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Editorial: Modeling-based approaches for water resources problems, volume II

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Editorial on the Research Topic
Modeling-based approaches for water resources problems, volume II

Modeling approaches are essential tools for investigating water resources problems. These approaches are used in theoretical research and in practical applications for understanding the complex processes controlling water resources problems, performing predictive studies, developing new water management strategies, designing systems and making decisions. Models for water resources problems can be classified into two categories: physics-based models (Miller et al., 2013), and data-driven models (Moyers et al., 2023). In physics-based models, the processes of water resources are described by partial differential equations, which are solved using either analytical or numerical methods. Data-driven models use observational data to construct generalized representations of the underlying problems with specific techniques such as data mining, machine learning or pattern recognition.

Physics-based models are generally suitable for forecasting applications, as they are grounded in physical laws. However, these models are often computationally demanding because they require calibration to fit their outputs with observed data. The calibration process often requires numerous forward simulations and necessitates sensitivity analysis to decrease the number of parameters by identifying the most influential ones (Song et al., 2015). In addition, as input parameters are often subject to uncertainty, reliable predictions require an uncertainty analysis to evaluate effects of the imperfect knowledge of input parameters on model outputs (Moges et al., 2021). This computational burden limits the applicability of physics-based models for large-scale or regional studies (Panthi et al., 2022). On the other hand, data-driven models are usually more efficient (Panthi et al., 2022). Once trained with available data, they can directly establish a functional relationship between inputs and outputs. Some techniques used by data-driven models, such as deep learning neural networks, have high performance on Graphics Processing Unit (GPU) cards. Nonetheless, the performance of data-driven models depends heavily on the quantity and quality of training data (Fahs et al., 2022). Data-driven models are known to be less reliable when used to forecast conditions that fall outside the scope of their training data.

Despite advancement in development and application of numerical models for water resources problems, there is a need for significant effort to improve their reliability, applicability and efficiency. The main challenges include:

- Designing innovative mathematical models that incorporate emerging physical processes, and analyzing the mathematical properties of the resulting equations, such as the existence and singularity of solutions.
- Implementing advanced and appropriate numerical methods and computational strategies to enhance the robustness and computational efficiency of models.
- Designing new numerical tools that leverage advances in computational technologies, such as GPU acceleration and parallel programming.
- Developing new analytical or semi-analytical solutions that serve as benchmarks for model validation.
- Applying models in real-world field studies to explore coupled physical and (bio)chemical processes, such as water flow, heat transport, geochemistry, and surface-subsurface exchange and gain deeper insights into system behavior.
- Implementing new techniques for enhancing model-data interaction.
- Applying models for system optimization problems and developing appropriate optimization techniques.
- Using new machine learning techniques to develop surrogate models that improve the applicability of physics-based models in inverse problems and for sensitivity and uncertainty analyses.
- Developing efficient and appropriate strategies for sensitivity and uncertainty analysis.
- Performing new laboratory experiments to validate models by comparing simulation results with experimental observations.
- Using hybrid approaches that combine advantages of both data-driven and physics-based models.
- Developing methods that deal with the heterogeneity of parameters and variables.

This Research Topic gathers recent advancements and innovative applications of numerical models for addressing critical water resources challenges. Five contributions were selected and published. The papers are mainly related to groundwater management and contaminant transport in aquifers. A summary and analysis of these papers is presented below.

Baalousha developed an efficient technique for parameter estimation and uncertainty analysis for groundwater flow in a heterogeneous karst aquifer null-space Monte Carlo method. The technique is applied to a karst carbonate aquifer in Qatar. It is based on the null-space Monte Carlo approach that allows for simultaneous estimation of parameters and quantification of uncertainties. Heterogeneity is considered using the pilot points approach. The results highlight the efficiency of the proposed strategy, and its applicability at real field scales, despite the considerable number of forward runs.

Su et al. investigated reactive transport in anisotropic domains. They developed a new numerical scheme to simulate diffusion-dominated solute transport in systems with dipping anisotropy. The suggested scheme is based on the multi-point flux approximation method (MPFA) that allows inclusion of full anisotropy. The developed code is verified against 2D and 3D analytical solutions and it is applied to an *in-situ* diffusion experiment and hypothetical deep geological repository. The results highlight the robustness and efficiency of the developed scheme and show the importance of anisotropy in determining long-term solute transport evolution in layered systems.

Burnett et al. developed a sustainable strategy for groundwater management of the Pearl Harbor aquifer in the state of Hawai'i. They used a simulation optimization framework to develop a tool that can help in establishing a suitable groundwater pumping strategy that allows for spring protection. The strategy aims at balancing human groundwater use with the natural spring discharge and the ecological impact of groundwater abstraction. The study presents a framework for determining optimal water pumping rates while respecting the state water policy that mandates specific constraints for social and ecological uses, and potable water demands.

Jari et al. investigated the efficiency of machine learning techniques for groundwater potential mapping. Groundwater potential refers to the ability of an area (i.e., a geological formation) to store and provide groundwater. They compared the performance of the Random Forest, Adaboost, K-nearest neighbors, and Gaussian processes by applying these techniques to the Tan-Tan arid region in Morocco. They demonstrated that ensemble learning models, especially Random Forest and Adaboost, achieved superior performance compared to individual models in mapping groundwater potential. The study showed that among several factors considered in the analysis, such as lithology and land use, the distance to the coast is the most significant parameter affecting groundwater potential.

Manewell et al. developed an efficient strategy for integrating aquifer test interpretations into parameters used by regional models. The newly developed strategy allows for efficient management of scale differences between aquifer tests and regional models. It proceeds via two sequential steps where a fine numerical grid is firstly used to include the aquifer tests, and the data space inversion is employed to endow regional model cells with appropriate model parameters. Numerical experiments are performed and demonstrate the effectiveness of the developed strategy. The paper suggests further research to improve the capacities of the proposed strategy by investigating posterior predictive uncertainties.

Author contributions

MF: Writing – original draft, Writing – review & editing. BA-A: Writing – original draft, Writing – review & editing. TG: Writing

– original draft, Writing – review & editing. MS: Writing – original draft, Writing – review & editing. CS: Writing – original draft, Writing – review & editing. AY: Writing – original draft, Writing – review & editing.

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