. It accounts for 70% of water use globally (UN Water, 2021-2022).
Industry and energy use 19% of global freshwater withdrawals, with major differences between developed and underdeveloped countries, while Europe industrial withdrawals is of 57% in Africa industrial extractions account for 5% (UN Water, 2022).
Groundwater dependence for domestic use is intensifying, almost 50% of global urban population demand is supplied by groundwater. Major challenges in developing countries are addressed from unplanned settlements that lack proper hydric infrastructure, low sewer coverage to lack of adequate data and management (UN Water, 2022).
Water panorama in every sector is still far from the ideal and the actions in one affect the others in several ways. Although these impacts are not always visible or measured their effects are significant. As a result, cross-sectoral perspectives are of great importance for bringing wider solutions.

3 Cross-sectoral Water Simulation and Optimization

Cross-sectoral analysis in environmental problematics have brought important insights for bridging knowledge gaps and creating more sustainable solutions. Cross-sectoral perspectives in water usage are not the exception, by establishing awareness of the interlinkages across sectors and giving visibility, models have been built with vital information that have boosted optimization and simulation outcomes.
Relationships across sectors are impactful, adaptation and mitigation actions by one sector can directly influence water demand, increase, or reduce water availability, change water quality for other sectors, and affect energy use. For example, pollution originated by agriculture "…has overtaken contamination from settlements and industries as the major factor in the degradation of inland and coastal waters." (UN Water, 2020). Chemicals, from fertilizers, are the most prevalent anthropogenic contaminant in groundwater globally. "Insecticides, herbicides, and fungicides, when improperly applied or disposed of, can pollute groundwater with carcinogens and other toxic substances." Persistent contamination of rural groundwater supplies with pathogens is estimated to affect 30% of the total domestic installations. (UN Water, 2022).
In small urban and rural settlements, use of water for agriculture and in some cases industrial applications results in reduced availability for domestic uses. (UN Water, 2020). These are some of the most noticeable relationships across sectors but many of them have not even been described. For this reason, it is essential that more studies may be performed from a cross-sectoral perspective.

3.1 Simulation and optimization

Some cross-sectoral investigations are summarized by author showing the optimization tools and the simulation models used in every study considering the principal variables and highlighting the contribution made in every research.

Wang et al. (2022) used the Leontief input-output model in an extended multiscale framework for identifying the characteristic energy-water-land links and trans-boundary relationships. This to reflect the connections across sectors and regions from a multisectoral perspective.

Yue et al. (2022) developed a stochastic multi-objective optimization model for crop-livestock-biogas-crop recycling through the coordination of resources allocation considering resources input reduction, agricultural wastes recycle, global warming mitigation, socio-economic security in order to promote sustainable circular agricultural development.

Deng et al. (2022) implemented a machine learning model using a multilayer perceptron in an Elman neural network for predicting the water level in the Dongting lake from a cross-sectoral perspective. Their contribution is to provide a reliable water level prediction for better hydric resources management.

The objective of Tian et al. (2022) was to understand the operational issues that can be found in complex water systems. Their contribution lays in partitioning large water distribution networks by creating partitions for the allocation of multiple sources, and for a multi-objective network decomposition. This optimization being achieved by a depth-first-search metaheuristic algorithm.

Dombrowsky et al. (2022) made an analysis of the effects of cross-sectoral policies by addressing challenges among different sectors. They deliver a process analysis of river conversion and rehabilitation, agricultural water consumption reduction, mitigation of contamination due to mining, catchment management strategy to manage water conflicts, competition coordination for scarce water resources.

Xiao et al. (2021) proposed a differential game model with a two-player finite-horizon representing both agricultural and industrial sectors. The objective was to minimize toxic gas emissions, pollutants, and damage while maximizing utility and production through cross-sectoral game theory.

Pronk et al. (2021) constructed different scenarios for water reuse optimization. Interlinkage description was a pivotal aspect for quantifying water use among sectors and propose a framework for cross-sectoral water reuse. Reusing industrial effluent for irrigation, industry, and aquifer replenishment.

Langergraber et al. (2021) had the objective of analyze the multi-functionality potential of nature-based solutions for water management. Maximizing the use and reuse of resources while reducing the need of external resource inputs. Creating an optimization framework for Nature Based solutions.

Krapez et al. (2020) detected agricultural water leakages from an airplane and drone using the Triangle/Trapezoid method. With the objective of reducing losses in water transmission through a feasible surveillance method for water transportation mains outside urban areas. This monitoring method provides important data for the system modelling and understanding.

Quesada et al. (2019) studied existent chemicals in water that potentially affect basins. The investigation highlights the need to monitor residual pharmaceuticals in water and its implications in cross-sectoral uses. Through a review of pharmaceuticals' current situation as emerging contaminants in surface water. It also provides detail in adsorption processes as an alternative to remove these compounds from aquifers.

Seibel and Kuhlmann (2018) developed the model of a pilot chemical plant using multi-objective optimization to minimize electricity purchase, maximize grid balancing services, maximize product sale, minimize cost of poor-quality water and minimize gas emissions using cross-sectoral resource optimization.

Chuenchum et al. (2017) performed rainfall projections under climate change scenarios, building a rainfall-runoff simulation within an Integrated Flood Assessment System. The main contribution with this simulation was the Regional Input-Output Model for determining the economic value of water.

Cook and Webber (2016) seek to improve irrigation efficiency in the agriculture sector to make significant volumes of water available for other purposes through the optimization of the resource conservation. The investigation contributed to the determination of water savings in the implementation of best management practices for irrigation efficiency across 2 counties in Texas.

Koutroulis et al. (2015) developed a hydrological simulation to assess the impact of climatic and socioeconomic futures on the water resources of a Mediterranean island, and constructed a cross-sectoral framework.

Wimmer et al. (2014) assembled an exploratory tool to investigate future adaptation needs in Europe's water-related sectors through the simulation of the effect of water management on agricultural productivity, hydric stress, demand.

The investigations listed above have intensely used simulation and optimization models for a more sustainable use of hydric resources contributing significantly to solve the complex water problem from a cross-sectoral water approach. Table 1 condenses some of the most relevant articles, however there are many more investigations that use cross-sectoral simulation and optimization models for water management and other resources.

The following Table 1 gives an overview of the simulation and optimization models for cross-sectoral water.

Table 1. Overview of models and authors.

Authors	Model	Simulation/Optimization
Wang et al., 2022	Leontief input-output model. Extended multiscale input-output model (EE-MSIO)	Optimization
Yue et al., 2022	Stochastic multi-objective optimization. Stewart model, analytic hierarchy process, carbon footprint.	Optimization

Deng B. et al., 2022	Machine learning model: multilayer perceptron, Elman neural network and optimization.	Optimization
Tian et al., 2022	Multilevel partitioning. Multi-objective network decomposition. Depth-first-search algorithm.	Optimization
Dombrowsky et al., 2022	Analysis of the effects of cross-sectoral water policies.	Simulation basis
Xiao et al., 2021	Differential game model, two-player finite-horizon, game theory	Optimization
Pronk et al., 2021	Scenario construction for water reuse optimization using Sankey diagrams	Optimization
Langergraber et al., 2021	Optimization framework for Nature Based Solutions	Optimization
Krapez et al., 2020	Triangle/Trapezoid method (T-VI) for detection of water leaks from airplane	Simulation
Quesada et al., 2019	Drug concentration determination, highlighting minimal, maximal, and mean values.	Simulation basis
Seibel and Kuhlmann, 2018	Simulation-based optimization, multi-objective optimization.	Simulation & optimization
Chuenchum et al., 2017	Simulation of runoff under climate change scenarios. Integrated Flood Assessment System. Regional Input-Output Model for economic value of water	Simulation
Cook and Webber, 2016	Water conservation optimization for more availability. Analysis and implementation.	Optimization
Koutroulis et al., 2015	Hydrological simulation to determine impacts of climatic and socioeconomic futures.	Simulation
Wimmer et al., 2014	Simulation of the effect of WAS on agricultural productivity, stresses on aquatic ecosystems, unsatisfied demand, domestic	Simulation

Cross-sectoral perspectives have contributed significantly to provide more accurate simulations and more impactful optimizations by properly addressing pivotal interactions among sectors which has also potentiated the use of intelligent tools such as Machine Learning, Big Data, among others.

3.2 Variables

To determine the interrelations across sectors it is vital to properly identify the most relevant variables and parameters within the system. The presented investigations consider these variables.

- Economic: service and goods utility, savings, energy, treatment, damage, infrastructure, pumping costs, GDP.
- Pollutants: CO2 NO2 emissions, chemical, fertilizers, drugs present in water and soil, water quality.
- Volume: treated water, leakages, aquifer levels (superficial and underground water), water reuse, domestic, agricultural, and industrial water use, water demand.
- Physical: soil, atmospheric, water temperature, humidity, pressure.
- Energy: type of energy, use, cost, demand, generation.
- Social: policies, management, socioeconomic growth, innovations, strategies, stakeholders, organizational objectives.

Other variables are also of pivotal importance and therefore taken into consideration according to the needs and circumstances of every problem. Some variables will take precedence in determined cases. It is important to notice that as the number of interactions increase, the variables to be considered will augment as well. This resulting into more complex models, that will require to incorporate additional tools for properly and effectively manage information and insights.

3.3 Opportunities in cross-sectoral models

Cross-sectoral approaches are still scarce as compared to other perspectives that have been widely implemented. For there are many gaps yet to fill. Among the opportunity areas that can be found in the present review are: cross-sectoral coordination policies, sustainable intensification schemes that minimize hydric stress, identification of non-obvious connections across sectors and boundaries, solutions for megacities' size and complexity, optimization, and decision support tools for different scenarios and weight objectives, considering more connections, activities, procedures, and elements along with the condition variability among sectors.

Other opportunity areas are also important to highlight, one of them is the lack of generalization and portability of models and methods to apply techniques in different aquifers and maximize coordination in cross-sectoral environmental policies (Deng B. et al., 2022). Control and monitoring of cross-sectoral water pollution including setting objectives in stages at all levels with adaptation options are still missing and a significant challenge to face. And it is also required to implement further optimization techniques to empower strategies.

Dombrowsky et al. emphasize that "coordination at process level does not necessarily translate into coordinated outcomes" (Dombrowsky et al., 2022) for it is also critical to redefine objectives, and actions in a dynamic way. It is difficult to determine causality of many problems while providing efficient, cost-effective solutions for surveillance, simulations (Krapez et al., 2020). Collaborative governance, quantitative approach, optimization techniques for supporting management are yet in an initial stage and completely scarce in developing countries. Multifunctionality is rarely implemented in nature-based solutions.

Furthermore, data collection, adaptable design approaches, inter-basin data transfer and analysis are major challenges to be tackled. Although Industry 4.0 tools have enabled more efficient information acquiring, techniques and methodologies for identifying relationships across sectors supported by accurate data are needed alongside with optimization techniques for supporting cross-sectoral approaches.

Simulation and optimization models are valuable tools for obtaining more significant results and can provide instruments for fulfilling the mentioned gaps while offering a wider vision of the systems. Cross-sectoral perspectives can deliver important information that traditional approaches can miss as it can be seen in Figure 1, where the cross-sectoral analysis not only brings data about each sector but the one pertaining the relationships among sectors.

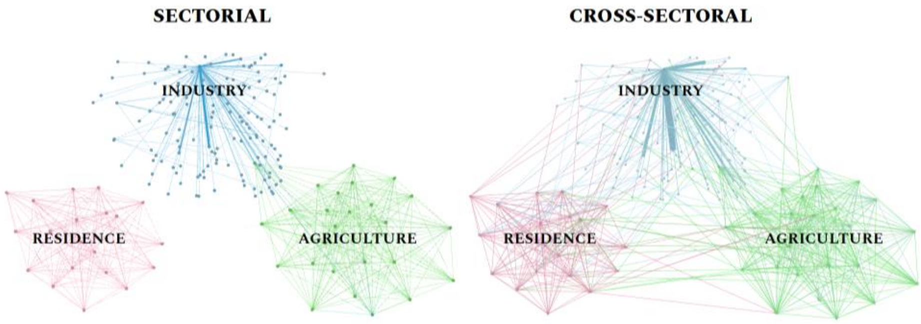

Fig. 1. Sectors analyzed separately vs cross-sectoral analysis.

The sectorial perspective focuses on the collaboration and coordination among the activities or procedures of its own sector, as it can be seen in the left network representation shown in Figure 1, where the nodes denote the physical spaces, activities or operations and the arcs represent the water inputs and outputs from one node to another. Within this kind of perspective, it is considered that the situation in other sectors can be tackled as a separate problem and that solving those problems individually then bringing those solutions together can constitute a difference on the whole system. While this is in part true, complex problems such as the one addressed here require a special treatment for understanding the aspects that will provide the necessary information to ideate strategies and solutions that bring significant results. On the other hand, the cross-sectoral approach seen in the right network representation takes on account what sectorial perspective is considering plus adding the connections between the nodes pertaining to Residential, Industrial and Agricultural sectors, as it is shown in Figure 1. Nonetheless, considering these relationships increases the challenges for not only constructing the models but for implementing the solutions given that the computational, mathematical, and operational complexity is increased. Even more robust and flexible tools are required to be created in order to face the challenges associated to a cross-sectoral simulation and optimization.

4 Conclusions

Simulation and optimization models are vital for solving complex problems such as the ones related to water. Those models require a balance between complexity and simplicity. While simpler models contribute to the generation of faster solutions, they can often misrepresent the system leaving vital aspects outside of the analysis. On the other hand, models that take on account more elements tend to increase the level of complexity leading to higher costs of implementation, more computing time, and additional problems associated with data collection and analysis. Nonetheless, due to the nature of the global hydric problem it is required to have more impactful solutions. Solutions that can only be achieved through a better understanding of the actual system that tools like simulation can offer. Cross-sectoral approaches provide information that is commonly set aside because of the additional complexity and work needed. This information bridges considerable gaps that otherwise would remain unattended. For it is important to continue simulating and optimizing from a cross-sectoral systemic perspective.

The present review condenses some of the various cross-sectoral water investigations that have been developed in recent years and highlights the gaps that are still pending to bridge. Future research will aim to empower the use of optimization and simulation models in cross-sectoral water for fulfilling hydric needs and contributing to understand the system dynamics more fully.

This article raises to highlight that cross-sectoral perspectives can change the paradigms of model construction and problem-solving in more than one problem as the one stated in this work, and that this approach can lead to other ways of handling and managing information in problems and in developing more sustainable systems.

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