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*Editorial*

# Groundwater Hydrological Model Simulation

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## 1. Introduction

The management of groundwater resources commonly involves challenges and complexities, which are taken on by researchers using a variety of different strategies. In particular, groundwater numerical modelling is a widely-used and effective approach to simulating and analysing groundwater dynamics under varying conditions. Models are set up to investigate particular features of the groundwater system that need to be better understood; they are generally implemented in order to test conceptual hypotheses arising from field observations of the system. For this reason, numerical models need to be supported by proper field data acquisition and elaboration, a correct conceptualization of the natural system, optimal selection of the computer code and solver, and an effective calibration process. Despite their wide use, each model is different from the others, and modellers must find the best technique to solve specific problems and meet specific objectives. One area that has especially promoted innovation in modelling technique is the study of climate change—it poses new challenges and requires investigation techniques to adapt to new needs.

This Special Issue aims to gather contributions emphasising different aspects of groundwater modelling, focusing on the latest developments and applications for water resources management, including innovative applications of traditional models, the implementation of new open source platforms for groundwater modelling, and the use of artificial intelligence to explore data and expedite the calibration process.

The Special Issue comprises 10 articles and 1 review paper, with contributions from over 47 authors. Geographically, the case studies concern 5 countries extending over 4 continents (United States of America (North America); Ethiopia and Tunisia (Africa); Italy (Europe); Nauru (Oceania)), with very different features (e.g., urban environment, carbonate mountain areas, coastal aquifers).

Specifically, the topics covered by the contributions collected in this SI include:

- the interactions between groundwater and the underground infrastructures in urban areas;
- the use of groundwater models to determine the origin of groundwater contamination;
- the testing of modelling approaches to simulate the impact of climate change;
- the testing of modelling techniques to optimize groundwater management;
- the development of open source software and tools to manage groundwater models;
- application of geostatistical tools to reduce model error and improve predictions;
- comparative studies among numerical models and machine learning techniques.

The SI offers a wide overview of recent applications of groundwater modelling harnessing a variety of techniques. The common goal of all the studies is to test methodologies that can be used to find optimal solutions for supporting stakeholders in adopting proper measures to manage groundwater. Depending on the case study, these measures are aimed at: reducing the damage due to flooding of urban structures; ensuring water supply while guaranteeing a sustainable water balance; evaluating and managing the effect of climate change on sensitive ecosystems; preventing the degradation of good-quality resources; reducing the threat of saltwater intrusion.

## 2. Overview of the Contributions of the Special Issue

The paper "Quantifying Groundwater Infiltrations into Subway Lines and Underground Car Parks Using MODFLOW-USG" [1] investigates the interaction between groundwater and underground infrastructures in a portion of urban Milan (Italy). The authors developed a steady-state MODFLOW-USG model which combined the use of Wall (HFB) and Drain (DRN) packages, for simulating underground infrastructures (i.e., subway lines and public car parks). The model was calibrated against a condition of high water levels. The quantification of groundwater infiltration shows agreement with historical information about submerged structures, giving confidence that the model can be used to predict infiltration related to water table oscillation and, thus, be a support in the design of dewatering systems or other proposed solutions to secure urban structures from potential infiltration damages.

In the contribution "Differentiating Nitrate Origins and Fate in a Semi-Arid Basin (Tunisia) via Geostatistical Analyses and Groundwater Modelling" [2], a MODFLOW-2005 groundwater flow model and a MODPATH advective particle tracking model have been combined with geostatistical analyses based on data from hydrochemical and hydrogeological characterization. Modelling is applied to a multi-aquifer groundwater flow system to verify the hypothesis of geogenic origin of $NO_{3-}$ in the semi-confined aquifer. While the uppermost unconfined aquifer is contaminated by $NO_{3-}$ by anthropic activities, models result show that the leakage of $NO_{3-}$ through the aquitard is negligible. Authors conclude that the high $NO_{3-}$ concentration in the deepest aquifer is associated with pre-Triassic evaporite dissolution and, thus, has a natural origin. These findings based on the model application should help guide proper management of the contaminated aquifers.

The paper "Groundwater Modelling with Process-Based and Data-Driven Approaches in the Context of Climate Change" [3] investigates the application of alternative modelling approaches (process-based, data-driven, and integrated data-driven/process-based) to simulate the effects of different climate scenario on three porous aquifers. Results distinguish key characteristics for each aquifer, such as the ability of storage capacity to mitigate the effects of dry climate conditions or the dramatic sensitivity of a system to climate extremes. In general, the study highlights that choosing the modelling approach based on the specific aquifer features is fundamental to obtaining a modelling tool efficient in supporting groundwater management actions aimed at mitigation of the effects of climate change.

In the paper "Simulation of heat flow in a synthetic watershed: The role of the unsaturated zone" [4], the authors applied a coupled flow (MODFLOW-NWT) and transport (MT3D-USGS) model for simulating unsaturated/saturated heat transport due to atmospheric warming via a synthetic three-dimensional representative watershed. An important novelty of the research is the focus on the unsaturated zone (UZ) and the effect of variable depth–to–water table on heat flow to the water table and surface-water features. The approach is computationally efficient and gives rise to a flexible tool for evaluating the temperature response to warming and trends of heat transport across the watershed. The research highlighted that: (1) the heat flow forcing function is the product of infiltration temperatures and infiltration rates; (2) the UZ has a strong damping effect on the warming signal; (3) the warming is buffered also at discharge points, where shallow and deep flow converge; (4) the stream baseflow response to heat forcing is influenced by the lateral extent of the riparian zone. The authors conclude that explicit representation of the UZ in models is important to realistically evaluating the impacts of climate change on fragile ecosystems such as riparian zones or stream habitats.

The paper "Evaluation of Fresh Groundwater Lens Volume and Its Possible Use in Nauru Island" [5] presents a particular case study concerning the groundwater system characterization and modelling of the Nauru Atoll Island (Pacific Ocean). After a large-scale study for detecting the location of freshwater lenses, a local-scale study was made, aimed at quantifying the freshwater lens thickness and volume for supply uses through a geoelectrical tomography survey, and a 3D density-dependent numerical model implemented in SEAWAT. The main scientific finding is that freshwater in small islands can unexpectedly accumulate right along the seashore and not in the centre of the island. Furthermore, the calibrated model can be used to design sustainable groundwater exploitation systems that avoid the exacerbation of saltwater intrusion.

The paper "ORGANICS: A QGIS Plugin for Simulating One-Dimensional Transport of Dissolved Substances in Surface Water" [6] describes the development and testing of a QGIS plugin, which simulates the concentration of a contaminant along the profile of the watercourse. Attempting to embed surface water solute transport modelling into GIS by inputting the entry point concentration and the average speed of surface water, this tool allows GIS experts to perform first level yet fast simulations of the concentration of the pollutant in surface water bodies. The code is open source and free, which facilitates the reproducibility of the run analyses.

The paper "Simulation of Heat Flow in a Synthetic Watershed: Lags and Dampening across Multiple Pathways under a Climate-Forcing Scenario" [7] is a continuation of companion research already presented in [4]. The processes of overland flow, infiltration through an unsaturated zone (UZ) and groundwater flow discharge to a surface-water network are simulated by a synthetic flow and transport watershed model under a 30-year warming signal. Quantitative results for the transient distribution of heat flow conditions demonstrate the dampening effect of the UZ in the warming transferred to the water table (about 40% of the warming applied to watershed infiltration) and the dampening effect of the aquifer on the heat discharged to the stream network (about 10% of the original warm-up signal). Despite the subsurface lag and storage effects, simulated temperatures in surface waters increase due to the addition of heat by storm runoff which bypasses the UZ. The relevance of this study lies in the fact that provides a possible workflow for climate-change modelling application, allowing for a detailed analysis of warming trends at the groundwater/surface water interface, which are areas of great importance for aquatic ecosystems.

In the paper "A Stepwise Modelling Approach to Identifying Structural Features That Control Groundwater Flow in a Folded Carbonate Aquifer System" [8], the authors set up a procedure to test a numerical modelling technique in a carbonate aquifer characterized by a complex geological structure that constitutes a source of good quality water for human consumption. Three models were implemented by gradually adding complexity to the model grid using an equivalent porous medium approach: single layer (2D), three layers (quasi-3D), and five layers (fully 3D). This was done in order to find the best match with the observed aquifer outflow to the river. The Newton–Raphson formulation for MODFLOW-2005 was used to solve numerical instabilities. Results demonstrated that folded and faulted geological structure control groundwater flow dynamics, and thus need to be adequately represented by a full-3D model. These findings are relevant in applications involving the management of groundwater in corrugated carbonate, which are often exploited for water supply.

In the paper "Using GIS and Remote Sensing Techniques: Case Study of West Arsi Zone, Ethiopia" [9], remote sensing data and geographic information system tools are used to evaluate the groundwater potential of the study area. By means of a chain of GIS tools, parameters influencing groundwater were extracted, mapped, and elaborated in a GIS environment; the procedure was validated by means of borehole data. Results show that the method provides a fast and accurate technique to detect the groundwater potential of an area, furnishing a tool for optimize the planning of groundwater exploitation.

The paper "Minimizing Errors in the Prediction of Water Levels Using Kriging Technique in Residuals of the Groundwater Model" [10] describes an application of the kriging geostatistical tool to the groundwater level residuals of a MODFLOW model developed in the Edwards–Trinity (Plateau) aquifer (Texas), aimed at improving predictions at unsampled locations. The average absolute model error was reduced from 31 m to 5 m, while the average residual standard error decreased from 9.7 to 4.7 m. The authors argue that their procedure makes model results more reliable, allowing design of more informative monitoring systems, and ultimately leading to more efficient management of groundwater resources.

The paper "Improving Results of Existing Groundwater Numerical Models Using Machine Learning Techniques: A Review" [11] presents a review of papers comparing the use of numerical and machine learning methods for groundwater level modelling. The review highlights the advantages or disadvantages of both techniques, depending on the objectives of the model. A promising strategy is to use both methods as complementary to each other: machine learning techniques can improve the calibration of numerical models whereas process-based numerical models are suitable to understand the physical system and, on turn, select proper input variables for machine learning models. Furthermore, machine learning models can provide rapid and effective solutions for groundwater management and are computationally efficient tools to correct head error prediction of numerical models.

The approaches and techniques featured in this SI are a sample of the many innovations being applied to groundwater modelling in order improve water management and to respond to short- and long-term threats to water supply.

**Conflicts of Interest:** The author declare no conflict of interest.

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