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Modeling for sustainable groundwater management: interdependence and potential complementarity of process-based, data-driven and system dynamics approaches

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Abstract

Groundwater systems are vast natural water reservoirs used to support human water demands and ecosystem services. Various modeling approaches have been developed to help manage these complex highly-dynamic systems. This paper discusses the strengths and limitations of three modeling approaches, namely: process-based, data-driven and system dynamics modeling. For demonstration purposes, the three modeling approaches are applied to the Konya Closed Basin, a large agricultural region with semi-dry climate located in central Turkey. Process-based modeling is grounded in the theory-based representation of the governing processes but is somewhat limited by the computational effort and the difficulty of defining the required input parameters that characterize the heterogeneous aquifer system. Process-based models are shown to be powerful tools for resource management purposes provided climatic and water demand scenarios are accurately defined. Data-driven models are efficient tools for the management of groundwater resources but are highly dependent on the availability of large training data sets encompassing the spectrum of possible system responses. The high efficiency of surrogate modeling approaches makes them ideal tools for incorporation into applications such as real-time decision support systems and digital twin platforms. System dynamics modeling examines the groundwater exploitation problem within a socio-economic context that involves multiple stakeholders and their decision making. It combines groundwater flow models with socio-economics and endogenous decision rules to conduct scenario analysis and support policy development. The analyses and model demonstrations presented in this paper underscore the interconnectedness and complementarity of these three modeling approaches and the need for more integrated use of these modeling approaches for enhanced multi-sectoral management of groundwater systems.

Key words: process-based modeling, system dynamics modeling, data-driven modeling, water resources management, irrigated agriculture

1. Introduction

Groundwater is a widely accessible resource that is increasingly playing a vital role in providing freshwater for domestic use, industry, and agriculture and for sustaining ecosystems (Ben Salem et al., 2023; Berghuijs et al., 2022). Groundwater systems possess relatively large storage volumes, estimated to be as much as 100 to 1000 times annual recharge, thus providing a high buffering capacity to mitigate against seasonal as well as annual fluctuations in precipitation, particularly in arid and semi-arid regions (Margat and van der Gun, 2013). As a result, global groundwater extractions have increased dramatically to more than 1000 Gm^3/year. This constitutes about 26% of the total global water use, including the water supply for 40% of irrigated lands worldwide (Gleeson et al., 2016; Siebert et al., 2010). The utilization of groundwater for irrigation has boosted economic growth and food production of many regions of the world (Lejars et al., 2017, Butler and Whittemore, 2024). Nonetheless, the widespread overexploitation of groundwater has also placed significant stress on this vital resource, leading to the depletion and contamination of many aquifer systems worldwide. These stresses pose significant risks to human health, socio-economic development and the environment, thereby threatening the sustainability of this vital resource and raising issues of intergenerational inequity. Climate change is further intensifying these challenges by instigating shifts in global temperatures and precipitation patterns which in turn affect groundwater recharge (IPCC, 2021; Green et al., 2011; Secci et al., 2021; Secci et al., 2023). It is imperative to recognize climate change as an external factor influencing groundwater quantity and quality and to urgently assess the impact of future climate change scenarios on groundwater resources.

Groundwater systems are highly dynamic and complex systems with spatially variable properties, difficult to estimate extraction and recharge rates, and highly temporal interactions with surface water bodies (Saatsaz and Eslamian, 2020). Direct monitoring is often limited to small fractions of the aquifer volume. As a result, modeling of subsurface systems has increasingly become an indispensable tool for the management of groundwater resources. Modeling is utilized to address a wide range of issues relating to both water quantity and quality, including the management of groundwater resources and assessing the impact of climate change on this vital resource (e.g., Jódar et al., 2024; Mundetia et al., 2024; Rajaveni et al., 2016).

The term modeling is very loosely used and can mean different things to different users (Konikow and Bredehoeft, 1992). A model is defined as a representation of the real system and can be broadly classified as physical, conceptual, mathematical or numerical. The development of models involves continuous tradeoff between the incorporated level of realism, generalization and functionality (Levins, 1966). As a result, all models involve some form of simplification and loss of precision and, hence, there is no single correct model of a system (Cuddington et al., 2013). In the analysis of groundwater systems, like other fields, widely varying modeling approaches exist. Physical models are typically simplified small-scale representations of the real system normally constructed to examine specific flow or pollution transport processes. Conceptual models depict the governing processes and relationships between variables. Conceptual models are often utilized as an intermediate step for developing mathematical models that provide a more quantitative representation of the flow and transport processes. Numerical models are generally developed when model complexity prohibits the use of analytical tools for the solution of mathematical models.

Modeling, the focus of the current study, varies widely in its purpose and underlying formulation. In the context of groundwater resources management, three modeling approaches will be examined in this study: process-based modeling (PBM), data-driven modeling (DDM) and system dynamics modeling (SDM). PBM is built on fundamental concepts such as the principles of conservation of mass, energy or momentum, often expressed in terms of governing partial differential equations. PBM relies on the latest physical formulations for the relations between dependent and independent variables. Their main challenges often include the computational effort involved and the need to quantitatively define the input parameters describing the governing process.

In recent decades, with the advancement of computational power, there has been a growing reliance on DDM to address complex problems. These models are particularly effective in capturing crucial relationships between inputs, including geological properties, boundary conditions, pumping rates, climatic data and outputs, such as groundwater levels, contaminant concentrations, or groundwater flow rates. This capability enables swift simulations and facilitates decision support.

Whereas most groundwater models focus on the simulation of flow and contaminant transport, there are other processes that also have significant impact on this resource. SDM (Forrester 1961, Sterman 2000), simulates nonlinear interactions and constructs feedback systems that better explain the broader dynamic nature of the systems including human, social and economic components. This modeling approach, which has its roots in the management of complex industrial processes, has evolved into a scientific practice with applications in various fields of research including socio-hydrological problems.

The rest of the paper is organized as follows. Section 2 gives an overview of the application of these three modeling approaches (PBM, DDM and SDM) to groundwater related problems and how they evolved over the years. Section 3 presents an application of these models that were developed for the management of the groundwater system of the Konya Closed Basin, one of the major agricultural regions of Turkey that is facing groundwater resources depletion due to overexploitation. Section 4 discusses the strengths, limitations and complementarity of these three models

2. Overview of Groundwater Modeling Approaches

2.1. Processed-Based Modeling

PBM are mathematical representations of one or several processes or mechanisms that describe the functioning of a well-delimited system (Buck-Sorlin, 2013). The processes are based on well-established scientific understanding, typically expressed in terms of one or more differential equations. PBM can be found in diverse disciplines such as forestry studies (Gonçalves et al., 2021), climate change modelling

(Wilson et al. 2021), soil sciences (Mu et al., 2020; Pierson et al., 2022), genetics and molecular biology (Gross, 2024) and economics (Smart et al., 2007). PBM are also widely used in the field of hydrology with the development of some models as well as debate among researchers on the challenges of these type of models and how they can be overcome going back to more than 5 decades (Clark et al., 2017). In the following subsection, we focus on the evolution of PBM relating specifically to the field of subsurface hydrology.

The use of numerical models for the management of groundwater resources traces back to the middle of the 20th century (Bredehoeft, 2012; de Marsily, 1986; Freeze, 2022). Earlier efforts focused on developing analytical solutions of the governing equations for simplified input parameter distributions and boundary conditions. With the development of computers, starting in the 1960's, numerical models that describe groundwater flow became gradually available (Bredehoeft, 2012). In the 1970s, numerical techniques such as the finite difference and finite elements were employed to solve the governing partial differential equations. However, the progress in these endeavors was constrained by the computational capabilities of the computers of that era. Further computational developments along with increased interest of hydrogeologists in utilizing numerical models for the solution of groundwater flow and contaminant transport problems led to the development of public domain PBMs such as MODFLOW (McDonald and Harbaugh, 1988), SUTRA (Voss, 1984), and MT3D (Zheng, 1990). These publicly accessible models allow for the simulation of the transient three-dimensional groundwater flow and contaminant transport for complex geometries and boundary conditions and for spatially variable input parameters. Some of these models remain in use to this day, albeit with a number of enhancements.

Models that can simulate saturated as well as unsaturated flow were also developed like the widely used HYDRUS computer code (Šimůnek et al., 2022). Such models are particularly of interest to simulate aquifer recharge and irrigation-related problems. Groundwater PBMs were also expanded to simulate multiphase flows such as those related to the remediation of groundwater contaminated with non-aqueous phase liquids (NAPLs). Computer codes capable of simulating multiphase flow include T2VOC (Pruess et al., 1993) and UTCHEM (Delshad et al., 1996). The governing equations describing multiphase flow are highly non-linear and coupled, including the occurrence of complex interphase mass transfer processes such as evaporation and dissolution, making them particularly difficult to solve.

Recognizing that the input parameters required by these models are always associated by some uncertainty due primarily to the heterogeneity of the subsurface environment and to the absence of exhaustive data to fully define their spatial patterns, the field of stochastic subsurface hydrogeology emerged with original works including Freeze (1975), Dagan (1989) and Gelhar (1993). Stochastic hydrogeology rapidly evolved into a broad field of study with extensive research activity and field applications (e.g., Kitanidis, 1997; Rubin, 2003) that are continuing to this very day (Renard et al., 2023).

PBM is also used for solving the inverse problem (de Marsily et al.1999, Carrera et al. 2005; Sun, 2014; Zhou et al. 2014). In the typical forward groundwater flow problem, input parameters such as the storativity and hydraulic conductivity are defined over the entire domain and the governing equations are solved to yield the dependent variable such as the hydraulic head or concentration.

The tremendous development in the field of quantitative hydrogeology in recent decades has made PBM an indispensable tool for the management of groundwater systems (Keller et al., 2023). PBM can help in the interpreting of field data and for enhanced understanding of the complex spatially distributed groundwater flow systems. Modeling has been used for the estimation of water budgets (e.g., Forootan et al., 2014; Aderemi et al., 2022; Glose et al., 2022). The spatial distribution of budget components such as the recharge may not be easily determined from measurements but can be estimated through model calibrations. Models have also been used to estimate the safe and sustainable yields of pumping wells. Such estimates can help in the sustainable use of groundwater resources and for extending aquifer lifespans. Modeling has been shown to be useful as part of a Decision Support System that targets improved management of limited water resources and/or protection of water resources from contamination or seawater intrusion (Kazakis, 2018). Numerical models are also suitable for sensitivity analyses and for risk assessment. With climate change expected to drastically influence water availability in many regions of the world, groundwater modeling has been used to assess the impact of climate change as well as other anthropogenic factors (Munir et al., 2024, Guevara-Ochoa et al., 2020).

Recognizing the importance of the interaction of surface and groundwater bodies, an increasing number of coupled process-based surface/subsurface hydrology models have been developed (Shen and Phanikumar, 2010; Ahmadi 2023). Numerous studies have shown that surface water bodies are strongly interconnected with groundwater resources but that this connection is dynamic, bidirectional and complex. Therefore, in many applications it is crucial to develop coupled surface-subsurface models for enhanced management of water resources. The most commonly used models that can simulate surface water/groundwater interactions are: SWAT-MODFLOW, GSFLOW, MIKE SHE, and HydroGeoSphere. Such models can for example help in assessing the impact of land use and vegetation changes (Öztürk et al., 2013), the impact of shallow water tables and irrigation practices on soil salinization (Nick et al., 2024) and the benefits of different water management practices such as enhanced irrigation systems or cropping changes (Wei and Bailey, 2019; Glose et al., 2022, Guevara-Ochoa et al., 2024).

2.2. Data-Driven Modeling

DDM is a particularly powerful type of surrogate modeling because it enables learning from data that is too expensive to analyze using traditional methods, or, in the worst case, makes it possible to create surrogate models for systems that would otherwise be controversial to model. Data-driven modeling techniques use input-target datasets to map how the system works and to create a simplified model that can be used to predict the system's behavior. These datasets can be generated from the complex system itself through simulations or experiments, or they can be collected from historical data. Once the input-target dataset is available, a data-driven modeling technique can be used to find linear or non-linear relationships. This model can then be used to predict potential outputs for any given set of input parameters.

The heterogeneous nature of aquifer properties introduces a substantial number of parameters which can slow down the simulations of PBMs. This hinders their use in integrated modeling for real-time decision support, especially for analyses involving multiple scenarios. A thorough analysis of surrogate models in groundwater studies is presented by Asher et al. (2015) which sheds light on the prevalent use of DDMs in predicting groundwater levels and addressing groundwater contamination issues.

Groundwater flow predictions leverage statistical methods, spatiotemporal geostatistics, and machine learning techniques. Notably, these models require only an initial training phase that makes use of historical or simulated data pertaining to the driving factors, such as precipitation and temperature, along with their corresponding responses, such as groundwater levels. (Bierkens et al., 2001; Bloomfield and Marchant, 2013; Varouchakis and Hristopulos, 2013; Secci et al., 2021; Secci et al., 2023)

Groundwater contamination represents another facet of DDMs applied to groundwater problems. Specifically, DDMs have been considered in three key areas: contaminant transport modeling, groundwater vulnerability assessment, and addressing inverse problems. The first area involves models that aim to simulate and predict the movement of contaminants through aquifers. They integrate extensive datasets, encompassing groundwater quality measurements, geological information, contaminant source data, and vital hydrogeological parameters (Douglas and Efendiev, 2006; Opher et al., 2009; He et al., 2019; Yu et al., 2020; Rodriguez-Galiano et al., 2014).

Groundwater vulnerability assesses the susceptibility of groundwater to contamination from diverse sources. It involves understanding the hydrogeological characteristics, identifying potential contaminant sources, and assessing pathways through which contaminants can enter the groundwater (Arthur et al., 2007; Sajedi-Hosseini et al., 2018; Atenidegbe and Mogaji, 2023). For the solution of groundwater inverse problems, Barati Moghaddam et al. (2021) and Gómez-Hernández and Xu (2022) have contributed critical reviews that comprehensively analyze four decades of efforts made in this field.

2.3. System Dynamics Modeling

System dynamics emerged in the 1950s as a model-based discipline to explore dynamically complex managerial problems. Since its inception, marked with the seminal works of Jay. W. Forrester (Forrester, 1961; Forrester, 1968), it has matured into a systems approach that addresses the root causes of chronic socio-economic problems with an endogenous focus (Sterman, 2000; Barlas, 2009). Being a model-based approach, advances in system dynamics have been highly influenced by developments in digital computation, as well as in mathematics and statistics (Sterman, 2018). Today, applications of system dynamics stretch over contemporary teams in corporate and business management, public policy and resource management, and sustainability. System dynamics theory delves into the issues of systemic model conceptualization/identification, formal model characterization, numeric computation, validation, scenario building, policy analysis and implementation. Barlas (2009) comprehensively covers the philosophical and methodological aspects of system dynamics. A short methodological outline for modeling is presented in Feola et al. (2012).

In parallel to the theory and practice accumulated in system dynamics in the 1960s, Stanford Watershed Model (Crawford and Linsley, 1966) and the Susquehanna River Basin Model (Hamilton, 1969) are considered to be the first applications in water resources management. Winz et al. (2008) argues that the systems approach to water resources management (Biswas, 1976; Rogers and Fiering, 1986) and integrated water resources management have created a larger space for the uptake of SDM in water resources management. Wurbs (1994), in their review of computer models for water resources management, cite the stock and flow based STELLA II (High Performance Systems, 1985) simulation platform of its time as one of the software that is in use by practitioners with the capabilities of “flexibility in realistically representing real-world system concerns”, and “analysis, display and communication” but also caution that the model building and maintenance can require large time and effort. Ford (1996), Saysel et al. (2002), Stave (2003) and Martínez-Fernández and Selma (2004) can be cited among earlier applications, sharing common principles and goals pertaining to system dynamics, such as dynamic problem orientation, multi-sectoral model boundary selection comprising the hydrological as well as socio-economic elements of a policy problem, feedback-rich model conceptualization, and model construction, analysis and implementation with the purpose of learning and system design. Today, with the emerging literature on food, water, energy nexus underlying the possible trade-offs and co-benefits in resource provision (FAO, 2014; Simpson and Jewitt, 2019) and the socio-hydrological modeling (Blair and Buytaert, 2016) demanding a holistic, multi-sectoral modeling approach for learning and management, rather than “problem solving”, system dynamics is now facing larger opportunities to respond to the needs as such in research and practice.

There are more recent inspiring applications of system dynamics in groundwater management studying semi-arid, water stressed geographies in Iran, New Mexico, and Turkey. Bakhshianlamouki et al. (2020), Ravar et al. (2020), and Naderi et al. (2021) adopt a nexus approach to water resources management by developing dynamic feedback models for multi-sectoral policy analysis, the former with a focus on Lake Urmia restoration and conservation, and the latter for sustainability measures in Gavkhuni and Qazvin plains in Iran, respectively. Bai et al. (2021) study socio-hydrology in New Mexico with a focus on agricultural water management in Rio Grande in New Mexico, analyzing policies extending from water sector to agriculture. Langarudi et al. (2021) extend the work in Rio Grande to southern New Mexico. Akhavan and Goncalves (2021) focus on groundwater use and sustainability in pistachio farming in the Rafsanjan of Iran. Their analyses are particularly interesting to show “better before worse” consequences of popularly received supply side solutions in water resources management. Mir et al. (2022) study the "limits to growth" in the fossil water dependent agricultural sector in Sistan of Iran.

3. Application to the Konya Basin

3.1. Study Area and Data Availability

The three modeling approaches described above- PBM, DDM, and SDM were applied to the Konya Closed Basin The basin, located in Central Anatolia, is the biggest endorheic basin in Turkey, covering an area of about 50,000 km^2 (Figure 1).

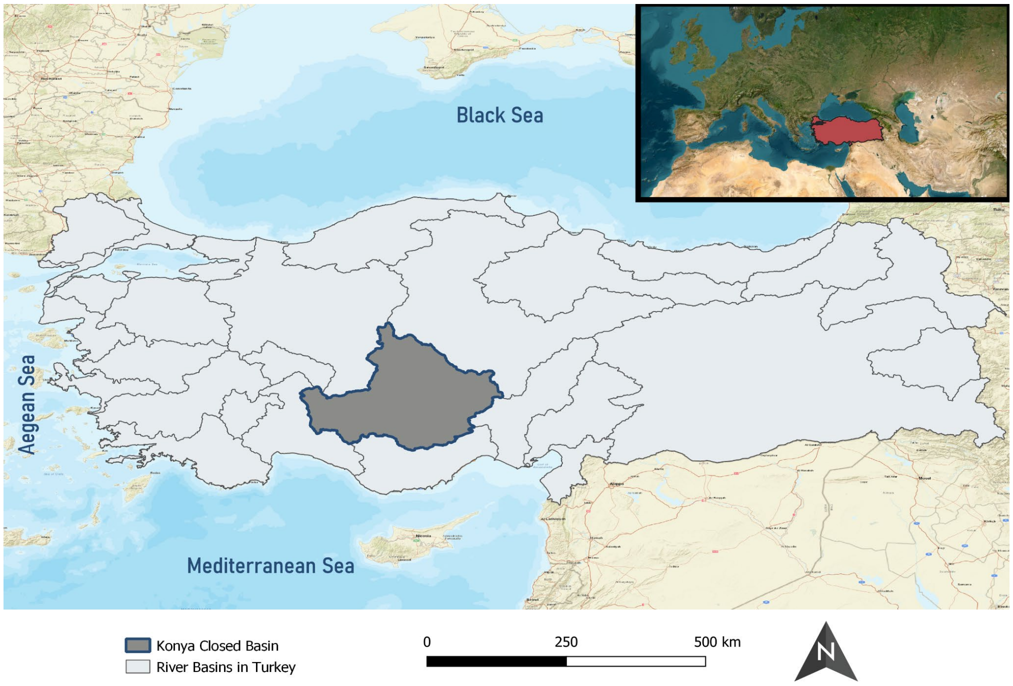


Figure 1. Map of Konya Closed Basin

The basin is characterized by a semi-arid continental climate with hot and dry summers and cold and moderately moist winters. The current average precipitation is about 380 mm/year with irregular temporal and spatial distribution. The higher precipitation rates are over the mountainous areas located in the southern and eastern portions of the basin with lower rates in the central plain. On the other hand, the potential evapotranspiration over the basin is about 1400 mm/year (Bayari et al., 2009).

The basin is a major agricultural region with around 90% of the cultivated land used for grain production mainly wheat, barley, sugar beet and corn (Figure 2). Historically, mostly dry agriculture was practiced (Saygin et al., 2023). However, the past 2 decades witnessed a steady transition to more profitable and water-demanding crops such as corn and sugar beet (Yilmaz et al., 2021). Today, irrigation is the primary driver of water consumption in the basin, estimated to constitute more than 90% of the basin's water demands. Since surface water resources are limited, groundwater is widely used to supply the water deficiency. The number of wells in the basin is estimated as more than 100,000, with about two-thirds unlicensed (Yoloğlu, 2023). The overexploitation of the groundwater resource has led to a sharp decline in groundwater levels, placing significant pressure on the food production, economic viability, and ecosystem services of the basin (Özturk et al., 2023). Projected climate change is expected to further exacerbate the situation.

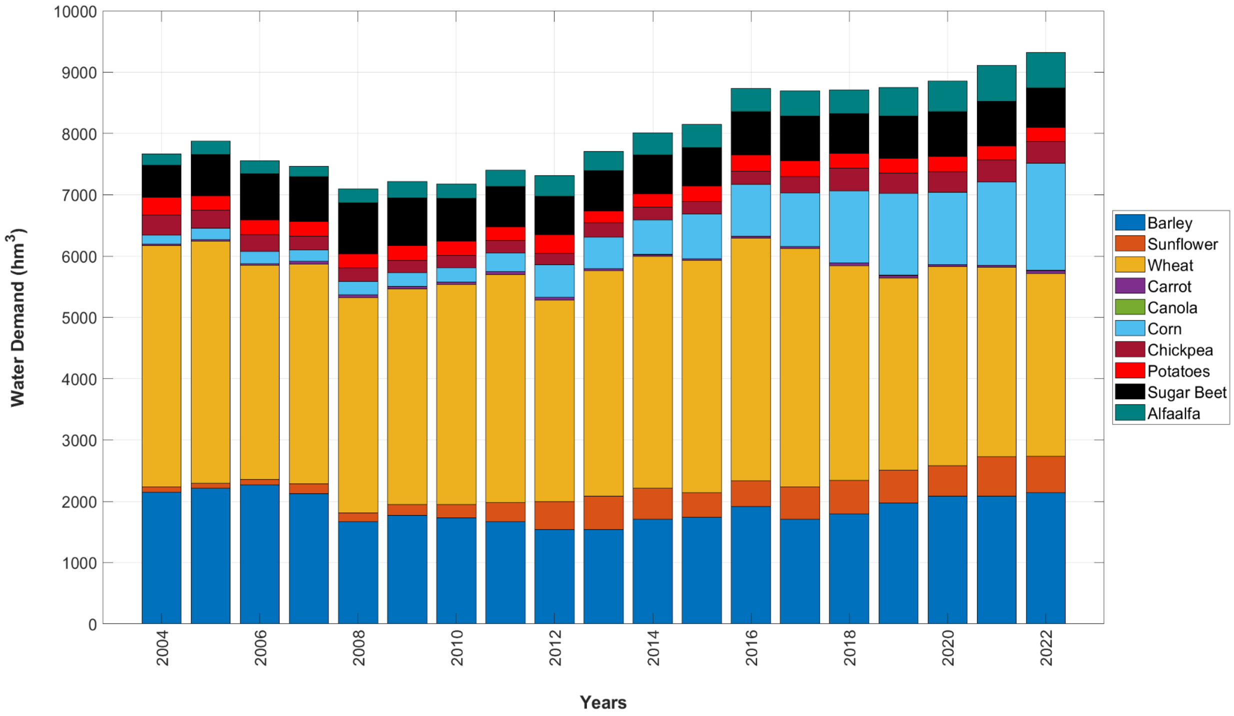


Figure 2. Water demand of the various crops cultivated in the Konya Closed Basin

The basin includes two primary aquifer systems: a shallow, fresh-water Neogene aquifer system and a deeper saline aquifer system, separated by low permeability Paleogene rocks. The fresh-water Neogene aquifer system has variable thickness extending to more than several hundred meters in some locations (Bayari et al., 2009). Geologic maps and well logs show the presence of a thin alluvium, mostly silty loam, overlaying the Neogene aquifer system with mountainous regions located along the edges of the basin. The hydraulic conductivity in the basin varies between 0.43 and 593 m/day based on data from 81 pumping tests located mostly in the central valley of the basin. The current hydraulic head varies from about 910 m above mean sea level in the central portions of the basin to more than 1200 m in the mountainous region at the east boundary of the basin. Since pumping wells are generally unmetered, groundwater extraction rates were estimated as described below indirectly from published official data on the cultivated areas of each crop and from water demand data of different crops for the Konya region (TUIK, 2023). These water demand calculations were performed on a monthly basis. Additionally, farmers' decisions on crops, irrigation methods, and irrigation level based on multiple factors, such as costs, prices, and groundwater and crop regulations, were also utilized in model development.

The three modeling approaches, which have different capabilities and hence use different datasets and scenarios, are discussed in the following sections.

3.2. Process-Based Model

3.2.1 Model Description

The PBM was developed using the MODFLOW program coupled with the UZF1 module (Niswonger et al., 2006) which simulates vertical water flow in the vadose zone along with horizontal flow in the underlying aquifer system. The advantage of using the coupled saturated/unsaturated model is that it does not require the definition of the spatially distributed recharge rate into the aquifer which is difficult to estimate; instead, the model internally calculates the net recharge to the aquifer from the spatially and temporally-dependent surface water (precipitation and irrigation) and the crop-dependent evapotranspiration. Details of the model are given in (Yoloğlu, 2023). The transmissivity and storativity were estimated from a series of pumping tests and spatially interpolated over the entire basin using kriging. As this is a closed basin, no-flow boundary conditions were assumed along the outer boundary. Past daily precipitation distributions for the period from 2000-2023 were spatially interpolated from 18 meteorological stations located within the basin. As noted above, because pumping wells are generally not metered, the groundwater extraction rates were estimated indirectly from crop cultivated areas and the water demand data of the different crops (TUIK, 2023). Potential evapotranspiration rates were defined based on published data for the Konya basin (TAGEM, 2017). Water demand calculations were performed on a monthly basis.

The model was calibrated using monthly observed water level from 29 wells for the period from 2000-2022. The irrigation efficiency, defined as ratio of the effective water use to the actual water withdrawal, was designated as the primary calibration parameter. The irrigation efficiency is the product of conveyance efficiency and field application efficiency (Brouwer et al., 1989). Typical values are in the range of 0.2-0.3 for low efficiency conditions to about 0.6 for high efficiency irrigation systems (Rai et al., 2017). The efficiency values determined from model calibration ranged from 0.3 for years 2000-2004 to 0.65 for years 2015-2022. These values reflect the gradual transition by farmers to more efficient irrigation since 2010 due to water-authority incentives.

3.2.2 Model Output and Analysis

Figure 3a shows the simulated head distribution at the end of year 2022. It is observed that the heads in the central area of the domain are lowest with flow from the boundary regions of the domain towards the valley in the central portions of the domain. The average long-term drop in groundwater levels in the central area is estimated to be 0.62 m/yr. The significant decline in groundwater levels underlines the unsustainable use of available water resources with potentially serious impacts on food production and livelihood of the inhabitants of the region.

The calibrated PBM was then used to investigate the impacts of different groundwater use practices for different climate change scenarios. Seventeen regional climate models from the EURO-CORDEX project under two climate pathways (RCP 4.5 and RCP 8.5) were considered for the period of 2023-2040 (Todaro et al., 2022). Five different water management scenarios were developed based on surveys with farmers, NGOs, and water authorities. These management scenarios considered the impact of (i) enhanced irrigation technology, (ii) roll back of corn cultivation, a recently expanded crop with relatively high water demand, to 2005 levels and (iii) inter-basin water transfer. For each scenario, 34 simulations were performed, each corresponding to one of the 17 available RCMs under the two climatic pathways, RCP 4.5 and 8.5. For demonstration purposes, results of two scenarios are presented here.

Figure 3b shows the water level distribution for December 2040 for the business as usual scenario, characterized by the absence of substantial alterations in policy or behavioral pattern. This scenario assumed that the trend in cropping that occurred in the years 2000-2022 continues into the future. The irrigation efficiency for the business as usual scenario is also assumed to continue to increase at a rate equal to that observed in the last two decades. The figure shows the simulated heads averaged over the 17 RCMs. The spatially averaged monthly head corresponding to the 17 RCMs is plotted in Figure 4a. The blue dotted line on the figure shows the calibrated model result between 2000 and 2022 with the black line depicting the median head for the RCP 4.5 and RCP 8.5 climatic pathways. A fan plot is used to depict the variability of the simulation of the various RCMs under the two climatic pathways. The model predicts that the rate of groundwater drop will gradually increase in the coming years as a result of expanded irrigation lands and crop types. The average annual drop in groundwater level between the years 2023 and 2040 ranged between 0.02 and 0.39 m/year for individual climate projections, with an average of 0.28

m/year. Future rates of groundwater drop are smaller than historical values corresponding to years 2000-2010 because of the switch to more efficient irrigation systems.

Figures 3c and 4b show the corresponding head distribution for the scenario corresponding to the roll back of corn cultivation to 2005 levels and replacing it with wheat, a winter crop more suitable for the semi-dry climate of Konya. This scenario also considers the continued trend in enhanced irrigation efficiency that has been occurring in recent years. It is observed for this scenario that the average groundwater levels are close to steady. These results demonstrate the type of analyses that can be conducted with the PBM that can help decision makers and water authorities in managing available water resources.

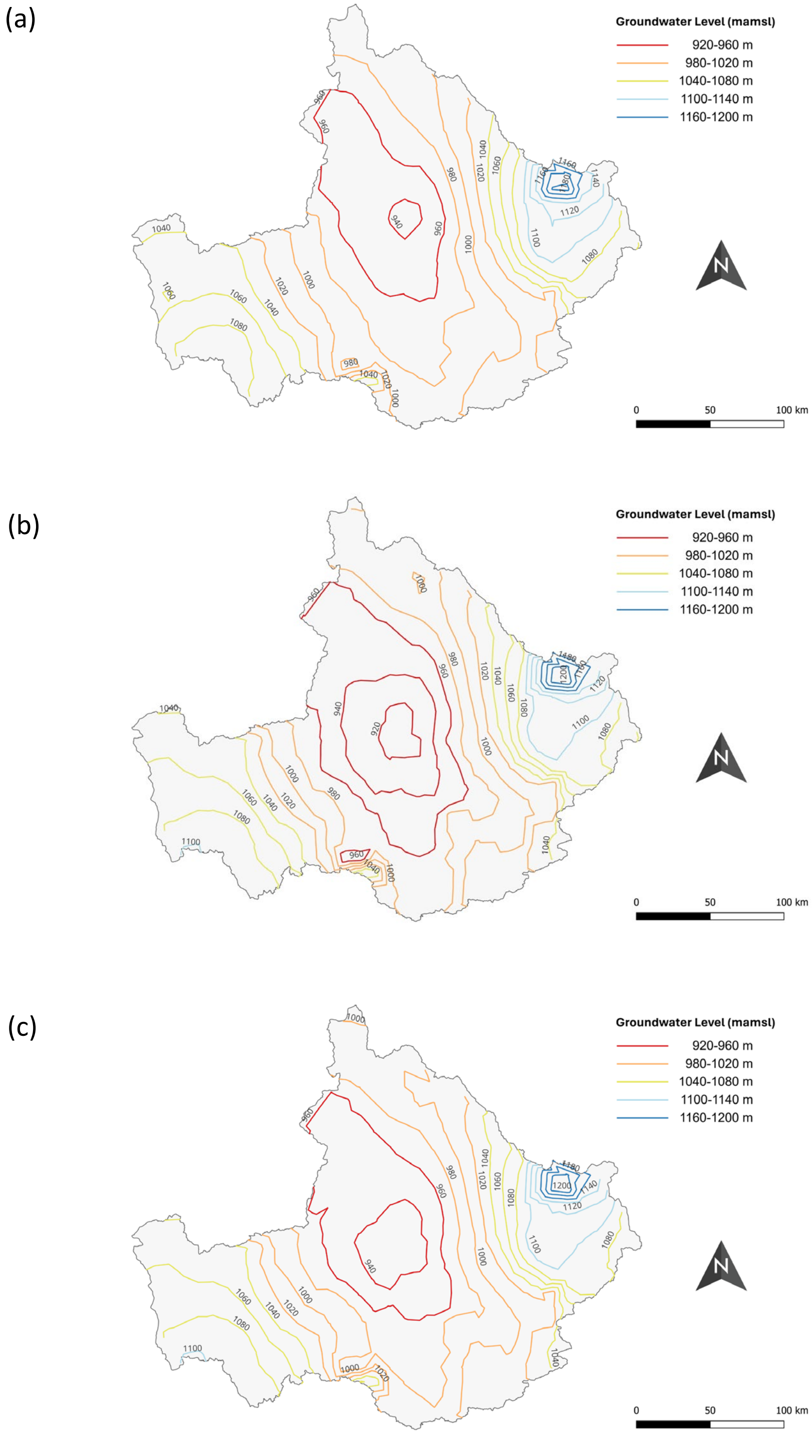


Figure 3. Simulated groundwater level in meters above mean sea level for (a) end of year 2022 at the end of the calibration process (b) end of year 2040 based on 17 RCMs under RCP4.5 climatic pathway for the business as usual scenario (c) end of year 2040 based on 17 RCMs under RCP4.5 climatic pathway for the reduced maize and enhanced irrigation scenario.

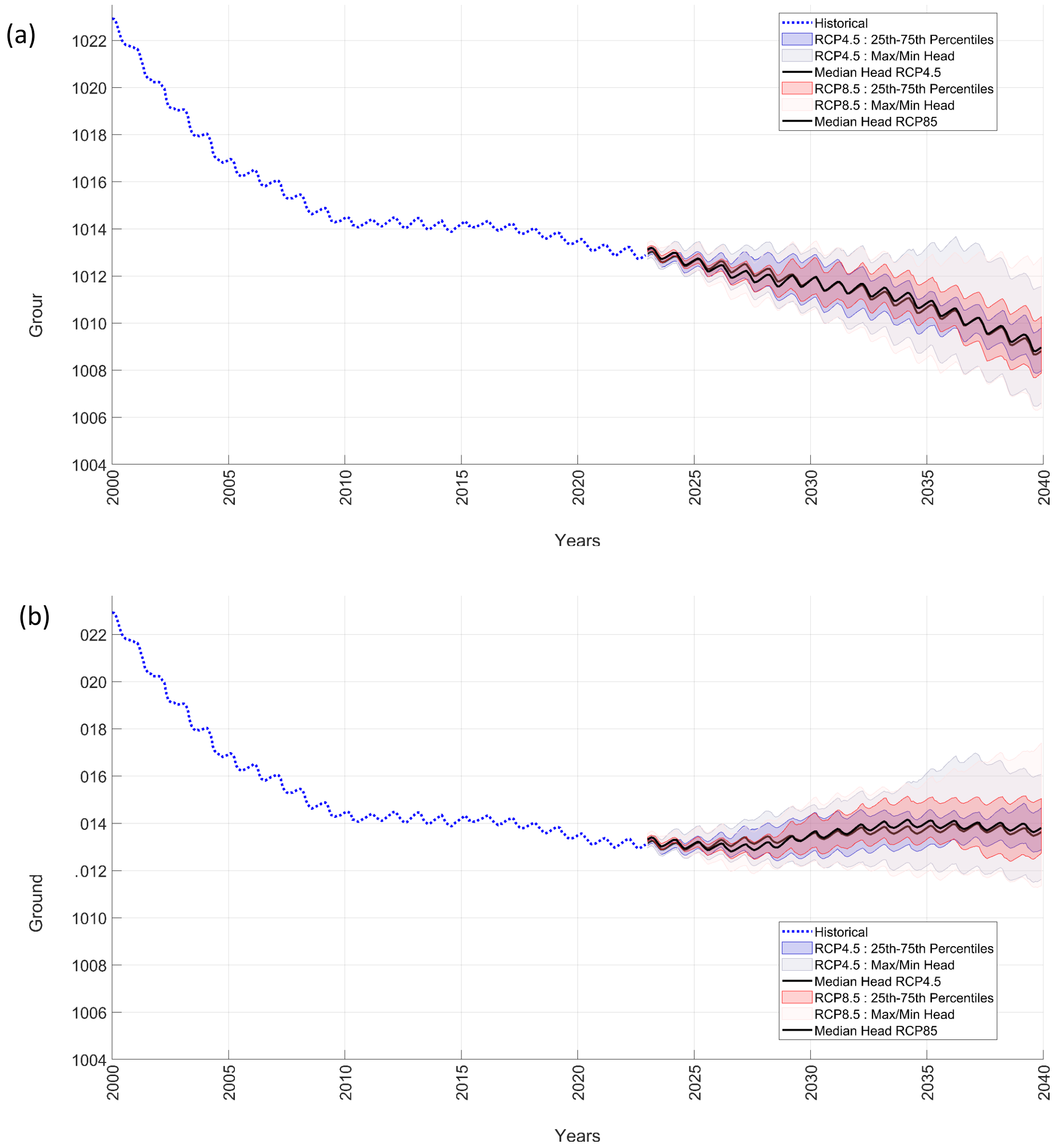


Figure 4. Predicted groundwater level in meters above mean sea level averaged over the entire basin for RCP 4.5 and 8.5 under (a) the business as usual (b) reduced maize and enhanced irrigation scenarios.

3.3. Data-Driven Model

3.3.1. Model Description

The implemented DDM , is an easy-to-use tool based on an artificial neural network(ANN). Details of the mathematical concepts are available in Secci et al. (2022). The model predicts monthly groundwater levels at 30 control points in the Konya Close Basin (Figure 5) until year 2040, considering various climate change and agricultural practice scenarios. The climate scenarios consider changes in precipitation, while the agricultural scenarios consider possible changes in crop types and irrigation patterns.

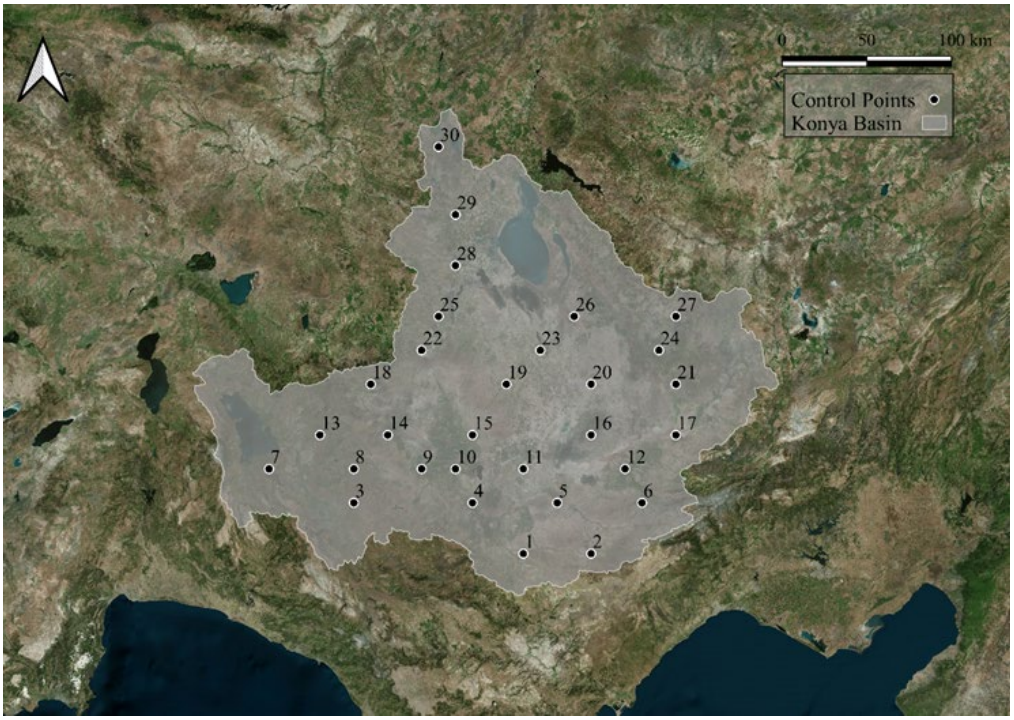


Figure 5. Konya closed basin (Turkey) and the 30 control points

In the application to Konya Closed Basin, the neural network consists of three layers: input, hidden and output. The ANN has three input features, incorporating two multiplicative coefficients—one assigned to historical precipitation (precipitation coefficient) and the other to historical crop water demand (crop coefficient)—and time. A hidden layer comprising 10 neurons processes this input with the desired output consisting of the groundwater levels at the 30 monitoring points (see Figure 5).

For training purposes, a dataset of 100 combinations of precipitation and crop coefficients was generated using the Latin Hypercube Sampling method (McKay et al., 1979). The precipitation coefficient ranged from 0.6 to 1.4, indicating a precipitation variation between -40% and +40% compared to the observed period. Concurrently, the crop coefficient ranged from 0.75 to 1.25, corresponding to a water demand varying between -25% and +25% of the historical one. For each combination, the PBM was executed from 2020-2040, generating monthly head data at the 30 monitoring points. The initial head distribution for this simulation was based on the December 2019 head data obtained from the calibrated PBM.

The input data, comprising 100 combinations of precipitation, crop coefficients, and time, along with the corresponding output (monthly heads at the 30 control points), constituted the dataset employed for training the network. Since the simulation covers a period of 20 years (2020-2040), each combination simulated by the full model produces 240 values of monthly heads for each of the 30 control points. Therefore, for each control point, the total size of the training dataset is 24,000 (100 combinations multiplied by 240 outputs each). The training dataset was partitioned into training (70%), validation (15%), and testing (15%) sets and standardized for stabilizing neural network training, mitigating issues such as vanishing gradients, and accelerating model convergence. The hyperparameters were calibrated manually with a batch size of 128, number of epochs equal to 50. The early stopping was selected as regularization criteria to prevent overfitting, while the learning and decay rates were set as 0.001 and 0.05, respectively.

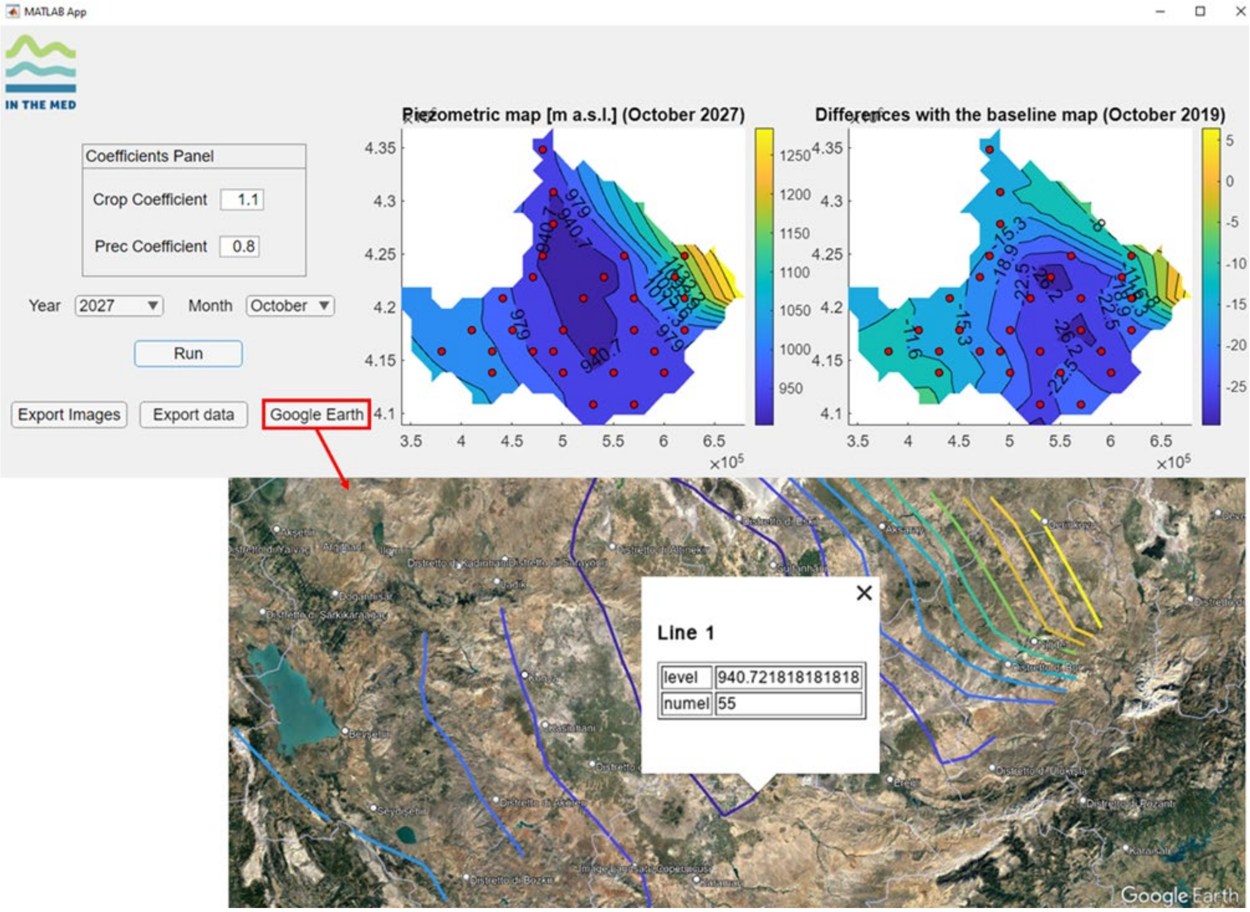
3.3.2. Model Output and Analysis

The mean square error of the overall network performance is 20.74 at the initial iteration, decreasing to 0.0061 at the final step of the training. This signifies a substantial decrease of at least three orders of magnitude compared to the initial loss calculated with randomly initialized weights and biases. In addition, the training, validation and test phases yielded means square error values of 0.0060, 0.0061 and 0.0062, respectively. While these results might raise concerns about overfitting due to the strong performance in the training phase, the consistent loss value associated with the validation dataset confirms effective training. This is further supported by the neural network's robust ability to generalize when confronted with data unseen during the testing phase.

Furthermore, the quality of the implemented model was also assessed in terms of the Coefficient of Determination (R^2), which quantifies the proportion of the variance in the dependent variable that is predictable from the independent variable(s). The R^2 values approach unity for the training, validation and testing phases (0.9626, 0.9634, 0.9635) indicating a remarkably high level of predictability in capturing the variance within the data.

The ultimate goal of the DDM was to develop an accessible and user-friendly tool that utilizes the trained neural network to predict groundwater levels. Figure 6 shows the user interface of the ANN tool that was developed in MATLAB (MathWorks, 2022). The left-hand panel allows users to simply select the precipitation and crop coefficients and specify the period for which the results are required. Clicking the "Run" button invokes the fully trained ANN, which uses the user-provided input features to generate the desired output. The results are presented in the form of a piezometric head map. The monthly groundwater levels at the 30 control points are provided by the ANN, while the final piezometric map is generated by spatial interpolation of the network's output. Additionally, based on the user-defined simulation period, the algorithm automatically creates a map that shows the differences between the obtained piezometric map and the baseline map from 2019 for the selected month.

The tool allows the user to export the images and the data associated with the 30 control points and the interpolated values to a text file. Finally, the resulting maps can be visualized as a contour plot superimposed over Google Earth Pro (Google LLC, 2023).



Coefficients Panel

Crop Coefficient 1.1

Prec Coefficient 0.8

Year 2027

Month October

Line 1

level	940.721818181818
numel	55

Figure 6. Piezometric map generated by the ANN tool

3.4 The System Dynamics Model

3.4.1 Model Description

The SDM explores the socio-economic and behavioral drivers of unsustainable groundwater use and aims to build a shared understanding of sustainable future pathways in the Çumra district of the Konya Closed Basin. Çumra is about 2200 km^2 and is considered one of the most agriculturally productive regions of the basin. To that end, the model was developed in parallel to three model group building workshops, in a living lab context (Andersen et al., 2007; Ceseracciu, 2023) with the participation of multiple stakeholders, including local farmers, water management authorities, chambers of agriculture, regional development administration, irrigation unions and cooperatives, academics, and environmental and agricultural NGOs.

First, desktop research was conducted for problem and stakeholder identification. Then, two field trips were organized to acquaint the research team with the stakeholders and initiate the living lab, followed by two participatory modeling workshops. The first workshop aimed to arrive at a shared understanding of the problems and to identify potential policy intervention points, representing the ideas and preferences of the diverse stakeholder groups. The second workshop focused on developing the seeds of a conceptual model through a joint examination on the nature of the relationships between variables. Building on the outputs of the workshops, the research team focused on formal model building, and then organized a third field trip for testing and validation of the model with selected stakeholders. In a third and final workshop, the stakeholders had the opportunity to explore the long-term impacts of multiple policy alternatives (as specified in the previous workshops) on a simulation platform through a model interface designed for that purpose and discuss the outcomes, reflecting back on their previous opinions. Further details regarding the group model building process are presented in Uygur (2023).

Figure 7 shows the conceptual model, where the causal interactions between the variables are presented with black arrows. Irrigation demand is driven by the crop land cover, farmers' crop yield goal, and marginal productivity of irrigation, i.e., crop yield return to water. Whether the demanded irrigation water can be supplied from groundwater depends on groundwater availability (remaining groundwater reserves) and accessibility (capacity of existing extraction infrastructure). Groundwater component is incorporated in the model with a single stock, representing the saturated zone. It is depleted with extraction and fed by recharge and lateral flow. Groundwater extraction infrastructure includes wells and pumps, which are adjusted annually based on irrigation demand. The crop yields are determined by the level of irrigation. Farmers update (i) land allocation of crops based on the relative profitability of crops and (ii) crop yield goals based on past experience. Production costs and generated revenues for the unit production of each crop are compared to determine the profitability of crops relative to one another. Though the total agricultural land is constant in the model, the size of the cultivated land changes due to the fallow practice in non-irrigated lands, and the share of each crop is adjusted continuously; more land is spared for more profitable crops. The red arrows represent potential policy interventions, aiming either to control groundwater supply directly (for example, enforcing a groundwater extraction quota or restricting well digging), or to decrease the demand for groundwater (for example, incentivizing less water demanding crops or enforcing crop rotation schemes). A publicly available user-friendly interface is published on the web (https://exchange.iseesystems.com/public/izel/inthemed-final-model---eng/index.html#page1), on which stakeholders run their own policy experiments with various options such as crop rotation, surface water transfer, extraction limits, and repricing of crops.

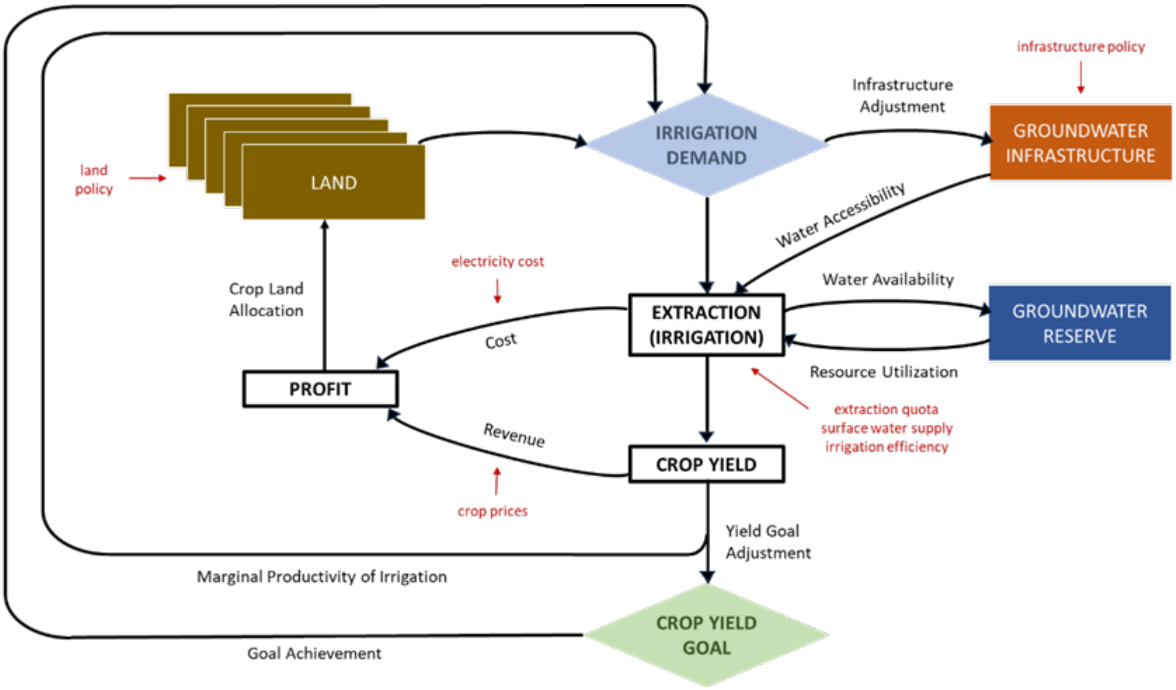


Figure 7: System dynamics conceptual model

The model was developed on STELLA Architect (ISEE Systems, 2023). It comprises groundwater hydrology, as well as farmer decisions on crops, irrigation method, and level of irrigation based on multiple driving factors, such as costs, prices and groundwater and crop regulations. The time unit of the model is one year, and the simulation horizon is 36 years from 2004 to 2040. The presented outputs in Figure 8 are simulated by solving the system of coupled ordinary differential equations using Euler's integration method with a computation step equal to 1/32. The integration method and time steps were based on criteria presented in Sterman (2000, Appendix A).

Prior to model based policy analysis, various validation tests were applied to the model. Socio-economic components were tested with indirect structure testing (Barlas, 1996) and with respect to socio-economic data on land use, crop choices and yields. Moreover, SDM had a coarse, spatially lumped representation of the groundwater resources. For these reasons, the calibrated PBM described in Section 3.1 was employed for the partial validation of the groundwater component of the system dynamics model (Homer, 2012). In an experimental procedure, 42 runs were taken from the PBM to estimate the parameters for the recharge and lateral flow rates in the system dynamics model. A detailed explanation of the partial validation process is provided in Uygur (2023).

3.4.2 Model output and analysis

Figure 8 presents the results of the base run, compared to an integrated policy. In the historical period (2004 through 2022), the unirrigated land shrinks as irrigation practices are adopted in the region. With irrigation, crop yields increase over time, rendering irrigated agriculture more profitable and more attractive. The increased demand for irrigation water requires infrastructure building; new wells are drilled and the average pump power increases. As a result, increased extraction leads to a continuous decrease in the groundwater table.

The policy scenario starting from 2025 includes interventions debated by various stakeholders and do not necessarily reflect on potential enforcement problems. They are formulated as follows: the unit electricity and green plants prices are decreased by 30% and 20% respectively, cereal and sugar beet prices are increased by 60% and 75% respectively, a 2-year rotation scheme is enforced for the green plants (as the current practice in some irrigation cooperatives in the region), 350 hm^3 of surface water is supplied for agricultural irrigation through the Mavi Tunnel, a recently constructed inter-basin water transfer project, well drilling is prohibited in the 2025-2030 period, and a pumping quota of 90,000 m^3/well/year is enforced.

As can be viewed in Figure 8, the integrated policy scenario has rather counterintuitive results; it negates the general belief in the basin that groundwater protection and maintaining the economic benefits of agriculture (a win-win case for the environment and the farmers) are mutually exclusive. Under this scenario, there is a significant improvement in groundwater level, compared to the base run. The crop pattern changes drastically due to both the changes in the price and the crop rotation; while the area for green plants decreases to one third of that of the base run, irrigated cereal and sugar beet become more favorable for farmers with higher prices. The total irrigated land is reduced by 13% and converted to unirrigated land. The decrease in overall water demand can be observed through the groundwater infrastructure; both the number of active wells and the average pump power are lower under the policy scenario compared to the base run. Additionally, even though lower irrigation levels lead to a declining trend in sugar beet and green plants' yields, the average profit substantially increases under this policy set, partly because of the increased crop prices and partly because the decrease in the unit electricity price reduces farmers' overall costs.

Indeed, there might be numerous other policy scenarios that different stakeholders may consider superior to this one, which implies that the "best" policy option is value-laden and dependent on the prioritized goals. For this reason, the model interface was a useful tool at the third workshop, where a diverse stakeholder group discussed their favored policies and their implications in the long run. Discussions of issues that are 'elephant in the room', such as the number of unlicensed wells in the basin and crop irrigation rates were facilitated through experimentation with the SDM by the end users and the water managing authorities.

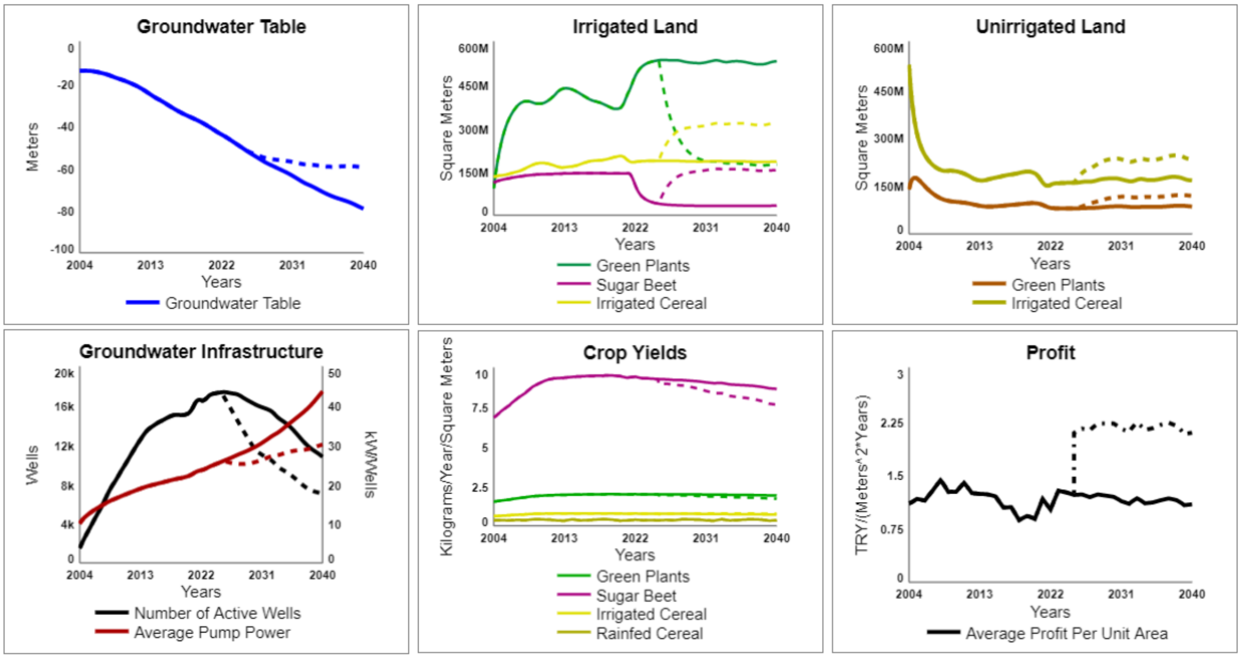


Figure 8: Key system variables in base run (solid lines) vs. the integrated policy scenario (dotted lines)

4. Discussion

The PBM, DDM and SDM approaches applied to the water-stressed Konya Closed Basin bring forth significant outcomes for sustainable groundwater management. Below it is argued that, while these modeling approaches have considerable differences with respect to their purposes, model formulations, model building processes, information sources, and validity and success criteria, their specific implementation in Konya has been interdependent and demonstrates potential complementary. In this section, first the generic differences and similarities of the three approaches are introduced. After that, their strengths and limitations, with reference to their specific implementation in Konya, are summarized. Last, the issues related to interdependence and complementarity during their implementation are summarized.

4.1 Differences and similarities

4.1.1 Overarching purposes

The PBM serves as an important tool that can aid in management of groundwater resources. It aims at understanding the hydrogeologic conditions, constrained by available site-specific data, for the study area that is highly dependent on groundwater resources. By considering alternative scenarios of exogenous changes such as pumping rates, land use and climate, the PBM, after calibration against observed historical data, can be utilized for predictive purposes, for example by estimating future groundwater levels and water budget. The DDM aims for a practically applicable, fast operating tool for predictive purposes. In that respect, it yields a useful tool to perform 'what if' analyses of the impact of exogenous inputs (ex. pumping and precipitation) on resulting outputs (ex. groundwater heads). SDM aims at policy exploration and design with respect to selected key performance indicators. It can internally generate socio-economic scenarios (e.g., increasing pumping) under a selected set of exogenous choices (e.g., crop prices). Though it is used to generate foresight to the future, it is rarely used for point-in-time predictive purposes, fundamentally because its behavior is generated by its high order, multi-loop nonlinear structure rather than exogenous drivers of change.

4.1.2 Mathematical formulations and computational effort

PBM is built on contemporary theory in the mature field of hydrogeology with decades of experimental work and analyses. The model is formulated with spatially distributed partial differential equations, solved numerically on computer platforms, often requiring long computation times. It is not a black box, but a causal modeling approach relying on the latest representation of hydrogeologic conditions and flow through porous media processes. DDM screens the regularity of patterns or intricate relationships among huge data sets using machine learning techniques, statistical analyses, and pattern recognition algorithms, amenable to fast computation. Differently from PBM, it operates by adopting a black-box approach that prioritizes predictive accuracy over explicit causal or theoretical understanding among the variables of concern. SDM builds on elicitation of variables with empirical/theoretical meaning and assessment of their causal connection and feedback processes formulated in terms of differential equations. In non-spatial SDM with aggregated agents, computation time is hardly a constraint. Individual mathematical formulations are based on multiple theories, as well as controllable empirical truths. In this regard, SDM is more similar to PBM with its causal/theoretical nature.

4.1.3 Modeling process

Available PBMs are often highly complex, spatially distributed constructs of the governing hydrogeological processes. They are often packaged in re-usable codes to be implemented for different cases and for relatively different purposes. Typical applications of PBM do not cover model building from scratch but utilize available, already verified codes. For each application of DDM, tasks, such as data collection and preprocessing (handling missing values, removing outliers, and normalization), are required. Feature selection or engineering is then performed to extract the most informative variables for the modeling task. An appropriate modeling technique is subsequently selected from a wide range of approaches such as regression models and ANNs, tailored to the nature of the problem. The SDM is typically built from scratch for a specific model purpose. In the case of SDM, model building benefits from generic model structures and archetypes that have been developed for models with relatively different purposes, theories from diverse disciplines of interest for the specific project, and empirical knowledge often enhanced with various forms of stakeholder involvement.

4.1.4 Data needs and use

Respective differences in purposes, model formulation and modeling processes create different needs and uses of data for each of the three approaches. Availability of large-scale quantitative data enhances the usefulness and predictive capacity of PBM. On the other hand, because of its reliance on widely studied processes, PBM is not totally bound to data availability. Based on its theoretical structure, it can operate with limited direct measurements supplemented with inferred or measured data derived from previous studies performed under similar hydrogeologic conditions, albeit with some increase in level of uncertainty. Unlike traditional approaches that rely heavily on predefined mathematical equations or theoretical frameworks, DDM derives its insights directly from the data itself. This means that the effectiveness and reliability of DDM are entirely contingent upon the quality, quantity, and representativeness of the data available. Every aspect of the modeling process, from model selection to parameter tuning, hinges on the characteristics of the dataset at hand. Therefore, meticulous attention is paid to data collection, preprocessing, and feature engineering to ensure that the data accurately reflects the underlying phenomena being modeled. SDM benefits from a mix of quantified (numeric) and qualitative data and often operates with limited data sets compared to the needs of its holistic, large boundary view of socio-environmental systems. Whenever quantitative data sets are available, they are primarily used to set the problem orientation and reference behavior of the model. While prior estimation of model parameters is performed, due to limited data and structural uncertainty, many parameters are indirectly estimated through model simulation tests.

4.1.5 Validity and success criteria

Validity and success criteria of the three modeling approaches are also differentiated. PBM is built on established and developing theories, often relying on re-usable, therefore tested, computer codes. Hence, for most PBM applications, the model structure and code is not rigorously scrutinized. The model quality and usefulness is tested through model calibration whereby model input parameters characterized with high levels of uncertainty are adjusted, within acceptable constraints, to improve agreement between model output and key dependent variables subjected to imposed boundary and initial conditions. The model calibration process benefits from sensitivity analyses performed to assess the behavior and sensitivity of the model output to key model input parameters. The validity of a DDM is typically assessed by testing its performance on unseen data, achieved through a process of training-validation split and subsequent evaluation. Initially, the available data is partitioned into a training set, used to train the model, and a validation set, used to evaluate its performance. The model is then trained on the training set, learning patterns and relationships within the data. Following training, the model predictions are compared to the actual values in the validation set using appropriate performance metrics. Additionally, the model can be tested on entirely new, unseen data to validate its generalization ability. In SDM, although the model is a causal representation of the system being analyzed, the underlying theories can be insufficient, ambiguous, and the socio-environmental reality overly complex to be sufficiently formulated in model structure. Therefore, every case specific application of SDM needs to go through the process of confidence building on its theory-like structure. Hence, first structural validation tests are implemented. Models with sufficient confidence in model structure then go through behavior validation tests to check whether the model produced patterns match with real life data sets. Beyond visual, descriptive judgements on pattern matching, statistical measures for means, trends, periods and amplitudes are commonly used.

4.2. Demonstrated strengths and limitations

The versatility in incorporating various data types enhances the PBM's accuracy, adaptability, and reliability, making it a valuable tool for simulating and predicting the complex dynamics of groundwater systems in response to different scenarios and external factors. Its reliance on well-established physical processes enhances user confidence and its reception among stakeholders and water resources managers. The PBM developed for the whole Konya Closed Basin provided an estimate of the temporal water balance for past conditions and future scenario analyses, to serve as one of crucial information for sustainable groundwater management. It utilized geologic maps, well logs and pumping test data to define the spatial distribution of the hydrogeological properties of the aquifer system. The model incorporated extensive precipitation data from various monitoring stations for simulating spatially and temporally dependent meteorological conditions and long-term historical groundwater data for model validation and calibration. The basin lacked direct measurements of groundwater extraction data, like many aquifers worldwide (Butler et al., 2023). For that reason, the model used an indirect estimate of groundwater extraction rates, with calculations based on the documented spatial distribution of cultivated areas of the various crops, their water demands and on irrigation efficiency scenarios.

A limitation encountered during the development of PBM of groundwater resources was the need for an estimate of aquifer recharge. Because of lack of reliable estimates of the recharge, this parameter was designated as a calibration parameter. To circumvent this requirement, the developed PBM for the Konya Closed Basin was extended to incorporate vertical water flow in the vadose zone in addition to horizontal groundwater flow. As such, the recharge in this model was an intermediate model output calculated from the applied surface water and evapotranspiration rate instead of defining it as input to the groundwater model.

The calibrated PBM was then used to assess the impact of climate change and the impact of different pumping scenarios management changes on the sustainability of groundwater resources. A limitation of PBM at this stage of analysis was its dependence on exogenous scenarios, either perpetuating past trends or building wishful futures, disregarding the socio-hydrological response to changing groundwater conditions in the long term.

Recent advancements in smart tools like surrogate DDMs have bolstered decision support systems capabilities remarkably by reducing computational time, which is useful for making timely decisions in dynamic environments. Surrogate DDMs expedite results without compromising accuracy, thus promoting cost-effectiveness, and improving organizational performance. The surrogate DDM for Konya Closed Basin offered easily interpretable results and is integrated with a user-friendly interface, making it accessible to governmental authorities, farmers, NGOs, and many other stakeholders indirectly involved in the groundwater debate, without the requirement for an in-depth understanding of the complex physical dynamics.

Despite their benefits, the black-box nature of surrogate DDMs, such as ANNs, may lead to skepticism about their reliability, invoking distrust among the end users of the tool. Emerging methods, such as incorporating physical constraints during training, aim to enhance model interpretability (Raissi et al., 2019; Secci et al., 2024). Furthermore, if high-quality and sufficient data are not available to adequately describe various scenarios within an appropriate training range, the DDM cannot be effectively trained. In fact, one limitation of DDM in this study was its entire reliance on the PBM, calibrated to historical data, for the generation of a consistent range of data needed for training the ANN to simulate different scenarios that exceed the historical precipitation and water demand datasets. Nevertheless, once trained, the DDM can prove to be beneficial for Decision Support System and can also potentially serve as a calibration model for the SDM, thereby significantly reducing the computational burden associated with this process.

SDM is a robust methodology for the analysis of dynamically complex problems with an endogenous focus. SDM allows for a multi-sectorial approach in groundwater management, incorporating various elements of socio-hydrological complexity. The SDM for Konya Closed Basin had focused on the administrative unit Çumra in and benefited from stakeholder knowledge and judgment at various stages of the study. It created future water use scenarios considering multiple system wide decisions in feedback, such as crop choices, factor use, infrastructure development and technological efficiency changes in response to changing groundwater conditions. For example, SDM relaxed the best irrigation practice and full resource accessibility assumptions subtle in scenarios perpetuating the past or building wishful futures. In that respect, SDM partly covers the factors leading to the paradox of irrigation efficiency (Grafton et al. 2018). The model interface for policy exploration and reduced simulation time enabled its use in a workshop setting to facilitate communication and learning among the stakeholders.

The SDM had a simplified representation for groundwater hydrology, in a non-spatial “box model” accumulating the lateral and vertical recharge minus pumping on an annual basis. This overly simplified representation of groundwater hydrology risked SDM’s messages being highly generic, rather than empirically grounded. To overcome this limitation, SDM benefited from PBM for partial validation of its hydrological component. Specifically, the flow parameters for SDM were estimated with simulation tests running the SDM and PBM in parallel under experimentally designed conditions of isolated and comprehensive flows with extremely high and extremely low irrigation conditions. The PBM outputs of these experiments were used to estimate SDM flow parameters.

4.3 Interdependence and potential complementarity

The Konya Closed Basin application and ensuing discussion demonstrates the different modeling perspectives can be utilized to examine water-related issues and identify optimal management strategies. The PBM rooted in scientific principles, provided a detailed understanding of underlying processes that are crucial for accurate representation of complex systems. The DDM offered a valuable alternative for tasks requiring rapid predictions and optimization. The SDM examined long-term groundwater management from a socio-hydrological perspective. The output of PBM is used to train DDM, and for partial validation of SDM. DDM once calibrated, can also be used for partial validation of SDM. SDM driven scenarios can be used by PBM and DDM to predict future groundwater conditions. In future applications, researchers can pursue enhanced coupling of these three approaches.

5. Conclusions

Numerical modeling has evolved into a vital tool for the management of groundwater resources. This paper traces the development over the past decades of three modeling approaches: PBM, DDM and SDM for the analysis of groundwater systems. We discuss these three modeling approaches in terms of their objectives, model formalism and computation, modeling process, data requirements, validation, computational effort and model use. To illustrate the strengths and limitations of these approaches, we describe their application to the Konya Closed Basin, a major agricultural region of Turkey that faces significant water stress due to over-exploitation of groundwater resources.

The three modeling approaches examined in this study have significant differences in various dimensions. The application to the Konya plain illustrates their strengths and limitations, but also their interdependence and suggested complementarity of these approaches. Depending on the specific purposes of individual modeling projects, one or more of these approaches can be pursued. By combining the strengths of PBM, DDM, and SDM, a synergistic effect can be achieved. This integrated approach not only enhances predictive accuracy but also fosters a comprehensive grasp of the studied phenomena. Moreover, the synergy enables researchers and practitioners to navigate the trade-off between computational efficiency and model fidelity, ensuring a balanced and informed decision-making process. Therefore, the collaboration between PBM, DDM and SDM presents a nuanced and effective approach for advancing modeling methodologies across diverse applications. To make use of their strengths, future model development efforts can focus on enhanced coupling of these modeling approaches. Recognizing the strengths and limitations of each approach, a hybrid modeling strategy emerges as a powerful path forward.

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