Chapter 9: CONCLUSION

9.1 Introduction

This chapter brings together the key findings, limitations, and future research directions stemming from this doctoral thesis on large-scale simulation optimization for sustainable river-aquifer exchanges. The primary focus of this research was on developing and evaluating computational tools for simulating and optimizing river-aquifer exchanges within large-scale groundwater systems, through integrating numerical models, S-O frameworks, and decision-making tools.

While the overarching aim of this thesis was to investigate the spatio-temporal variations of R-A exchanges under different groundwater pumping scenarios, it also investigated the WEFE nexus framework by employing large-scale S-O techniques, deep learning models, and multi-criteria decision-making approaches. The R-A exchanges exhibited significant spatial and temporal variations influenced by groundwater pumping, seasonal streamflow fluctuations, and aquifer properties. These variations directly impact the sustainability of water resources by altering recharge rates, modifying flow regimes, and influencing the availability of water for competing uses. The limitations of employing large-scale S-O models were addressed in the lower Ain River basin, which included the selection of optimal metaheuristic algorithm, decision variable reduction for large-scale models, and introduction of surrogate models. A GUI named PyGWMO was established for the stakeholders to navigate through the whole process and make informed decisions in the context of groundwater management. Through comprehensive modeling and analysis, the thesis provides valuable insights into the dynamic interplay between groundwater extraction, stream-aquifer exchanges, and their implications for sustainable water resource management.

9.2 Specific conclusion of each objective

This thesis addressed namely five objectives, each contributing to a holistic understanding of the R-A exchange optimization:

- Objective 1: Developed an integrated simulation-optimization (S-O) model for managing groundwater pumping-induced R-A exchanges. This involved creating a 3D transient MODFLOW model capable of simulating groundwater flow, an MT3DMS model for nitrate transport, and R-A interactions. Sensitivity analysis was performed to identify the key hydrogeological parameters that affect the GW flow and R-A exchanges. Further, the calibrated simulation model was integrated with different optimizers in a Python based GUI PyGWMO. The hyperparameters for the metaheuristic algorithms were tuned. Finally, the developed framework was successfully applied to the Lower Ain River Basin in France.
- Objective 2: Explored optimal groundwater management strategies using a multi-objective S-O framework developed previously. The conflicting objectives of maximizing GW discharge from the aquifer and R-A exchanges were optimized simultaneously. Three different GW model boundary conditions and four different metaheuristic algorithms were used to derive Pareto-optimal solutions, balancing groundwater extraction with R-A exchange enhancement. The pareto fronts were compared using convergence and diversity metrics and it was found that MOPSO performs better in achieving more converged and spread-out solutions than others. It was also observed that boundary conditions and domain size significantly influence the results of simulation optimization models.

- Objective 3: Evaluated the feasibility of PINNs and ML models as groundwater surrogate models for predicting the head values based on the input data of space, time, and hydrogeological parameters. It was found that while ML models perform better than PINNs for complex domains, PINNs were suitable for simpler cases. The surrogate model of the S-O was also developed to quantify the impact of introducing ANN directly to the SO model. It was found that the ANN-SO model performs better in terms of both convergence and diversity, and the hypervolume is increased up to 50% for some models.
- Objective 3: Developed a methodology for reducing significant decision variables in groundwater optimization problems. First, the decision variable space was studied, incorporating the uncertainties of clustering algorithms, GW model domains, and variable bounds. The variable importance was calculated in the S-O model through statistical analysis, explainable artificial intelligence, and generalized additive modeling. The study found that a few critical decision variables have large correlations with the objective functions while others did not affect the results much. By using a weightage approach, the delineation of development zones and environment zones was done. Further, a new methodology to reduce the large decision variables through aquifer parameter clustering was achieved in the GW SO problem. At last, the impact of the number of decision variables on the S-O results was studied, demonstrating the efficiency of parameter-based clustering techniques for simplifying complex problems.
- Objective 5: Developed a many-objective optimization model to optimize socio-economic demands and environmental constraints within the water-energy-food-environment nexus. Nexus thinking in the context of this thesis emphasizes a paradigm shift from singular objectives, such as maximizing groundwater extraction, to a broader focus on enhancing system efficiencies, identifying synergies, and managing trade-offs

within the nexus. The interconnected nature of river-aquifer exchanges and groundwater usage underscores the necessity of adopting a holistic nexus approach, which has been an implicit consideration in water resource management long before the WEFE nexus framework gained prominence. A WEFE nexus management model was developed, which included the objectives of maximizing the GW extraction, minimizing the nitrate-affected agricultural areas, maximizing the food yield, and minimizing the energy requirement for GW supply. Further, this model examined the impact of fulfilling these objectives on R-A exchanges. Finally, the pareto fronts obtained were studied and a scenario comparison was done to evaluate the WEFE sustainability with respect to R-A exchanges and GW extraction. While the extensive body of work on hydrology and groundwater modeling provides a strong foundation for WEFE nexus research, this framework offers a unique opportunity for broader application and collaboration.

9.3 Research findings

The findings of this thesis underscore significant advancements in modeling, optimization, and decision-making for sustainable groundwater and river-aquifer exchange management. The integrated S-O model developed in this study proved to be a reliable tool for simulating R-A exchanges, nitrate transport, and groundwater flow dynamics. By incorporating complex hydrological processes and their interactions, the model offers valuable insights for designing sustainable water resource management strategies that balance competing demands.

The application of metaheuristic algorithms, including MOPSO, NSGA-II, and MOEA/D, demonstrated their capability to identify Pareto-optimal solutions in multi-objective groundwater management scenarios. These algorithms effectively revealed trade-offs between competing objectives, such as maximizing groundwater extraction and sustaining

R-A exchanges, providing critical decision support for resource allocation under conflicting priorities.

Clustering techniques were successfully employed to reduce the dimensionality of decision variables without compromising the quality of the optimization solutions. This approach facilitates the scalability of large-scale optimization problems by significantly reducing computational complexity while preserving the integrity of the decision-making process.

Machine learning models, particularly ANN with MLP architecture, were utilized as surrogate models for groundwater head prediction and optimization. These models improved computational efficiency by approximating the responses of complex numerical models, enabling rapid evaluation of alternative management strategies while maintaining high predictive accuracy.

Finally, the many-objective optimization framework applied to the WEFE nexus provided a comprehensive analysis of critical trade-offs among water supply, energy consumption, agricultural productivity, and environmental protection. These findings emphasize the interconnectedness of these sectors and offer actionable insights for achieving sustainable resource management in the context of increasing demands and environmental constraints.

9.3.1 Implications for Integrated Water Management

This thesis has direct implications for policymakers, stakeholders, and researchers involved in sustainable groundwater management. The integration of numerical modeling, deep learning, and S-O frameworks for nexus management provides a robust methodology for managing water resources in complex systems.

Policy Recommendations: The study advocates for policies that balance groundwater extraction with different environmental sustainability indicators by incorporating R-A exchange dynamics, nitrate contamination, food yield, and energy consumption into regulatory frameworks.

Technological Adoption: Adopting novel techniques like PINN and machine learning for predictive modeling offers practical tools for data-driven decision-making. The clustering algorithms and visual techniques to represent high-dimensional datasets are an add-on.

Blue-Green Zone Prioritization: Spatial modeling and sensitivity analysis provide actionable insights for prioritizing areas for interventions to mitigate aquifer depletion. Policymakers can identify the vulnerable areas and better plan land use with more informed decision-making for increased recharge and baseflow revival of the disconnected rivers. The decision variable space provides crucial insights not always evident in the objective space, emphasizing the importance of decision variable analysis for robust groundwater management.

Decision Support system: The PyGWMO model provides easy-to-implement GW management problems with the liberty to choose different optimization techniques and clustering algorithms and provides intuitive graphs while running and after the optimization model. Post-processing is easy as it gives the results in a .csv format. Decision makers can easily identify the trade-offs between the management goals.

9.4 Limitations

Despite the significant contributions, this thesis has several limitations that warrant consideration. The research primarily focuses on a single case study, the Lower Ain River Basin (LARB), which may limit the direct transferability of the findings to other hydrogeological contexts with differing characteristics. Additionally, the numerical models used in the study are simplified representations of real-world systems, and while they provide valuable insights, they may not fully capture the complexities and uncertainties inherent in natural systems. The parameter estimation process relies on the availability of data, which may not fully account for the heterogeneity of subsurface conditions or the limitations of existing datasets. In these simulations, nitrate was treated conservatively—

without accounting for denitrification, plant uptake, or microbial reduction—in order to focus on hydrological transport and to isolate the influence of groundwater pumping and stream leakage on nitrate migration. This approach does not reflect the full biogeochemical complexity of nitrate behavior. The current model does not simulate unsaturated flow or multi-phase processes. In this thesis, the scope was limited to the saturated zone dynamics and on direct stream-aquifer interactions. However, I agree that in many hydrogeological contexts, particularly those with deep unsaturated zones or significant land-surface inputs, the vadose zone plays a critical role in nitrate attenuation and temporal lag effects. Furthermore, although effective, the optimization algorithms employed in the study can be computationally intensive for large-scale problems. While surrogate models were utilized to reduce computational burdens, challenges remain in achieving greater efficiency for expansive optimization tasks. The WEFE nexus model employed in this thesis simplifies the intricate relationships between water, energy, food, and environmental systems and does not comprehensively address all socio-economic and policy factors that influence resource management. Lastly, the study's scope was limited to numerical simulations, and field verification of the optimal strategies proposed in the research was not conducted, leaving room for further validation through practical implementation.

9.5 Future scope

Future research should address the limitations identified in this thesis and explore additional research directions to enhance the robustness and applicability of the proposed methodologies. Field verification of the optimal solutions obtained from the simulation optimization model in real-world settings is essential to validate the efficacy and practicality of the models. Future work should incorporate reactive transport models that consider redox processes, microbial respiration, and the role of organic matter. Kinetic models for nitrate reduction, including first-order or Monod-type decay, are indeed welldocumented in the literature and will be essential for making future simulations more realistic. Incorporating stochastic methods and uncertainty analysis will help better account for parameter and model uncertainties inherent in groundwater systems, thereby improving the reliability of predictions.

Developing and integrating more advanced surrogate models, such as autoencoders and DeepOnet, can significantly enhance computational efficiency, particularly for large-scale optimization problems (Ullah et al., 2020; Zhang et al., 2024). Autoencoders reduce the dimensionality of high-dimensional optimization problems, allowing for more efficient surrogate model construction. They have been shown to outperform other techniques like Principal Component Analysis regarding modeling accuracy. DeepONet is designed for learning nonlinear operators, which is crucial for solving high-dimensional stochastic problems. The MultiAuto-DeepONet model combines autoencoders with DeepONet to handle multi-resolution inputs and improve efficiency by reducing trainable parameters (Cui et al., 2022; Y. Zhang et al., 2022). Adaptive optimization algorithms that dynamically respond to changing hydrogeological and socio-economic conditions should also be explored to improve the flexibility of management strategies (Kayhomayoon, Babaeian, et al., 2022; Milan et al., 2021). Multi-scale modeling approaches that capture both local and regional dynamics of groundwater systems, and river-aquifer interactions will enable a more comprehensive understanding of these systems.

Incorporating policy frameworks that integrate the WEFE nexus approach can provide a holistic perspective for water resource management, addressing interconnected challenges across sectors. Stakeholder engagement is another critical aspect, and incorporating stakeholder preferences and feedback into the decision-making process will enhance the practical applicability and acceptance of the proposed solutions(Cao et al., 2024; Mendonça et al., 2023b; Radmehr et al., 2024). Developing high-resolution models that account for riverbed heterogeneity will also improve the quantification and understanding of river-aquifer exchanges. Lastly, integrating real-time sensor data into simulation-optimization models can facilitate the adaptive management of river-aquifer systems, ensuring more responsive and effective strategies for resource sustainability.

9.6 Concluding remarks

This doctoral thesis contributes to sustainable water resource management by developing a framework that addresses complex interactions between groundwater and surface water systems. The framework enhances the understanding of R-A exchanges, provides optimization strategies, and demonstrates the potential of integrating surrogate models and many-objective optimization techniques for more efficient decision-making. **This research provides a robust methodology for developing and managing groundwater resources, particularly in subbasins where river-aquifer systems are crucial for water supply and ecosystem health.** By addressing the limitations and pursuing the identified future research directions, the scientific community can further enhance our ability to manage these vital resources sustainably.

This research aimed to enhance sustainable groundwater management while maintaining R-A systems' ecological and hydrological balance.