ABSTRACT

Groundwater management is an inherently wicked problem, characterized by interdependencies between multiple objectives. This complexity is particularly pronounced in regions where groundwater is vital for ecosystem maintenance and socio-economic development. The interconnections between rivers and aquifers (R-A exchanges) play a crucial role in groundwater-dependent systems by sustaining river baseflows during dry periods. This thesis presents an integrated many-objective simulation-optimization (S-O) framework to evaluate the basin-scale Water-Energy-Food-Environment (WEFE) nexus, aiming to develop sustainable water management strategies that balance groundwater extraction, energy consumption, and socio-economic goals. This research advances our understanding of such systems' complex dynamics by applying the S-O framework to the Lower Ain River Basin (LARB), an alpine river with significant R-A exchanges.

A transient three-dimensional groundwater flow model (MODFLOW) was coupled with a nitrate pollution transport model (MT3DMS) to capture the hydrogeological processes influencing the basin. The methodologies employed in this research integrate numerical modeling, metaheuristic optimization, and machine learning. MODFLOW and MT3DMS provided the foundation for simulating groundwater flow and nitrate transport, calibrated using field data and refined through sensitivity analysis. Metaheuristic-assisted S-O models were then employed to analyze trade-offs between net groundwater extraction and R-A exchanges, generating Pareto fronts to visualize these trade-offs. These fronts were evaluated using various performance metrics, revealing insights into the optimal balance

between conflicting objectives. Additionally, surrogate models, including Artificial Neural Networks (ANNs) and Physics-Informed Neural Networks (PINNs), were explored to predict groundwater heads and replicate the results of the S-O framework. This thesis also focuses on decision variable (DV) space analysis, employing aquifer parameter clustering to reduce dimensionality and enhance computational efficiency. A many-objective nexus management model was subsequently developed to assess the impact of WEFE nexus management on R-A exchanges, providing actionable scenarios for sustainable decision-making.

The results demonstrate a distinct trade-off between R-A exchanges and groundwater extraction, underscoring the need for balanced management strategies. Optimizers like MOPSO showed superior performance, with its non-dominated solutions exhibiting better convergence and spread across the Pareto front than NSGA-II and MOEA/D. Surrogate models such as ANNs and PINNs, alongside advanced machine learning techniques like XGBoost and Support Vector Machines (SVMs), were utilized to reduce computational burdens in large-scale S-O frameworks. The findings indicate that ANN models, particularly those with multi-layer perceptron (MLP) architectures, outperform PINNs in predicting groundwater heads, especially in complex domains. PINNs struggled to capture viable distributions of groundwater head variability, highlighting the challenges of applying such models to dynamic, heterogeneous systems. This study further identified key decision variables significantly impacting optimization outcomes, providing a foundation for targeted management interventions.

The objectives of the thesis span multiple facets of groundwater management. The first objective was to design a regional S-O model capable of estimating groundwater head, R-A exchange dynamics, and nitrate loading to optimize these exchanges under varying discharge scenarios. The second objective involved evaluating and comparing the performance of various metaheuristic algorithms, identifying their strengths and limitations based on Pareto front metrics. The third focused on reducing decision variables in groundwater optimization, employing clustering and explainable AI (xAI) techniques to identify the most impactful variables. The final objective was to develop a many-objective optimization model for balancing socio-economic and environmental demands within the WEFE nexus, particularly emphasizing R-A exchanges.

Metaheuristic algorithms, including MOPSO, NSGA-II, MOEA/D, and Pareto search, were applied to explore multi-objective trade-offs, leveraging a dynamic soft distance-based penalty for constraint handling. Decision variable dimensionality was reduced through clustering methods, informed by xAI techniques, to improve optimization efficiency. Lastly, the WEFE nexus was integrated into the framework, providing a many-objective optimization approach to balance competing demands.

The key findings of this thesis highlight the effectiveness of the developed S-O framework in modeling R-A exchanges and optimizing groundwater management strategies. The framework, enhanced by a user-friendly graphical user interface (GUI), facilitates accessibility for policymakers and stakeholders. Comparative analysis of optimization algorithms identified MOPSO as the most effective in achieving convergence and diversity, while NSGA-II and Pareto Search exhibited robust performance across diverse scenarios. The research also demonstrated that ANN models outperform PINNs in predicting groundwater heads, particularly in complex and dynamic domains. Decision variable analysis revealed critical parameters influencing optimization outcomes, enabling targeted strategies to improve resource management. Furthermore, aquifer parameter-based clustering was introduced as an innovative approach to reduce the dimensionality of decision spaces without compromising solution quality. The many-objective optimization model applied within the WEFE nexus framework successfully quantified trade-offs among water supply, energy use, agricultural productivity, and environmental protection, offering comprehensive insights for integrated resource management.

This thesis concludes that the developed framework is a robust decision-making tool for balancing groundwater extraction and R-A exchanges under the WEFE nexus framework. It provides a foundation for sustainable water management strategies by integrating advanced modeling, optimization, and decision-support techniques. Future research should address existing limitations, such as uncertainties in aquifer parameters and model inputs, by incorporating stochastic methods and expanding the application of parameter-based clustering techniques. Enhancing the real-time adaptability of models through sensor data integration and exploring the integration of socio-economic and policy considerations are crucial directions for advancing the research.