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Research Article

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DOI: https://doi.org/10.21203/rs.3.rs-599210/v1

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Multi-Objective Optimal Model for Sustainable Management of Groundwater Resources
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Abstract

Increased abstraction from the aquifer, in addition to the progressive drawdown of groundwater table can increase the concentration of pollutants. This research, optimal scenario for withdrawing water from wells is proposed for the aquifer sustainable development. The aquifer quantitative and qualitative simulation was carried out with the GMS model. The developed code in MATLAB2018b provides the link between the simulation and the NSGA-II optimization tools. Optimal scenario was chosen based on applying the Multiple-Criteria Decision Making (MCDM) and Berda Aggregation Method (BAM). The results show that reducing the current withdrawal rate to 51.55% can establish the quantitative and qualitative stability of the aquifer. The spatial and temporal distribution of nitrate concentration after applying the optimal discharge of wells shows that the nitrate concentration in central and eastern parts of the aquifer have greatly reduced. The developed structure can be used to improve the quantitative and qualitative status of any aquifer.

Keywords: Karaj aquifer, Nitrate concentration, GMS simulation model, NSGA-II, Multi-objective optimization, Sustainable development, MATLAB code
1. Introduction

Groundwater resources are one of the main and most important components of water supply in the domestic, agricultural, and industrial sectors. Lack of precipitation, high potential of evapotranspiration, increasing consumption along with their development during the past decades have caused an increasing pressure on water resources, especially groundwater resources in arid and semiarid regions (Safavi et al., 2010).

In Iran, more than 300 plains out of 609 plains in this country due to intensive use of groundwater have been declared as "forbidden plains". In these plains, with extensive withdrawals and overwater capacity from aquifers, these underground reservoirs face a negative water balance of nearly 5 MCM (Million Cubic Meters) per year. A total of 500 BCM (Billion Cubic Meters) of strategic underground reservoirs have been identified in Iran. Of this amount, 200 BCM is brackish water and only 300 BCM in terms of quality can be used by various consumer sectors. So far, for various reasons, significant amounts of these resources of more than 110 BCM (more than 36% of static volume of groundwater reservoirs) have been extracted (IWRMC, 2017). Excessive withdrawals, drilling of illegal wells, insufficient monitoring of the amount of withdrawals beyond the exploitation permission has led to significant decrease well yields, decrease in GWTL, reduction in groundwater discharge to streams, increase in pumping costs, decrease in groundwater quality, land subsidence in a number of plains (Rejani et al., 2009; Zhang et al., 2014; Xiang et al., 2020).

It is not possible to create sustainability in quantitative and qualitative conditions of groundwater resources in many arid and semi-arid regions, but it is possible to minimize the adverse effects of over-abstraction by using appropriate operation policies for these valuable water resources.

For this purpose, many studies have been proposed and successfully applied to real-world groundwater systems since the 1970s to manage groundwater resources and create sustainable
conditions using simulation and optimization tools. In these models, due to the lack of access to important quality parameters such as nitrate and the complexities of aquifer quality modeling, the water quality of the aquifer is usually less considered in development of operation polices of groundwater. Typically, these models use an aquifer simulation model (which can be an analytical solution or well-known codes such as MODFLOW) and an optimization tool to solve groundwater resource management problems. Also, in these studies, optimization tools are different according to the number of decision variables, the complexity of the problem, and the number of objectives. By implementing these groundwater management models, it is possible to provide scenarios of aquifer operation (Ahlfeld and Pinder (1992); Ebraheem et al., 2003; Karamouz et al., 2005; Karamouz et al., 2007; Ayvaz and Karahan (2008); Esteban and Dina (2013); Farhadi et al., 2016; Banihabib et al., 2019; Nazari and Ahmadi (2019); Sabzzadeh and Shourian (2020); Norouzi Khatiri et al., 2020). In this section, as an example, the approaches considered for groundwater management by some researchers are mentioned.

Rejani et al. (2009) proposed a non-linear transient hydraulic management model (model 1) and a linear land allocation optimization model (model 2) for the Balasore coastal basin groundwater management. The first and second developed models have been sued to optimize the pumping rate and determining the optimal cropping patterns for maintain groundwater levels within the desired limits, respectively. The results obtained based on the developed policies for wet, normal and dry years show that the pumping schedules and cropping patterns differed significantly under the three scenarios, and the groundwater levels improved significantly under the optimal conditions compared to the existing condition. Also, the net annual return from the basin during three strategies increased to 257% (in wet period), 167% (in normal period), and 112% (in dry period) of the present net annual return.
A GA based simulation-optimization model was presented by Sedki and Ouazar (2011). In developed model, the optimal groundwater exploitation strategies in Rhis-Nekor Plain with the objective of maximizing groundwater withdrawals to supply water demands has been considered. This study shows that the proposed pumping strategy can capture an important amount of the nonbeneficial fresh water discharging to the sea for local water supply.

Majumder and Eldho (2016) examined the effectiveness of cat swarm optimization (CSO) for groundwater management using the combination of the analytic element method (AEM) and reverse particle tracking (RPT). In this study, three single-objective problems were considered where the objectives are defined as: maximization of the total pumping of groundwater from the aquifer, minimization of the total pumping costs, and minimization of groundwater contamination by capture zone management. The results obtained from applying the developed model to a two hypothetical case study show the superiority of CSO in comparison with other optimization algorithms.

A linkage between DSSAT, an agronomic model, and MODFLOW on an annual time step in order to assessing groundwater conservation strategies in groundwater-irrigated regions was prepared by Xiang et al. (2020). Due to the significant increase in aquifer recharge by municipal and agricultural wastewaters, one of the parameters that usually increases in groundwater and has adverse effects on humans is nitrate. This parameter enters the water sources through different ways such as contact of water sources with sewage or discharge of agricultural return flow into the river and most importantly oxidation of nitrogenous organic materials such as proteins. Therefore, it is necessary to pay attention to the simulation of this parameter and provide solutions and policies to improve the quality of groundwater resources in the development of aquifer management.
models. The concept of optimal use of groundwater resources, considering the development of nitrate pollution, is a relatively new concept that has received less attention.

Ayvaz (2010) introduced a linked simulation–optimization model to determine the source locations and release histories together with the potential source numbers. In the proposed model, MODFLOW and MT3DMS packages were used to simulate the process of flow and transfer of groundwater; then, they integrated the models with the optimization model based on the heuristic harmony search. The results of this study show that the prepared model can be used to solve the inverse pollution source identification problems.

Peña-Haro et al. (2011) presented a structure based on nonlinear programming and groundwater flow and mass transport numerical simulation for stochastic optimization of control strategies for groundwater nitrate pollution from agriculture under hydraulic conductivity uncertainty. The research of this study shows that a stochastic analysis allows providing more reliable groundwater management strategies than deterministic models.

Alizadeh et al. (2017) developed a fuzzy multi-objective compromise methodology based on MODFLOW and MT3D simulation models, NSGA-II, and Fuzzy Transformation Method (FTM) in order to determine the socio-optimal and sustainable policies for hydro-environmental management of kavar-Maharloo aquifer. The results indicate the proper performance of the proposed model for determining the most sustainable allocation policy in groundwater resource management.

For quantitative and qualitative modeling of groundwater systems and their simulation within water resources management optimization models, it is necessary to establish the link between the simulation model and the optimization in a desirable way. In previous studies, due to the software limitations of developed groundwater simulation models such as GMS in accessing their input and
output files, the following approaches for using the results of the aquifer simulation model was used in the optimization process: response matrix method (Rejani et al., 2009; Pena-Haro et al., 2009; Pena-Haro et al., 2011; Salcedo-Sánchez et al. 2013; Tabari and Soltani, 2013; Tabari and Yazdi, 2014; Rashid et al., 2014, and etc.), using analytic element models to simulate an aquifer under limited and special conditions (Gaur et al., 2011; Majumder and Eldho, 2016, and etc.), use meta-models to communicate between simulation and optimization models (Rogers and Dowla, 1994; Karamouz et al., 2007; Tabari, 2015; Alizadeh et al., 2017), create or modify MODFLOW and MT3DMS codes (Wang and Zheng, 1994; GAD and Khalaf, 2013; Elci and Tamer Ayvaz, 2014; Sreekanth et al., 2015; Luo et al., 2016; Ayvaz, 2016; Ghaseminejad and Shourian, 2019; Norouzi Khatiri et al., 2020 , and etc.).

Review of the previous studies on optimal quantitative and qualitative management of groundwater resources indicated that in the developed models, the use of an aquifer distributed simulation model instead of using simplified relationships to simulate quantitative and qualitative parameters is essential to better description the behavior of groundwater resources. Also, adopting management strategies in the abstraction of the aquifer and its control can be very effective in improving the quantitative and qualitative conditions of the aquifer. Accordingly, in this study, with the aim of achieving sustainable development in the quantitative and qualitative operation of the Karaj plain aquifer, the multi-objective management model was developed based on the GMS simulation model and the NSGA-II multi-objective algorithm. In this model, the accuracy of quantitative and qualitative aquifer simulation has direct effects on the results of the optimization model. Therefore, by preparing code in MATLAB environment for direct connection of the multi-objective optimization model with the GMS simulation model by direct access to the input and output files of this simulation model, the aquifer was simulated and calibrated as a cell by cell.
It should be noted that the development of a multi-objective quantitative and qualitative model of the aquifer to provide optimal operation policy for each active well and to determine the monthly harvesting from them using the extensive groundwater simulation model is considered as one of the innovative aspects of this study. Also, controlling the concentration of nitrate quality parameter in the developed management model is another new aspect of this study, which has been considered simultaneously with the quantitative management of the aquifer (preventing the progressive drawdown in GWTL and excessive withdrawals). The results obtained from the implementation of the proposed approach show the high performance of aquifer operation policies in order to create quantitative and qualitative sustainability during a short-term planning period. Therefore, applying the proposed approach in other aquifers can reduce the operating costs of groundwater and compensate the water depletion of groundwater, and provide the sustainable and stable operation of aquifers.

2 Materials and methods

2.1 Study area

Due to the importance of studying critical areas with special political, social and regional sensitivities, in this study, the aquifer of Karaj plain has been selected as case study. This region needs special attention in meeting water supply and controlling groundwater pollution due to its strategic location (Fig. 1). The Karaj plain has experienced a large population density in recent year due to its proximity to the capital of IRAN, Tehran. This has led to an increase in abstraction from groundwater resources and as a result a significant decline in GWTL and decrease in water quality of the Karaj plain aquifer. It should be noted that this region is the biggest destination of immigration in Iran after
Tehran city. The area of case study is 255 square kilometers and is located in the aquifer of Karaj plain with an average altitude of 1274.14 meters above sea level and 48 kilometers northwest of Tehran. The hydrogeological and hydrogeochemical characteristics of case study are fully described in the paper of Chitsazan et al. (2017).

In order to investigate the quantitative and qualitative behavior of the aquifer of Karaj plain, it is necessary to first prepare an aquifer simulation model and then be calibrated and validated. The time period considered for aquifer modeling is the 2010-2011 water year. The reason for choosing this water year is the completeness of aquifer hydrogeological and hydrogeochemical data. It should be noted that for quantitative and qualitative modeling of the Karaj plain aquifer under steady and unsteady conditions, quantitative and qualitative data related to the 2010-2011 and 2011-2013 water years has been used for calibration and verification, respectively.

In qualitative modeling of Karaj plain aquifer, due to the significant growth and development of urban and agricultural land use in this region, the nitrate parameter has been considered as one of the important and effective parameters in the qualitative degradation of groundwater resources. Spatial and temporal distribution of measured nitrate concentration in drinking wells located in the study area over a 14-year period (2000-2013) are presented in the paper of Chitsazan et al. (2017).
Fig. 1 a) Study areas of aquifers in Iran b) The field application site at Tehran-Karaj plain c) Location of the study area
2.2 The structure of the proposed approach

Preparation and development of groundwater resources operation scenarios for sustainable
groundwater abstraction and its quality improvement requires the definition of specific
management objectives. For this purpose, in this study, a novel approach based on the most
appropriate simulation and optimization tools was developed. In this approach, it is first necessary
to properly define the objective functions and constraints, and introduce them to the developed
model. In this study, three objective functions are considered, which are: minimize the sum of
drawdown of GWTL in drinking wells located in the study area during horizon planning (as first
objective function), minimize the sum of nitrate concentration in cells containing operation wells
during horizon planning (as second objective function) and minimize the sum of withdrawal rate
from wells during horizon planning (as third objective function). Due to the nonlinear and complex
relationship between groundwater level drawdown, harvesting from aquifer, and nitrate
concentration in each of the active aquifer cells, the mentioned goals do not work in the same
direction and are considered as conflict objectives.

A remarkable point in the proposed approach is the use of the distributed GMS model to simulate
the quantitative and qualitative behavior of groundwater in Karaj plain, which unlike lump models,
leads to an increase in the accuracy in calculating the GWTL and nitrate concentration parameters.

The mathematical form of the objective functions and constraints are defined as follows:

Objective function:

\[ \text{Minimize } Z_1 = \sum_{t=1}^{m} \sum_{z=1}^{n_{well}} \Delta H_{tz} \]  \hspace{1cm} (1)

\[ \text{Minimize } Z_2 = \sum_{t=1}^{m} \sum_{z=1}^{n_{well}} C_{well_{tz}} \]  \hspace{1cm} (2)

\[ \text{Minimize } Z_3 = \sum_{t=1}^{m} \sum_{z=1}^{n_{well}} Q_{well_{tz}} \]  \hspace{1cm} (3)

Constraints:
\[ Q_{\text{well}}_{tz} \leq Q_{\text{Cwell}}_{tz}, \quad z = 1,2,\ldots,n_{\text{well}}, \quad t = 1,2,\ldots,m \]

\[ \Delta H_{tz} = H_{tz} - H_{(t-1)z} \]  

(4)

\[ H_{tz} = f(Q_{\text{well}}_{tz}, R_t, H_{(t-1)z}) \]  

(5)

\[ C_{\text{well}}_{tz} = g(Q_{\text{well}}_{tz}, R_t, H_{(t-1)z}, C_{\text{well}}_{(t-1)z}) \]  

(6)

\[ Q_{\text{well}}_{tz} \geq 0, \quad z = 1,2,\ldots,n_{\text{well}}, \quad t = 1,2,\ldots,m \]  

(7)

\[ C_{\text{well}}_{tz} \geq 0, \quad z = 1,2,\ldots,n_{\text{well}}, \quad t = 1,2,\ldots,m \]  

(8)

\[ H_{tz} > 0, \quad z = 1,2,\ldots,n_{\text{well}}, \quad t = 1,2,\ldots,m \]  

(9)

where,

\[ \Delta H_{tz}: \text{The rate of GWTL drawdown associated with well } z \text{ in month } t \text{ (m)} \]

\[ Q_{\text{well}}_{tz}: \text{Amount of water withdrawn from well } z \text{ in month } t \text{ (m}^3/\text{day}) \text{ (as decision variable)} \]

\[ Q_{\text{Cwell}}_{tz}: \text{Current status of withdrawal from well } z \text{ in month } t \text{ (m}^3/\text{day)} \]

\[ R_t: \text{The amount of natural recharge of the aquifer in month } t \text{ (m/day)} \]

\[ C_{\text{well}}_{tz}: \text{Simulated nitrate concentration in well } z \text{ and in month } t \text{ (mg/l)} \]

\[ H_{tz}: \text{Simulated GWTL in well } z \text{ and in month } t \text{ (m)} \]

\[ f: \text{A function based on which the quantitative behavior of aquifer (based on GWTL parameter) is modeled.} \]

\[ g: \text{A function based on which the qualitative behavior of aquifer (based on nitrate parameter) is modeled.} \]

\[ n_{\text{well}}: \text{Number of wells in the study area} \]

\[ m: \text{Number of months in planning horizon} \]
In this part, introduced equations will be explained. In equation (1), which is the first objective function, the control of GWTL drawdown (equation (5)) in each well is considered. Based on this relationship, it is necessary to first simulate the GWTL time series using a validated aquifer model. In order to simulate the GWTL, the GMS model is used which is presented in the form of equation (6). This model is as a graphical user interface for MODFLOW simulation model. In fact, for each of the solutions that provided by the optimization algorithm, it is necessary to run an aquifer simulation model to determine the GWTL and its drawdown in each of the simulated cells. Based on equation (6), it can be seen that the parameters of recharge, discharge and GWTL of the previous month are needed as input to simulate the quantitative behavior of the aquifer in GMS model.

According to the mentioned explanations above can be found that the satisfaction of the first objective function can be effective in controlling the monthly GWTL drawdown in operation wells, reducing pumping costs, and improving the water quality of the aquifer in the long-term with increasing the saturated thickness of the aquifer. In other words, the first objective function plays an effective role in controlling the quantitative stability of the aquifer.

In equation (2), the second objective function of the proposed approach is realized, which is to reduce the nitrate concentration in the operation wells. In order to determine the nitrate concentration in each of the wells, it is necessary to run a calibrated qualitative model, which in this study is MT3DMS and is one of the packages of the GMS model, for different situations of well extraction. This value, which is determined based on equation (7), indicates the qualitative behavior of aquifer in the face of stresses due to water abstraction. In Karaj aquifer, the concentration of nitrate has increased to more than the permissible values due to the remarkable withdrawal by wells. Therefore, this groundwater overdraft was controlled by equation (4).
The third objective function of this study, which plays an important role in the quantitative and qualitative stability of the aquifer, is to minimize the amount of abstraction from operation wells. Indeed, in this objective function (equation (3)), the water supply demands of the region are not considered and long-term operation of the aquifer and attention to the stability of the aquifer in order to improve the water quality of the aquifer are considered as the priority of water withdrawal from wells.

Using these three objective functions, which are also complementary to the sustainable development of the aquifer, can be determine the optimal allocation values from each of the wells. Also, based on optimal allocation water can be provided necessary planning to water supply the shortage of demands from other water resources (such as surface water resources).

In order to solve the developed management model, initially, it is necessary to define the problem variables which are known as decision variables or unknowns of the model. In this study, the decision variables considered for each month are the monthly amount of water extracted from existing wells. As there are 2453 active operating wells in the Karaj plain, the total number of decision variables will be 58872 within three years planning horizon.

The reason for considering each of the exploitation wells as a decision variable is the independence in their exploitation, which is mainly managed by the private sector and it is not possible to integrate them regionally. In fact, in case of aggregation and determination of the optimal amount of water allocation, the optimal amount cannot be properly distributed among the stakeholders.

Also, reducing the number of wells and presenting it in the form of a limited number of wells to apply to the distributed model of the aquifer due to not applying the exact position of the harvest, it can lead to errors in simulating the quantitative and qualitative behavior of the aquifer. It should be noted that this approach can be very effective in developing optimal allocation guidelines from
each well for inclusion in the exploitation license and provide appropriate guidance to decision-makers in this area.

In this study, a short-term planning horizon (three-year) was considered in order to extract the best policies for operation of wells. Providing optimal aquifer operating policies for a long-term period is not practical for reasons such as changing exploitation approaches as a result of the managerial instability in the organizations in charge of the operation of Iranian aquifers and lack of adequate monitoring of aquifer resources.

To determine the optimal amount of these decision variables, we used the NSGA-II that is one of the most suitable optimization tools. According to this multi-objective optimization algorithm, first, an initial population of random values of water withdrawal from each well (as set of solutions) is generated. Then, the values of the objective functions are calculated for each of the solutions. Using the operators defined in the NSGA-II algorithm, the generated solutions are improved during successive iterations to satisfy the developed objective functions. This process continues until there is no change in the optimal trade-off curve. Under these conditions, it can be stated with great probability that the value provided for the decision variables is near to global optimal and can be used as scenarios for the exploitation of wells in the study area. Based on these optimal allocation amounts from different wells, can be formulated the optimal operation policies on a monthly or seasonal basis. To study the NSGA-II algorithm further, one can refer to Tabari and Soltani (2013) article.

Figure 2 shows the flowchart to achieve optimal trade-off between objective function and how to extract an aquifer operation policy based on the proposed methodology. According to this figure, to achieve the goals of this study, which is the sustainable qualitative and quantitative groundwater development during planning horizon, a structure based on the hybrid of GMS simulation model...
and the NSGA-II multi-objective optimization algorithm are proposed. Initially, in this structure, the quantitative and qualitative data sets of the studied aquifer (Karaj plain) are collected and monitored.

Then, the quantitative and qualitative simulation models of groundwater based on GMS tools were prepared and calibrated. Considering that the inputs GMS simulation model can be called from GIS (Geographic Information System) software, therefore, the digital aquifer layers such as the topography, bedrock, piezometric head, wells data, aquifer hydrodynamic coefficients, land use, the hygrometry and meteorology stations data, location of qualitative measuring points for nitrate concentration, and etc. were prepared in GIS environment and introduced to GMS model.

Since the proper simulation of the quantitative and qualitative behavior of the aquifer in the optimization process and the determination of the optimal values of the decision variables is of great importance, therefore, to increase the precision of the aquifer simulation results, a code that can be used to simulate the fully distributed of aquifer within the optimization model was prepared in the MATLAB2018b application environment. This code has the ability to call all input and output files of GMS software in MATLAB environment and is able to quantitative and qualitative modeling of aquifer for a short time (approximately 4 seconds) during a period of 24 months.

In developed MATLAB code, the user will be able to change the status of the stresses in the groundwater system (like recharge and discharge) using a file with the h5 extension in the GMS model and observe variation in GWTL and nitrate concentration after the implementation of GMS model. In this code, it is necessary to use a calibrated simulation model of aquifer, which indicates the actual behavior of the groundwater system in Karaj plain. For this purpose, the GMS model was first calibrated under steady and unsteady conditions to determine the status of variation in hydrodynamic coefficients of the aquifer. Then, to ensure the accuracy of the prepared aquifer
simulation model, the model was validated based on new data which have not been used in the calibration process.

By implementing the proposed coupled simulation-optimization model, the optimal trade-off curve between the objective functions is extracted. Each trade-off curve contains numerous optimal scenarios for operation of wells. Therefore, in this study, the MCDM methods were used to extract the most appropriate exploitation of aquifer scenario in terms of objectives.

In this study, the MCDM methods used to determine the superior scenario are: weighted aggregate sum product assessment (WASPAS), complex proportional assessment (COPRAS), technique for order preference by similarity to ideal solution (TOPSIS), compromising programming (CP), and modified TOPSIS (M-TOPSIS). Due to the different ranking of scenarios (points located on optimal trade-off curves) in each of the MCDM methods, the BAM method was used to aggregate the results of these five MCDM methods of ranking the solutions that generated by the NSGA-II algorithm and determine the final ranking of each scenarios. Details of the decision-making methods used can be found in the Banihabib et al. (2017) paper.

Based on the best scenario, the quantitative and qualitative behavior of aquifer is analyzed under optimal operation. In fact, according to the optimal values obtained from this scenario, deciding on existing operating conditions becomes easier and operating and decision-making managers can appropriately present short-term and long-term plans for sustainable operation of the groundwater system.
Fig. 2 The structure of the proposed multi-objective simulation-optimization model for sustainable operation of the aquifer

2.3 Aquifer simulation using prepared MATLAB code

In this study, due to the high application of the GMS model and its very appropriate accuracy in investigating the quantitative and qualitative behavior of the aquifer, code was prepared in MATLAB environment with the aim of establishing link between this software and multi-objective optimization algorithms. It should be noted that there are other methods such as using mfLab and directly coupling the compiled MODFLOW Fortran code instead of calling GMS in the developed multi-objective optimization management model that can be used for distributed modeling of the aquifer. In this study, due to the simplicity of using GMS model, its widespread use by researchers,
easy communication with MATLAB coding environment and proper execution speed, an approach based on simultaneous calling of the GMS model in the multi-objective optimization model has been used. The application of this method on a hypothetical aquifer has been investigated by Majumder and Eldho (2015).

GMS is an application software for creating and simulating groundwater models from Aquaveo. It features 2D and 3D geostatistics, stratigraphic modeling and a unique conceptual model approach. Currently supported models include MODFLOW, MODPATH, MT3DMS, RT3D, FEMWATER, SEEP2D, and UTEXAS.

The steps of aquifer simulation using the proposed MATLAB code are presented in the Fig. 3 flowchart. According to this figure, before establishing a link between the simulation model and optimization, it is necessary to be prepared a conceptual model of the studied aquifer (Karaj plain) based on data related to aquifer geometry and hydrogeological data such as bedrock, aquifer topography, discharge and recharge components, storage coefficients, and hydraulic conductivity of the aquifer, etc.
Fig. 3 The proposed MATLAB code structure to establish a link between GMS simulation model and multi-objective optimization algorithm and its position in calculating the objective functions of production populations by NSGA-II algorithm.
After collecting the required information and preparing a conceptual model, it is necessary to design a groundwater flow model for implementation. In this stage, the modeling boundary, number of stress periods and time steps, type of aquifer boundary conditions, cellular amounts of recharge and discharge, and other aquifer hydraulic parameters are determined. In order to groundwater system simulation with the finite difference method, it is necessary to divide the aquifer area into a smaller number of zones which is called a cell. According to the geological condition, topography, area of case study, and the amount of available data from the Karaj plain, the grid with cells 500×500 meters and 44 rows and 39 columns, and containing 1017 active cells in the UTM geographical coordinate system was prepared.

The Karaj aquifer is unconfined and spreads throughout the plain. A single layer model has been considered to simulate this aquifer, according to the condition and type of aquifer. The boundaries of the modeling area are determined mainly by the spatial distribution of the observation wells (piezometric wells). The northern borders of the study area adjacent to the southern heights of Alborz and its eastern border cover the Karaj river. In order to determine the direction of

**Fig. 4** Three-dimensional map of the aquifer area along with the conceptual model of the Karaj aquifer
groundwater movement and also to study the possible inflow and outflow fronts of groundwater, boundary conditions were determined using the hydrogeological feature and prepared the GWTL map in ArcGIS10.2 software. In terms of boundary conditions, considering that the trend of groundwater movement from north and northwest to south and southeast and in the direction of Karaj River, so the north and northwest borders were considered as the inflow to the groundwater and the southeast and south borders as the groundwater outflow (Fig. 4). After determining the boundaries of groundwater inflow and outflow of Karaj aquifer based on the observation wells data, these boundaries were introduced to GMS tools as General Head Boundary (GHB) due to the uncertainty of the volume of inflow and outflow from the boundaries of aquifer. In fact, using this package and determining the amount of hydraulic conductivity of the inlet and outlet boundaries and the level of groundwater at each time step, the amount of inflow and outflow from the aquifer is calculated.

Other parameters that have been introduced to the GMS tools for simulation of Karaj aquifer are: aquifer surface topographic, bedrock, initial hydraulic conductivity, monthly GWTL, location and value of well discharge, initial nitrate concentration, recharge amounts by surface water resources, agricultural return flow, domestic absorption wells and precipitation, and etc. As an example, the topographic cell map, bedrock, initial GWTL, the location of the operation wells and the position of the piezometers are presented in Fig. 5.

By performing calibration process under steady and unsteady conditions, the hydrodynamic coefficients of the aquifer and the longitudinal and transverse diffusion coefficients are calibrated and used for validation. In order to use the validated model during the optimization process, it is first necessary to call and store data related to the location and amount of withdrawal from wells
based on the validated simulation model. For this purpose, it is necessary to use the following code in MATLAB environment:

```matlab
Dwells=hdf5read('VerificationKarajAquifer.h5','/Well/07. Property');
```

In this code, “VerificationKarajAquifer” is the name of the validated groundwater simulation model.

The amount of decision variables undergoes many variations during the optimization process to achieve the optimal value, which is the satisfaction of the objective functions. Therefore, based on these variations, it is necessary to calculate the value of objective functions in proportion to them.

For this purpose, it is necessary for each variation in the decision variables, the original value (Dwells) replaced with new withdrawals values from wells and run a validated groundwater simulation model. The following command is used to open the validated GMS model in MATLAB environment and replacement of the new withdrawal values from wells:

```matlab
plist = 'H5P_DEFAULT';
fid = H5F.open(VerificationKarajAquifer.h5','H5F_ACC_RDWR', plist);
dset_id = H5D.open(fid,'/Well/07. Property');
H5D.write(dset_id,'H5ML_DEFAULT','H5S_ALL','H5S_ALL','H5P_DEFAULT', Dwellsnew);
H5D.close(dset_id);
H5F.close(fid)
```

With the implementation of quantitative and qualitative simulation model using the following command, the required parameters to calculate the value of the three defined objective functions, namely monthly GWTL and nitrate concentration are extracted for each active cell:

- Command to call the executable file of the aquifer quantitative simulation model:

```plaintext
command = 'D:\KarajModel_MODFLOW';
```
The process described above is repeated for each variation in the decision variables located on the chromosomes of the NSGA-II algorithm. With the completion of calculating the value of the objective functions for all chromosomes (a population), the selection, crossover and mutation and non-domination-sort operators are applied to the chromosomes in order to generate an improved population to achieve the optimal trade-off curve between the objective functions.
Fig. 5 Spatial distribution of aquifer modeling parameters, a) Aquifer topography (m) and position of piezometers, b) Aquifer bedrock (m), c) Initial GWTL (m) and location of operation wells
4 Results

For sustainable management of groundwater resources using the proposed model, it is necessary to calibrate the aquifer simulation model. Then, by implementing the multi-objective optimization model and extracting the operation scenarios of groundwater system, the optimal operation policies of wells can be determined. In this section, initially, the results of the aquifer quantitative and qualitative simulation model and then the analysis and discussion of the optimization management model results are presented.

4.1 Results of aquifer simulation model

By implementing a prepared quantitative simulation model under steady condition and based on the GWTL of observation wells for September 2010, first by manual method (trial and error), the initial hydraulic conductivity was somewhat calibrated. Then, according to the appropriate capabilities of GMS software in calibration of numerical models, for calibration of hydraulic conductivity (K) values, a number of pilot points are defined in the model and based on the values obtained from manual calibration, an initial value of K was assigned to each of these points.

In the next step, the software calculates the hydraulic conductivity values for all model cells by interpolating the initial values given for the pilot points and simulates the GWTL distribution in the study area by implementing the model using these values.

Finally, by comparing the observational and computational GWTL values at the observation wells, the computational error of the model is determined and the model tries to provide a better description of the distribution of this parameter in the study area by modifying the hydraulic conductivity values at the pilot points.

The interpolation method used for the hydraulic conductivity of pilot points is the kriging method, which has more capabilities than other existing interpolation methods (such as IDW) and provides
better control over the output results of the interpolation process. The calibrated values of the hydraulic conductivity for the modeling region are shown in Fig. 6. Also, the scatter plot and the bar chart diagram between the observed and simulated GWTL in piezometric wells in order to assessment the accuracy of the calibrated model results are drawn in Fig. 7. As shown in this figure, overall, relatively good agreement between the observed and simulated GWTL are found in all piezometers.

For simulation in unsteady condition, it is necessary to construct an unsteady model for the study area so that the temporal variation of the aquifer is assessed in this study. The time period considered in this model is one water year (2010-2011). In this model, the number of stress periods are 12. All hydrological parameters for different stress periods are assigned to cells of aquifer according to the data available in different months. By implementing a quantitative simulation model under unsteady conditions, the spatial distribution of the calibrated specific yield coefficient can be presented in Fig. 8. To evaluate the accuracy of the unsteady calibration results, the GWTL hydrograph in the studied piezometers are presented in Fig. 9. According to this figure can be found that the aquifer parameters have been well calibrated in order to modeling the real conditions governing the groundwater system of the Karaj plain.

In order to evaluate the prediction accuracy of the calibrated GMS model, the following statistical performance indices were used:

\[
MSE = \frac{\sum_{i=1}^{n} (x_{ml} - x_{ci})^2}{N} \tag{11}
\]

\[
MAE = \frac{\sum_{i=1}^{n} |x_{ml} - x_{ci}|}{N} \tag{12}
\]

\[
NRMSE = \frac{RMSE}{\bar{x}_{ml}} \tag{13}
\]

where, \(x_{ml}\) and \(x_{ci}\) are the measured and simulated values, respectively. Also, \(\bar{x}_{ml}\) is the average of measured values. The Normalized Root Mean Square Error (NRMSE) the RMSE facilitates the
comparison between models with different scales. The NRMSE which relates the RMSE to the observed range of the variable. Thus, the NRMSE can be interpreted as a fraction of the overall range that is typically resolved by the model. In all the above error indicators, the values closer to zero show that the model performance is more appropriate.

By calculating the above error indices for all aquifer piezometers, it can be seen that the calibrated model can simulate the quantitative behavior of the aquifer to assess the groundwater level with appropriate accuracy (Table 1).

Qualitative model of Karaj plain aquifer done for modeling monthly variations of nitrate concentration. For this purpose, MT3DMS model was used to aquifer qualitative simulation. Accordingly, the qualitative conceptual model of the aquifer was implemented on a quantitative unsteady model. According to the available data and in order to adapt to the prepared quantitative model, the qualitative data measured in the observation wells of the period 2010-2011 have been used to calibration of model. Using the manual method and changing the longitudinal dispersion parameter and the amount of nitrate entering the aquifer, the qualitative model was calibrated. Fig. 10 shows the calibrated value of the aquifer longitudinal dispersion coefficient. According to this figure, the value of longitudinal dispersion coefficient in the aquifer varies from 0.05 in the central and western parts to 0.26 in the southeastern parts of the aquifer.
Fig. 6 The map of calibrated hydraulic conductivity (m/day)
Fig. 7 The bar chart diagram (a) and scatter plot (b) between the observed and simulated GWTL in piezometric wells under steady condition.
Fig. 8 The map of calibrated specific yield coefficient (dimensionless)
Fig. 9 Comparison of observed and simulated GWTL hydrographs at the location of piezometers
Fig.9 (continue)
Table 1. Performance evaluations of piezometers during the calibration of GMS model

| Piezometer Name | MSE  | MAE  | NRMSE |
|-----------------|------|------|-------|
| p1              | 0.395| 0.4672| 0.0005|
| p2              | 0.670| 0.8027| 0.0007|
| p3              | 0.306| 0.4979| 0.0005|
| p4              | 0.157| 0.3026| 0.0003|
| p5              | 0.467| 0.6368| 0.0006|
| p6              | 0.359| 0.4978| 0.0005|
| p7              | 0.322| 0.5004| 0.0005|
| p8              | 0.793| 0.8618| 0.0007|
| p9              | 0.206| 0.3534| 0.0004|
| p10             | 0.190| 0.3688| 0.0004|
| p11             | 0.641| 0.7006| 0.0006|
| p12             | 0.242| 0.4301| 0.0004|
| p13             | 0.298| 0.4782| 0.0005|
| p14             | 0.291| 0.4674| 0.0005|

![Map with color scale showing flow conditions](image)
4.2 Results of developed optimization management model

In this study, an NSAGA-II multi-objective algorithm, developed in the MATLAB-R2018b environment, has been used to achieve the optimal trade-off curve between objectives. Parameters related to crossover and mutation operators were determined using trial and error method. Also, the tournament operator was used to select the parent's chromosomes. Since the initial population plays a vital role in time consuming of optimization process and distributing the solutions on trade-off curve, so in this study, the initial population with feasible solutions was identified. In the NSGA-II algorithm, the population size was considered to be 150. By implementing the developed three-objective simulation-optimization model on a computer with 16 gigabyte RAM and CPU core i7-9700, the optimal trade-off curve was determined.

Regarding the computational costs of implementing the proposed model, it can be stated that based on the properties of the mentioned computer, 64.58 hours are required to perform 500 iterations of the proposed model. It should be noted that the execution time of each aquifer simulation model based on MATLAB code is 3.1 seconds.

According to optimal trade-off curve, the minimum and maximum value of first objective function (sum of drawdown of GWTL in drinking wells) were 3554.8 m and 3742.5 m (equivalent to an average drawdown of 1.45 m and 1.53 m per well) in total planning horizon (three years), respectively. The minimum and maximum value of second objective function (sum of nitrate concentration in cells containing operation wells) were 3347638.5 mg/l and 3352001 mg/l (on average, 56.87 and 56.94 mg/l nitrate concentration per well and monthly), respectively. Also, the range of third objective function (sum of withdrawal rate from wells) are estimated between
226.11 MCM and 230.92 MCM, respectively. These minimum and maximum values of objective function are used to determine the priority of each of the solutions on optimal trade-off curve using MCDM methods.

4.2.1 Extraction of the superior solution based on MCDM methods

In this study, in order to determine the rank of each solution located on the optimal trade-off curve, seven MCDM methods called WASPAS, COPRAS, TOPSIS, $CP_{p=\infty}$, $CP_{p=2}$ and $CP_{p=1}$ have been used. By applying these decision-making methods to the optimal solutions, the rank of each solution based on each MCDM methods was determined as Table 2. According to this table, the ranking for the solutions is very different with miscellaneous MCDM methods, and it is not possible to provide the final rank. For this purpose, the BAM method was applied to select the final rank that has a higher Berda scoring.

Based on NSGA-II result can be found that 139 and 11 solution (of the 150 generated solution) are considered as non-dominate and dominate solutions. Therefore, ranking is done on 139 non-dominate solutions and if a solution has a rank of one, its Berda scoring will be equal to 138. Similarly, this Berda scoring can be easily calculated for other solutions. By performing this process for each MCDM method and extracting the sum of Berda scoring obtained for each solution, the final Berda scoring of solutions is determined. By sorting descending of scores, can be specified the final rank of each solution in the form of Fig. 11.
| Method | $CP_{p=1}$ | $CP_{p=2}$ | $CP_{p=\infty}$ | TOPSIS | $M-\text{TOPSIS}$ | COPRAS | WASPAS |
|--------|------------|------------|-----------------|--------|----------------|--------|--------|
| 1      | 120        | 118        | 74              | 117    | 20             | 4      | 23     |
| 2      | 60         | 17         | 35              | 60     | 78             | 40     | 82     |
|        | .          | .          | .               | .      | .              | .      | .      |
|        | .          | .          | .               | .      | .              | .      | .      |
|        | .          | .          | .               | .      | .              | .      | .      |
| 35     | 32         | 43         | 96              | 34     | 106            | 116    | 106    |
| 36     | 117        | 98         | 14              | 124    | 15             | 45     | 20     |
|        | .          | .          | .               | .      | .              | .      | .      |
|        | .          | .          | .               | .      | .              | .      | .      |
|        | .          | .          | .               | .      | .              | .      | .      |
| 75     | 124        | 130        | 88              | 119    | 24             | 51     | 18     |
| 76     | 107        | 103        | 77              | 103    | 42             | 93     | 37     |
| 77     | 84         | 42         | 1               | 89     | 44             | 47     | 53     |
| 78     | 22         | 53         | 112             | 20     | 119            | 109    | 115    |
| 79     | 101        | 83         | 38              | 102    | 37             | 20     | 38     |
|        | .          | .          | .               | .      | .              | .      | .      |
|        | .          | .          | .               | .      | .              | .      | .      |
|        | .          | .          | .               | .      | .              | .      | .      |
| 108    | 52         | 8          | 17              | 52     | 83             | 34     | 85     |
| 109    | 34         | 78         | 106             | 37     | 108            | 79     | 108    |
| 110    | 65         | 19         | 31              | 65     | 74             | 32     | 74     |
| 111    | 106        | 92         | 41              | 109    | 28             | 21     | 32     |
|        | .          | .          | .               | .      | .              | .      | .      |
|        | .          | .          | .               | .      | .              | .      | .      |
|        | .          | .          | .               | .      | .              | .      | .      |
| 138    | 69         | 27         | 56              | 69     | 71             | 80     | 70     |
| 139    | 75         | 46         | 62              | 75     | 65             | 81     | 65     |
Based on Fig. 11, it can be seen that solution 108 is in the first rank (selected scenario) in terms of satisfy three proposed objective functions simultaneously. Accordingly, the optimal decision variables in proportion to this solution, which contains optimal values of withdrawing from operation wells, are evaluated as a desirable alternative compared to another alternative located on the optimal trade-off curve. Based on the results of alternative number 108, can be extracted optimal amounts of groundwater abstraction from the aquifer for sustainable quantitative and qualitative development. Also, based on these values, the quantitative and qualitative analyzes are carried out on the status of each well to determine the effects of the proposed approach on improving the quantitative and qualitative status of the aquifer.

**Fig. 11** The Berda scoring of solutions
4.2.2 Investigation of the aquifer quantitative status under optimal abstraction conditions

Based on the selected scenario and considering the optimal allocation of existing wells, it can be concluded that for establishing stability in the quantitative and qualitative status of the aquifer, it is necessary to reduce the current abstraction (471.55 MCM) to 228.49 MCM (with a 51.55% reduction) over the planning horizon (Fig. 12). By applying the proposed approach, the quantitative behavior of the aquifer has dramatically improved, so that the reduction of the pumping of the wells has led to an increase of 4.6 m in GWTL (an average of 19 cm per month) over three years (Fig. 13).

The response of the aquifer to the reduction of pumping is indicative of the high sensitivity of the aquifer to the stresses on it. Therefore, in order to water supply demands of the study area, it is necessary to be planned other available surface water resources such as increasing the allocation of Karaj dam, increasing the amount of water transferred from Taleghan dam. Also, in order to achieve aquifer sustainable development, water consumption must be decreased in different sectors and water use efficiency increased in the agricultural section.

To observe the status of GWTL rise under optimal abstraction conditions, the GWTL hydrograph in the operation wells has been drawn in different positions of aquifer according to Fig. 13. The results show that in most parts of the aquifer, the GWTL is rising, and this is especially significant in situations where the number of wells is high. This is due to increase in the saturation thickness of the aquifer as a result of reduced withdrawal. It should be noted that this increase in the GWTL will reduce the cost of pumping and decreases nitrate concentration as a result of increased saturation thickness and dilution of the quality parameters (especially nitrate).

Histogram analysis of GWTL variation in 2453 operation wells shows that with the implementation of optimal withdraw policies, 24.13% of wells (592 wells) experience an increase
of 4.5-5 m in GWTL during the study period. Also, 13.82% and 13.98% of operation wells, which are equivalent to 339 and 343 wells, will benefit from an increase of 4-4.5 m and 5-5.5 m in their GWTL, respectively. Other wells, similar to Fig. 14, will have a GWTL rise. It is worth mentioning that after applying the optimal allocation results from wells, in 7 wells the GWTL increases to more than 12 m in three years.

Since the Karaj aquifer area is 254.25 $km^2$, an increase of 4.6 m in the GWTL, including a specific yield of 0.163, will lead to the annual addition of 95.3 MCM of water to the saturation thickness of the aquifer. This amount, which is equivalent to 41.7% of the total optimal withdrawal from wells, can lead to an increase in the static reservoir volume of the Karaj plain aquifer in the long-term.

Fig. 12 Comparison of the monthly withdrawal from wells under optimal and current conditions
Fig 13. The rate of GWTL variation after the implementation of the proposed model

Fig. 14 GWTL variation histogram in 2453 studied operation wells as a result of applying optimal withdrawal policy
4.2.3 Investigation of the aquifer qualitative status under optimal abstraction conditions

To investigate the qualitative status of Karaj plain aquifer in terms of nitrate parameter, the results of the extracted from the best scenarios, which derived from the optimal trade-off curve, are analyzed. For this purpose, first, the general process governing the qualitative status of the aquifer is described after applying the optimal pumping policies to the aquifer operation resources, and then details related to the qualitative variations made on wells during the planning horizon are presented.

A study on the time series of nitrate variations over the three years (2012-2014) shows that despite a significant reduction in the pumping of wells, the average reduction in nitrate concentration was about 3% (Fig. 15). This is due to the severe pollution of the Karaj plain aquifer as a result of the entry of urban and agricultural wastewater. If these optimal operating conditions persist, this reduction in nitrate concentration can be intensified by utilizing the municipal wastewater collection system over a period of 10 years and can be reduced to less than the permissible limit of nitrate in drinking water (That is 50 mg/l according to the World Health Organization (WHO) guideline). In other words, optimal withdrawal policies can lead to a significant improvement in the aquifer quantitative sustainability in the short term but to create the desired qualitative condition, more time is needed.
Fig. 15 Time series of nitrate concentration in Karaj Plain aquifer under optimal and current conditions

Qualitative zoning of the nitrate parameter under the conditions of optimal allocation and continuation of the current withdrawal process was drawn to evaluate the effectiveness of the proposed approach in improving the qualitative aquifer conditions (Fig. 16). Investigation of variation in nitrate concentration in the Karaj aquifer after applying the optimal operation policy values shows that nitrate concentration in the northern, western and eastern parts of the aquifer has been greatly reduced and it is in a more favorable condition. Continuation of optimal allocation policies can lead to quantitative stability of aquifer short-term and improve the qualitative aquifer status in terms of nitrate parameter. By calculating the levels covered by each of the nitrate concentration ranges (based on the nitrate zoning map shown in Fig. 16), can be found that the
zones with high concentrations of nitrate in the current conditions gradually replaced by zones with lower concentrations of nitrate and the general qualitative conditions of the plain are moving towards zones with low concentrations of nitrate. This is especially evident in areas with a large number of operation wells. For example, using the optimal values allocated to each well, the area of aquifer with a nitrate concentration of more than 110 mg/1 has been reduced from 5.38 km$^2$ to 0.67 km$^2$ (Fig. 17).

**Fig. 16** Nitrate concentration distribution a) in current status b) after applying the proposed model (March 2014)
In order to compare the efficiency of the proposed approach in improving aquifer qualitative conditions in terms of nitrate parameter, the time series of nitrate concentration for the two different operating conditions (continuation of the current situation of aquifer operation and applying proposed groundwater management model) were drawn in Figures 18 to 20. As shown in these figures, the effectiveness of the developed structure in creating the qualitative stability of the aquifer is quite evident. Recommendation to continue this process of optimal operation of wells can be significantly effective in reducing the concentration of nitrate, due to the decreasing slope of this parameter.

Fig. 17 The covered area of nitrate concentration with different ranges under optimal policy and current situation (March 2014)
Fig. 18 Nitrate concentration time series in well number 471 under two different operating conditions.

Fig. 19 Nitrate concentration time series in well number 725 under two different operating conditions.
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Fig. 20 Nitrate concentration time series in well number 2061 under two different operating conditions

5 Conclusion

This paper presented and developed a coupled optimization-simulation model for quantitative and qualitative sustainable management of groundwater resources in an arid and semi-arid area (Karaj plain aquifer). In the proposed model, three objective functions were formulated to minimize the sum of drawdown of GWTL in drinking wells, minimize the sum of nitrate concentration in cells containing operation wells, and minimize the sum of withdrawal rate from wells during planning horizon. Due to appropriate accuracy and widespread use of the GMS model in investigating the quantitative and qualitative behavior of the aquifer, code was prepared in MATLAB environment with the aim of establishing link between this software and multi-objective optimization algorithm (NSGA-II). In this code, the user will be able to change the status of the stresses in the groundwater
system (like recharge and discharge) using a file with the h5 extension in the GMS model and observe variation in GWTL and nitrate concentration after the implementation of GMS model. After calibration and validation of GMS model under steady and unsteady conditions and its use in multi-objective optimization model, the groundwater management model was implemented and the optimal pareto-front of solutions (scenarios) between the objective functions was extracted. In this study, seven MCDM methods were used to determine the rank of each solution and the BAM method was applied to select the superior scenario.

Analysis of optimal allocation values of wells shows that in order to create sustainability in the quantitative and qualitative status of the aquifer, it is necessary to reduce the total amount of aquifer withdrawal from 471.55 MCM to 228.49 MCM over the planning horizon. This reduction in abstraction has led to an average increase of 4.6 m in GWTL, which adds 95.3 MCM of water to the static reservoir volume of the Karaj plain aquifer.

The results obtained from nitrate concentration variation after the implementation of the proposed approach show that the area of aquifer zones with high nitrate concentration has decreased and the quality status of the aquifer have improved. Accordingly, the northern, eastern and western parts of the aquifer have experienced a decrease in nitrate concentration during the planning horizon. For example, the area of lands with a nitrate concentration above 110 mg/1 has decreased by 87.5% and reached less than 0.67 km².

Examination of the results obtained from the application of the proposed approach in the quantitative and qualitative management of the aquifer shows that the developed structure of the simulation-optimization model has a high performance in improving the quantitative and qualitative status of the groundwater system. In fact, the simultaneous application of the NSGA-II
and GMS models, and MCDM methods using the developed MATLAB code can be successfully used to manage complex aquifer systems that have significant operation resources.

Acknowledgements

The authors of this article would like to thank the Alborz Regional Water Company for providing quantitative and qualitative groundwater data on the Karaj plain aquifer.

Ethical Approval

This article does not contain any studies with human participants or animals performed by any of the authors.

Consent to Participate

Not Applicable

Consent to Publish

Not Applicable

Authors Contributions

Mahmoud Mohammad Rezapour Tabari: Conceptualization, Supervision, Methodology, Data acquisition, Writing- Original draft preparation

Mehdi Eilbeigi: Conceptualization, Methodology, Visualization, Editing of manuscript

Manouchehr chitsazan: Methodology, Supervision, Editing of manuscript

Funding

Not Applicable

Competing Interests

The authors declare that they have no conflicts of interest.
Availability of data and materials

Data and material would be made available on request.

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