



Editorial: Modeling-Based Approaches for Water Resources Problems

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Editorial on Research Topic

Modeling-Based Approaches for Water Resources Problem

Models are common tools for water resources problems. They are used in theoretical research for understanding the complex processes controlling water resources problems. Numerical models are also used in practical applications for several purposes such as predictive studies, management, designing systems and making decisions. Among different existing approaches, physics-based or mechanistic models are of significant importance (Miller et al., 2013). Despite the fact that mechanistic models require numerical techniques for solving the governing equations, they are irreplaceable in studies involving spatially distributed processes (Paniconi and Putti, 2015). Currently, mechanistic models are gaining increasing interest in studies related to climate change (Michel et al., 2022). These models capture real physical processes, and these processes are not likely to change due to climate change stresses. Thus, calibrated physics-based models can provide reliable predictions.

Field applications of mechanistic models require efficient simulators to deal with large time and space scales and a calibration procedure to fit simulations and field observations (Ataie-Ashtiani et al., 2020). Model calibration requires a sensitivity analysis to reduce the number of estimated parameters by identifying the most significant ones (Song et al., 2015). Because 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., 2020). Despite the significant progress in model development and applications, several research questions on the improvement of model applicability and reliability are still open. These questions cover new applications and will take advantage of the advances in computing technology. Current progress on modeling-based approaches for water resources problems combines efforts on:

- Developing new mathematical models to integrate new physical processes and investigating the mathematical characteristics of equations (i.e., solution singularity).
- Developing new numerical methods and computational techniques to improve model robustness and efficiency.
- Developing new analytical solutions for benchmarking purpose.

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- Implementing new techniques for model-data interaction and reliable surrogate models.
- Understanding what data is needed at what spatiotemporal resolution to make meaningful predictions.
- Implementing efficient techniques for sensitivity and uncertainty analysis.
- Conducting new laboratory experiments and comparing simulations to observations.
- Applying models in field studies to investigate multi-physical processes and provide new physical insights.

In this context, this Research Topic was aimed at collecting recent developments and applications on numerical modeling for water resources problems. Six papers were published. These papers cover wide ranging topics including geologic and chemical heterogeneity, the inclusion of geologic information in groundwater models, thermal-hydrological-chemical modeling of freeze-thaw cycles in permafrost systems, reactive transport modeling of CO₂ carbon capture and storage, new finite element methods in groundwater modeling, and integrated assessment modeling for decision making under uncertainty conditions.

A brief summary and analysis of these articles is provided below.

Raymond et al. studied the influence of physical and chemical heterogeneities on the release of acid rocks from waste rock piles. Significant heterogeneities in physical and geochemical parameters is created during the construction of waste rock piles due to the use of heavy equipment. The MIN3P-HPC model was used and applied to conceptual domains dealing with a single bench or multi-bench piles. Heterogeneity was considered by relating physical and chemical parameters to the grain size diameter which was assumed to be randomly distributed. The results indicated that the implications of heterogeneity and construction method are scale-dependent. For different construction methods, the heterogeneity decreases the peak mass loading rates 2 to 3-fold. Heterogeneity leads to longer acid rock drainage release.

Vahdat-Aboueshagh et al. used well log data to identify the geological characteristics in an aquifer. An appropriate approach was developed to interpolate well log data in order to create the stratigraphic structure. The approach was based on domain translation and faces interpolation. It was applied to the Chicot aquifer in Louisiana. A groundwater flow model of this aquifer was developed using MODFLOW. The model was used to investigate the hydraulic behavior of the aquifer. The result shows that pumping activities have reversed the hydraulic gradient and created an inland flow direction, indicating potential saltwater migration.

Yi et al. investigated thermal-hydrological-chemical (THC) processes during waste rock weathering under permafrost conditions. This paper studied mines in remote areas subject to permafrost. It investigated the effect of freeze-thaw cycles and the development of permafrost on drainage volumes and mass

loadings. Thus, the MIN3P-HPC model was used to perform THC simulations of a hypothetical pyrite-rich waste rock pile. The results show a potentially strong coupled effect of sulfide mineral weathering rates and a warming climate on the evolution and persistence of permafrost within waste rock piles and the release of acidic drainage.

Miotlin and Peeters predicted the fate of dissolved CO₂ in the Guarani Aquifer in South America. This aquifer is used for carbon storage, and dissolved CO₂ is expected to undergo geochemical reactions with minerals. However, it is unknown how much dissolved carbon may be immobilized. Thus, numerical simulations were performed with a reactive transport model (PHREEQC) to address this issue. The model predicted that more than a half of the CO₂ could be immobilized by precipitation. The input carbon concentrations and the plagioclase hydrolysis rate are the first parameters controlling the distribution of the carbon across the aquifer.

Etangsale et al. discussed the use to the Interior Penalty discontinuous Galerkin method for solving equations of groundwater flow in heterogeneous and anisotropic domains. The paper compared hybridized-, embedded-, and weighted-interior penalty schemes. The impact of the static condensation procedure in the performance of these schemes is investigated. Numerical experiments confirmed the superiority of the hybridized- and embedded schemes.

Rosello et al. analyzed integrated assessment models that can be used to inform decision making processes relating to water resources management. This study provided guidance on using models under uncertain conditions. The approach was based on (1) invoking a decision support framework, (2) characterizing misalignment with an existing integrated model, and (3) designing adjustable solutions that align model output with immediate information needs. This approach was applied to the Brahmani River Basin in India. The results showed that this approach could be used for rapid feedback early in the planning design process to raise awareness about potential issues to be explored prior to further investments.

AUTHOR CONTRIBUTIONS

MF wrote the first draft of the manuscript. BA-A, TG, MS, CS, and AY reviewed, revised, and edited the manuscript. All authors approved the final version of the manuscript.

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