Chapter 1: INTRODUCTION

1.1 Background and motivation

The rising demand for groundwater (GW) resources and ecosystem services, driven by rapid economic growth and population expansion, poses significant challenges globally. This intensifying demand directly or indirectly contributes to ecological degradation, endangering food security, water availability, and ecosystem health. Furthermore, rapid population growth in agricultural and industrial activities has significantly increased groundwater reliance. Global groundwater demand has tripled over the last five decades while its availability has steadily declined. The global groundwater footprint is about 3.5 times the actual area of aquifers, with about 1.7 billion people living in areas where groundwater resources and/or ecosystems are under threat (Hansen et al., 2017). This unsustainable extraction has led to severe depletion of aquifers and a decline in their ability to sustain ecological processes, including the crucial exchange between rivers and aquifers (R-A exchanges).

1.1.1 River-Aquifer Exchanges and its significance

River-aquifer exchanges are critical processes that influence the quantity and quality of water resources in various regions. These exchanges occur when water flows between rivers and adjacent aquifers, as groundwater discharges into the river (gaining conditions) or river water infiltrates the aquifer (losing conditions). This can be seen in Figure 1.1. These exchanges' spatial and temporal variability can be influenced by several factors, including geological and geomorphic features, river stage fluctuations, and climatic conditions (Boano et al., 2008).

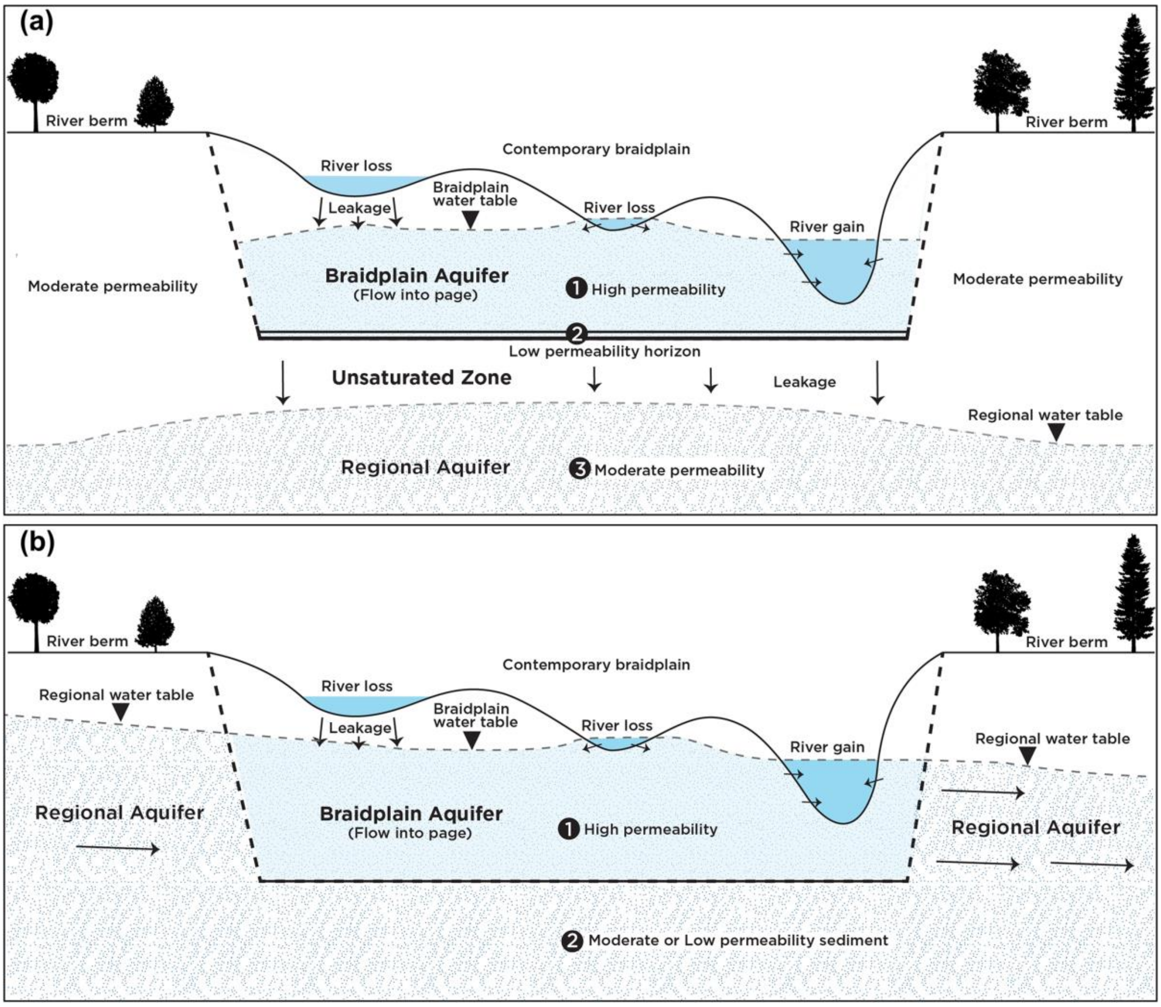

Figure 1.1 Conceptualization of (a) hydraulically disconnected from the regional groundwater system and (b) hydraulically connected to the regional groundwater system Source: Wilson et al. (2024)

The importance of R-A exchanges can be divided into:

a) **Hydrological Significance:** River-aquifer exchanges are critical for maintaining river flow, especially during low-flow periods, and for recharging aquifers during high-flow periods. Groundwater inflows, or baseflow, sustain river discharge when surface water levels are low, ensuring streamflow continuity. Conversely, rivers contribute to aquifer recharge through downward infiltration during high-flow periods or in losing stream conditions, replenishing groundwater reserves. This bidirectional exchange mitigates drought risks and ensures reliable water availability across hydrological regimes. In regions with significant seasonal variability, the interplay between surface and groundwater systems acts as a natural buffer, stabilizing water supply for various human and environmental needs.

b) **Ecological Importance:** Water exchange between rivers and aquifers forms distinct hydro-biological environments that control nutrient dynamics and thermal conditions, essential for diverse biological activities. Groundwater nutrient influx boosts primary productivity in river ecosystems, promoting aquatic flora and fauna growth. Groundwater inflows also moderate thermal conditions, maintaining favorable environments for temperature-sensitive species and supporting aquatic biodiversity. These exchanges influence habitat conditions, underpinning the ecological integrity of riverine systems, ensuring species survival, and enhancing ecosystem resilience.

c) **Environmental significance:** River-aquifer exchanges are vital for the life cycles of many aquatic organisms, particularly those with specific habitat requirements. For instance, fish species like salmon depend on hyporheic zones (the interface between river water and groundwater) for critical life stages such as nesting and reproduction. The hyporheic flow provides oxygen-rich and thermally stable environments, ideal for spawning and egg development. Due to over-extraction of groundwater or altered flow regimes, disruptions in R-A exchanges can jeopardize these habitats, threatening such species' reproductive success and survival. Protecting and managing these exchanges is thus integral to maintaining the ecological balance and ensuring the long-term sustainability of aquatic biodiversity.

In Europe, especially in the Mediterranean region, the summer air temperature is predicted to rise to 4 °C (Wawrzyniak et al., 2017), with a significant decrease in runoff and recharge. Due to the decline in mean discharge and extended low flow periods, the stream temperature will rise, affecting the water budget and surface water availability (Dole-

Olivier et al., 2019; Suanez et al., 1998). During these high temperature-low flow periods, certain fishes seek refuge in cold water patches, often driven by GW upwellings (Dugdale et al., 2015). More generally, the exchanges between streams and aquifers have strong ecological significance. The R-A zone acts as a critical ecotone, connecting river and groundwater ecosystems, and is characterized by diverse gradients and high metabolic activity. This zone supports nutrient cycling, respiration, and the survival of macroinvertebrates. The riverbeds and surrounding sediments' physical characteristics can also affect the dynamics of river-aquifer exchanges. Understanding these complex interactions is essential for effective water resource management, especially in regions with variable climatic conditions and diverse geological settings.

1.1.2 The transdisciplinary Water-Energy-Food-Environment nexus

The production, utilization, and security of water, energy, food, and environment (WEFE) are deeply interconnected, forming what is known as the WEFE nexus. Water, energy, and food are closely linked. Water production requires energy, energy production utilizes water, and food production requires both water and energy. This interdependence means that actions in one sector often impact the others, necessitating a holistic management approach. For instance, intensive irrigation to meet the growing global food demand has led to significant water quality issues in rivers and groundwater. Nitrate contamination in groundwater seriously threatens ecological systems and human health. When nitrate nitrogen (NO3-N) concentrations exceed 50 mg/L, it becomes hazardous (Jiang et al., 2021). Excessive nitrate loading in aquatic systems promotes uncontrolled vegetative growth, disrupts ecosystems, and increases water treatment costs. Additionally, the pressure on arable land in many countries has escalated, creating challenges in improving water use efficiency and sustaining crop yields. These challenges are compounded by the increasing energy demands for water supply and food production, forming a complex nexus where changes in one element directly influence others, leading to intricate synergies and trade-offs.

A river serves as a critical link between various management goals, where the interdependence of water demands and constraints among stakeholders becomes evident. For instance, rivers connect multiple sectors, such as hydropower, agriculture, and fisheries, interacting with diverse actors like geomorphology, aquifers, and groundwater flow (Döll et al., 2010; Pagès et al., 2020). Excessive groundwater pumping alters river flow regimes, exacerbating variability in downstream sectors. Upstream hydropower operations, particularly hydropeaking, can significantly affect water availability for irrigation, impacting agricultural productivity and downstream ecosystems (Daufresne et al., 2007). Balancing sufficient R-A exchanges with optimal GW extraction rates is a multifaceted challenge influenced by regional hydrogeological conditions, climate variability, ecological dynamics, and human interventions (X. Cai et al., 2018). Anthropogenic activities serve as external factors, driving socio-economic benefits but complicating resource management. Therefore, effective GW and R-A management should emphasize an integrated approach within the WEFE nexus. Adopting a systematic nexus optimization framework allows for evaluating synergies and trade-offs across management plans, significantly achieving at least six of the 17 Sustainable Development Goals (SDGs) (Di Martino et al., 2023). The United Nations and the World Economic Forum have strongly advocated for the integrated management of food, water, and energy resources, emphasizing the need to optimize social benefits and protect the environment. This shift in resource management strategy highlights the emergence of a nexus approach in policymaking, which aims to address the interconnectedness and interdependencies of these critical resources. The WEFE nexus captures the intricate interrelationship among water resources, energy use, and food production, all essential for human well-being and sustainable development. Different methods have been employed to understand and optimize the conflicts among water resources, environment, and social-economic management goals. Numerical models such as HydroGeosphere, MT3DMS, FEFLOW, and MODLOW are extensively utilized for simulating flow dynamics and contaminant transport under varying conditions, including GW extraction regulations and the impacts of climate change (Mansour et al., 2023; Peña-Torres et al., 2022). Simulation-optimization (SO) methods are crucial in addressing practical challenges related to single and multi-objective optimization problems. It has been applied to various management goals relating to the WEFE nexus. For instance, to optimize the sharing of physical and virtual water for different water users while considering the environmental impact (Song et al., 2022; Zahedi et al., 2024); to optimize wastewater reuse by considering reuse supply and demands, costs and profits, while reducing pollutants (Lin et al., 2022; Mirzaie et al., 2021). At the same time, other scholars have focused more on the socio-economic advantages. For example, an integrated management model for saline water management, optimized irrigation strategies, local optimization to maximize the net benefit from agricultural water uses, and supply and water demands, including urban, agriculture, and industry (Mansour et al., 2024a; Morlet-Espinosa et al., 2023; Wang et al., 2024; Zhou et al., 2024). A few studies also contribute to the environmental and ecological aspects, such as the optimal design of renewable energy systems under nexus considerations, reservoir operation schemes, minimizing the environmental risks by nitrates, and in situ remediation design (Ma et al., 2022; Zhang et al., 2023). These studies have demonstrated the efficacy of S-O in addressing the macroscopic allocation of water supply and demand while accounting for certain socio-economic benefits. Moreover, S-O excels in its capacity to integrate the physical mechanisms governing the water cycle, hydrogeology and the impacts of water pollution at a regional scale. However, real-world GW management issues are often complex due to the nonlinear, multimodal, and nondifferentiable objectives and large-scale decision variables. Several MOMEA have been studied to overcome this, and their reliability and effectiveness have been proven in recent years. Integrating MOMEA(s) within numerical models has increased the application of S-O models in nexus management, extending beyond the limitations of predefined scenarios (Yu et al., 2024).

Investigating the intricate relationships among different nexus components within the interconnected S-O framework is valuable, yet it poses significant challenges. Prior uses of the S-O model have had a limited impact on quantifying and managing R-A exchanges and GW management. Nonetheless, an integrated S-O model that merges numerical simulations for river leakage with nitrate transport modeling in groundwater-fed river basins has yet to be utilized for optimizing basin-scale nexus strategies. Achieving a balance between accuracy and computational efficiency during large-scale multi-objective optimizations is crucial for the effectiveness of S-O in nexus management. Consequently, it is critical to establish a systematic approach for the scientific management of the WEFE nexus to facilitate optimal resource allocation and promote environmental sustainability. The lower Ain River Basin (LARB) in Rhône-Mediterranean basin, France faces significant water resource management and environmental sustainability challenges. Unregulated groundwater extraction and agricultural practices such as excessive fertilization have led to environmental issues, including nutrient pollution (NP) and changes in groundwater-surface water interaction dynamics. These pressures have impacted the river and basin's ecological balance and water quality. Numerous studies have qualitatively and quantitatively assessed these environmental impacts, providing valuable insights into the water systems, ecological challenges, and agricultural practices. (H. Ren et al., 2022; Suanez and Provansal, 1998) However, a comprehensive evaluation of the intricate WEFE nexus using a many-objective simulation optimization approach has yet to be applied in this region. Such an approach could offer a deeper understanding of the interdependencies and provide optimal strategies for sustainable water management in the basin.

1.2 Problem statements

The unsustainable groundwater extraction has disrupted the natural balance between surface water and aquifers, reducing baseflow contributions to rivers and intensifying hydrological and ecological stress. This decline in R-A exchanges poses critical challenges: it diminishes water availability during dry periods, affects water quality, and degrades aquatic and riparian ecosystems. These changes alter essential ecological processes such as nutrient cycling and thermal regulation, vital for sustaining biodiversity and maintaining habitat for certain species.

At the same time, escalating water demands for agriculture, energy production, and domestic use place immense pressure on groundwater resources. This competition is further complicated by the interdependencies within the WEFE nexus, where maximizing one objective often compromises others. For instance, hydropower operations upstream can reduce water availability downstream for irrigation and ecosystems, exacerbating trade-offs and leading to socio-economic tensions. More intensive agriculture leads to higher nitrate concentrations in GW and streams.

The challenge is magnified by hydrogeological system uncertainties, climate variability, land-use changes, and anthropogenic influences. These uncertainties affect the predictability of R-A exchanges, complicating the development of effective management strategies. Current models often fail to capture the dynamic interactions and feedback loops between surface water and groundwater systems, leading to suboptimal decisions that underutilize or overexploit resources.

While simulation-optimization (S-O) frameworks offer a promising solution by coupling predictive models with optimization techniques, their application to large-scale groundwater systems is computationally demanding. The uncertainty derived by choosing the optimal algorithm, decision variable handling, and multi-criteria decision-making in large-scale optimization is a critical challenge that can significantly impact the solution framework's robustness, accuracy, and computational efficiency. The complexity of these models often limits their scalability and real-time adaptability. Furthermore, most existing S-O approaches do not fully integrate the nexus approach, which could significantly reduce model accuracy and lead to a suboptimal management strategy.

This thesis addresses these critical issues by developing a computationally efficient S-O framework that quantifies trade-offs and synergies within the WEFE nexus to provide a holistic framework for sustainable groundwater management. The goal is to optimize groundwater extraction strategies while ensuring ecological sustainability and supporting socio-economic development.

1.3 Research design

This research explores several critical aspects of managing river-aquifer exchanges within the context of large-scale groundwater systems. First, it investigates the key hydrogeological and anthropogenic factors that influence R-A exchanges through numerical models, aiming to understand how these factors interact and impact water resource sustainability. Secondly, a significant focus is placed on applying multi-objective optimization techniques to balance competing objectives—maximizing groundwater extraction while sustaining R-A exchanges. Further, it also delves into identifying the decision variables that influence optimization outcomes most, providing insights into how these variables can be strategically managed to enhance resource efficiency.

The thesis also evaluates the potential use of surrogate modeling for improving computational efficiency and accuracy to address the computational challenges of large-scale S-O frameworks. Furthermore, the study examines the trade-offs and synergies within the WEFE nexus under various groundwater withdrawal scenarios. The significance of this research lies in its ability to address critical gaps in integrated water resource management.

1.4 Research aims and objectives

This thesis addresses the need for sustainable strategies by exploring numerical models, S-O frameworks, and decision-making tools. This thesis aims to develop and evaluate advanced computational tools in simulating and optimizing R-A exchanges within large-scale groundwater systems. These tools include groundwater numerical (qualitative and quantitative), predictive models, and large-scale many-objective optimization frameworks. The overarching goal is to enhance the sustainable management of groundwater resources while maintaining the ecological and hydrological balance of R-A exchanges. The specific objectives include:

Objective 1: Design and develop a regional S-O model to estimate groundwater head, R-A exchange dynamics, and nitrate loading. The framework for optimizing for R-A exchanges under different discharge scenarios is established.

Objective 2: To evaluate, compare, and select the most efficient optimization algorithm for S-O in the context of GW management problems. Metaheuristic algorithms suitable for large-scale optimization are tested and compared based on the pareto front.

Objective 3: To determine the feasibility of physics-informed neural networks (PINNs) as GW surrogate models. Developing a surrogate model for S-O, and its comparison based on the computational performance and accuracy.

Objective 4: To develop a methodology for studying the decision variable behavior in large-scale S-O models, thereby calculating decision variable importance and reducing large decision variables. An optimal number of decision variables and their impact on the S-O result was studied.

Objective 5: Develop a many-objective optimization model to optimize socio-economic demands and environmental constraints within the WEFE nexus and study its impact on the R-A exchanges.

1.5 Thesis structure and organization

This thesis consists of ten chapters. The core content of Chapters 2, 3, and 4 has been published in peer-reviewed journals, while Chapter 8 is currently under review. Below is a brief overview of the key topics covered in each chapter.

Chapter 1 defines the research scope of the thesis by establishing the theoretical background and motivation, the framework of reference, the core research questions, and the overarching strategy used to integrate the various components of the study.

Chapter 2 offers an in-depth review of the R-A exchange processes and explores various S-O methodologies used in groundwater management. It also comprehensively examines relevant techniques and frameworks applied in this research. Research gaps are provided in this chapter.

Chapter 3 focuses on developing and implementing numerical models to identify R-A exchanges, nitrate contamination, and GW flow budget. This chapter also develops the integrated S-O model and a graphical user interface (GUI) for future studies. This chapter also discusses the results of R-A exchange dynamics on the spatio-temporal scale. Sensitivity analysis is done to identify the most critical boundary conditions and aquifer parameters that have the most significant impact on R-A exchanges and GW heads.

Chapter 4, a multi-objective management model incorporating a MODFLOW-based simulator, is developed and implemented for the lower Ain River basin (LARB). The pareto fronts are compared based on convergence and diversity to choose the best algorithm for GW optimization.

Chapter 5 explores the decision variable space of groundwater S-O problems, incorporating various uncertainties and identifying the most influential pumping zones impacting R-A exchanges and GW extraction.

Chapter 6 introduces techniques to reduce decision variables in large-scale GW optimization problems for improved accuracy and robust results.

Chapter 7 describes the applicability of surrogate models in GW head and S-O result prediction. More specifically, it studies the feasibility of PINNs in GW head prediction for large-scale S-O models.

Chapter 8 develops and evaluates a large-scale objective WEFE optimization strategy and its impact on R-A exchanges as the management model for LARB.

Finally, **Chapter 9** concludes this thesis by summarizing its significant findings, limitations, and future scope.