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Coupled Quantity-Quality Simulation-Optimization Model for Conjunctive Surface-Groundwater Use

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Abstract Many water resources optimization problems involve conflicting objectives which the main goal is to find a set of optimal solutions on, or near to, Pareto front. In this study a multi-objective water allocation model was developed for optimization of conjunctive use of surface water and groundwater resources to achieve sustainable supply of agricultural water. Here, the water resource allocation model is based on simulation-optimization (SO) modeling approach. Two surrogate models, namely an Artificial Neural Network model for groundwater level simulation and a Genetic Programming model for TDS concentration prediction were coupled with NSGA-II. The objective functions involved: 1) minimizing water shortage relative to the water demand, 2) minimizing the drawdown of groundwater level, and 3) minimizing the groundwater quality changes. According to the MSE and R^2 criteria, the results showed that the surrogate models for prediction of groundwater level and TDS concentration performed favorably in comparison to the measured values at the number of observation wells. In Najaf Abad plain case study, the average drawdown was limited to 0.18 m and the average TDS concentration also decreased from 1257 mg/lit to 1229 mg/lit under optimal conditions.

Keywords Conjunctive use · Multi-objective optimization · Groundwater · TDS concentration

1 Introduction

Nowadays, conjunctive use of surface water and groundwater use could be considered as an effective approach for water supply. Overall, conjunctive use models have been formulated as

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optimization models (Hantush and Marino 1989). Conjunctive use models may be classified as: (1) classical methods, (2) simulation-optimization models and (3) evolutionary algorithms.

The SO modeling approach, a powerful tool, has been widely used to solve the complex water allocation problems (Katsifarakis and Petala 2006). The SO approach has been used extensively for the optimum conjunctive use of water resources problems to determine the best management plan according to a defined conditions (Karamouz et al. 2007).

Within the SO approach, response matrix and embedding techniques are the two common methods used to couple the simulation and optimization models (Gorelick 1983). Another approach applied to integrate the simulation and optimization models is the external linking of the numerical simulation model to the optimization model (Dhar and Datta 2009).

Generally, integration of a non-linear simulation model in a management model is difficult and complex and computational time to achieve the optimal solution may take large (Singh 2014). The required computational time can be reduced via approximations of the simulation model, or use meta-models as an alternative to actual complex numerical models (Bhattacharjya and Datta 2005). Common surrogate models are Kriging models, SVM ANN, GP, regression functions and radial-basis-function network (Sreekanth and Datta 2010).

Safavi et al. (2010) developed an SO model for conjunctive use of water resources in Zayanderood basin by coupling an ANN model with the GA. Triana et al. (2010) applied ANNs for efficient modeling of stream-aquifer system in an irrigated river basin to improve irrigation efficiency, reduce soil water salinity, and increase crop yields. ANN models were trained and tested using solution datasets from MODFLOW-MT3DMS models. A few studies in the field of hydrology and water resources have used GP models (Parasuraman and Elshorbagy 2008; Wang et al. 2009). Zechman et al. (2005) used a simulation-optimization approach for identifying a groundwater pollutant source. The numerical model was replaced by a GP surrogate model to reduce the computational burden and a GA applied as the optimization model.

Most studies on conjunctive use of resources involve multiple objectives. There are several multi-objective optimization methods such as weighting, E-constraint, goal attainment method and multi-objective evolutionary algorithms. To surmount weaknesses of weighting, E-constraint methods, multiobjective evolutionary algorithms have been developed.

Sreekanth and Datta (2010) linked GP and MNN models to a MOGA to derive the optimal management strategies in coastal aquifers. The results showed that the developed GP models compared to the MNN models have lesser uncertainty while the number of parameters used in the GP was much fewer than that those in the MNN models. Rezapour Tabari and Soltani (2013) applied NSGA-II and SGA to minimize the total costs and maximize the reliability of a conjunctive use system. The results showed that the NSGA-II model can be considerably reduce the computation burden of the conjunctive use models in comparison with the SGA model. Peralta et al. (2014) used ANNs-NSGA coupled model to optimize the conjunctive use for production, cost and energy considering dynamic return flow. The results demonstrated the efficiency of the developed SO model for complex nonlinear multi-objective optimization problems.

This study presents an innovative approach in coupling a surrogate hydrological model with multi-objective optimization models to search for optimal conjunctive surface-ground water use considering human-induced water conflicts. The developed model is capable of supporting decision makers to optimize the temporal and spatial distribution of conjunctive water use/extraction to ensure water resources sustainability in a complex real-world semi-arid region. The study area is Najafabad plain located in central Iran.

2 Methodology

The schematic representation of conjunctive use SO model developed in this study is shown in Fig. 1a.

2.1 Groundwater Flow and Transport Simulation Model

The finite difference flow and transport simulation models, namely MODFLOW (McDonald and Harbaugh 1988) and MT3DMS (Zheng 1990), were selected to respectively simulate the flow and pollution transport processes in the aquifer-river system. The governing equation for MODFLOW in transient conditions is as follow (Wang and Anderson 1982):

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = \frac{S}{T}\frac{\partial h}{\partial t} - \frac{R\,(x,y,t)}{T} \tag{1}$$

Where S is the storage coefficient, h is the pressure head (L), T is the transmissivity ($L^2\,T^{-1}$), t is the time (T), and $R\,(x,y,t)$ is the recharge function (LT^{-1}). The partial differential equation in the MT3DMS for simulation of three-dimensional transport of contaminant in groundwater is:

$$\theta\frac{\partial(C)}{\partial t} + \rho_b\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_j}(\theta v_i C) + q_s C_s - q_s' C - \lambda_1\theta C - \lambda_2\rho_b\overline{C} \tag{2}$$

where θ is the material porosity, C, C_s are the material concentration in aqueous phase and in the source, respectively (ML^{-3}), t is the time(T), ρ_b is the bulk density of medium (ML^{-3}), $\overline{C}$ is the material concentration in adsorbed phase (MM^{-1}), $x_{i,j}$ is the distance to a Cartesian coordinate axes (L), D is the dispersion coefficient tensor ($L^2\,T^{-1}$), v_i is the flow velocity in porous media or Darcy velocity (LT^{-1}), q_s is the source rate of water (T^{-1}), q_s' is the groundwater storage changes in transient conditions (T^{-1}), λ_1 and λ_2 are the first order biodegradation rate constant through dissolved and adsorbed phase (T^{-1}).

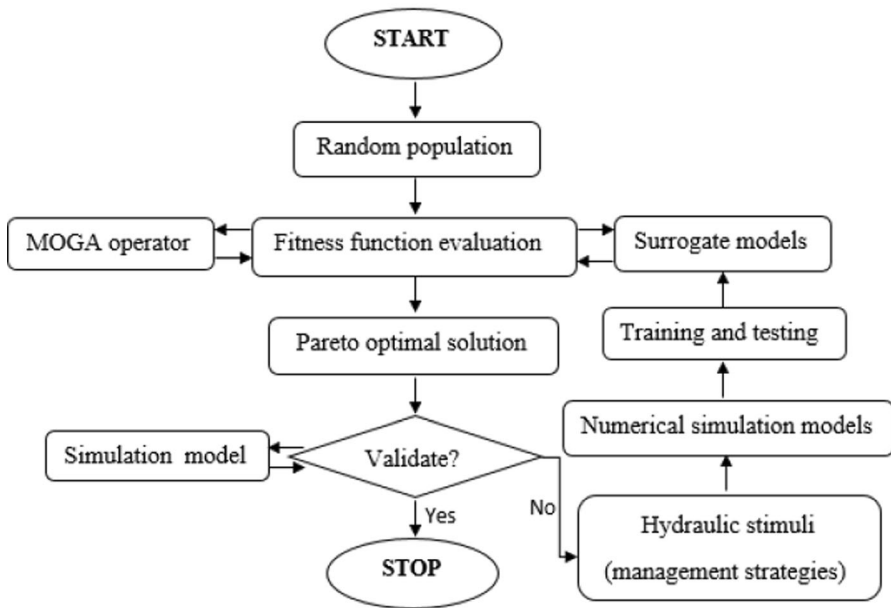### 2.2 Water Resources Allocation Model

Water resources allocation model uses numerical simulation model(s) to simulate surface water-groundwater interactions and response to different sets of assumed hydraulic stimuli (management strategies). The strategies and their corresponding response obtained from numerical models are used to train the surrogate models. Then, the trained surrogate models are employed during optimization as substitute simulators when developing the optimal strategies. The schematic representation of the developed water resources allocation model is shown in Fig. 1b.

2.2.1 Surrogate River- Aquifer Simulation Models

To reduce computational effort of the water allocation model, here we use two substitute simulators ANN and GP during optimization. Artificial Neural Networks are data-driven
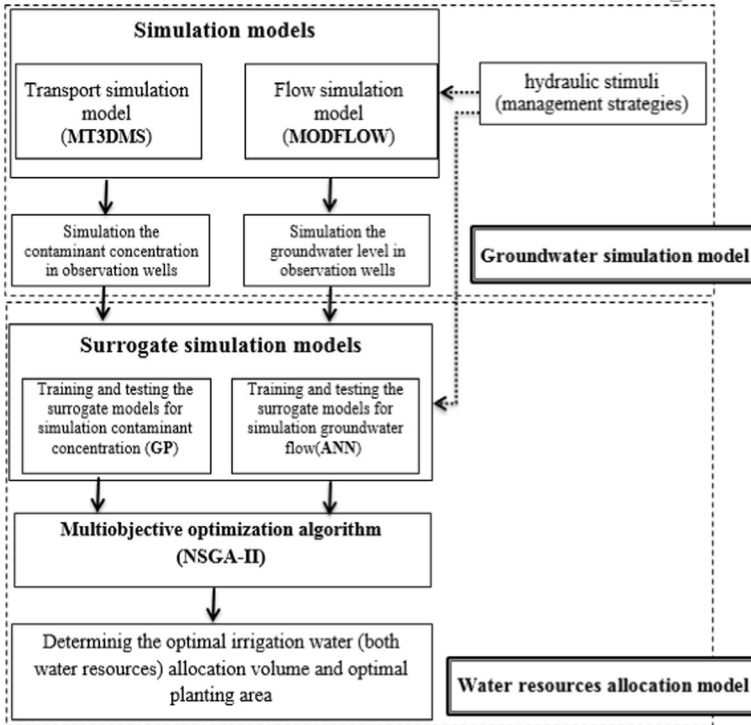
(a)

(b)

Fig. 1 Schematic representation of **a** the simulation-optimization model, **b** the water resources allocation model

models which by a network of interrelated nodes are able to determine the relation between inputs and outputs in a physical system. The activity rate of each connection is regulated by historical information (learning process) while the model can discover the rules between inputs and outputs (Delavar et al. 2005).

Genetic programming is a genetic algorithm applied by Koza for the first time in 1992. It employs Darwinian principle of natural selection to regression models over a series of generations (Sreekanth and Datta 2010). Generally, genetic programming is an artificial intelligence method based on the random iterative search to achieve an appropriate relation between independent variables and the dependent variable (Fallah-Mehdipour et al. 2013).

2.2.2 Multi-Objective Optimization Model

The present work employs NSGA-II for optimal allocation of water and land resources to dominant products in the region. NSGA-II (Deb et al. 2002) is one of the elitist multi-objective evolutionary algorithms. The search process, similar to genetic algorithm, is started with an initial random population (parents' population) of candidate solutions and produces a population twice the size of the initial population (parents' and children's population) by performing the basic GA operators of cross-over and mutation.

2.2.3 Optimal Conjunctive Use Formulation

The proposed S-O model considers three competing objectives are expressed as follows:

The first objective is to minimize the relative water deficit expressed by:

$$Z_1 = Min \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{X_{1ij} + X_{2ij} - \text{demand}_{ij}}{\text{demand}_{ij}} \tag{3}$$

where X_{1ij} is the discharge of stream water diverted at diversion point during month i for product j (m^3/month), X_{2ij} is the discharge of water pumped from wells during month i for product j (m^3/month), and demand_{ij} is the gross water demand during month i for product j (m^3/month).

The second objective is to minimize the annual groundwater level changes given by:

$$Z_2 = Min \sum_{i=1}^{I} \sum_{k=1}^{K} \frac{L_i(k) - L_1(k)}{\Delta L_{\max}} \left(\frac{a_k}{A} \right) \tag{4}$$

$$L_i(k) = \text{ANN}_k(\text{inputs}) \tag{5}$$

Where $L_i(k)$ is the groundwater level during month i and observation well k (m), $L_1(k)$ is the groundwater level in observation well k during the first month of simulation period (m), $\Delta L_{\max}$ is the maximum of annual permissible change of groundwater level in 2009–2010 period (m), a_k is the area of Thiessen polygon k (ha), and A is the aquifer area (ha). Here, $\Delta L_{\max}$ equals 0.86 m.

The third objective is to minimize the groundwater quality change represented by:

$$Z_3 = Min \; \frac{1}{12} \sum_{i=1}^{I} \sum_{k=1}^{K} \left(\frac{C_i(k)}{C_{max}}\right) / \left(\frac{a_k}{A}\right) \tag{6}$$

$$C_i(k) = GP_k \; \text{(inputs)} \tag{7}$$

Where $C_i(k)$ is the total dissolved solids concentration during month i and observation well k (mgr/lit), and C_{max} is the maximum permissible TDS concentration in the groundwater (mgr/lit). Here, C_{max} equals 450 mgr/lit (World Health Organization). Equation (5) and (7) also represents the coupling of the surrogate model with the optimization model to simulate the the groundwater level andcontaminants concentration respectively.

Constraints are expressed as follows:

$$\sum_{j=1}^{J} A_j \leq A_{\text{total}} \tag{8}$$

$$A_{\text{minj}} \leq A_j \tag{9}$$

$$\sum_{i}^{I} \sum_{j}^{J} X_{1ij} A_j / \eta_1 \leq SW_{\text{total}} \tag{10}$$

$$\sum_{i}^{I} \sum_{j}^{J} \left[X_{2ij}.A_j / \eta_2 - \beta_2 \left(X_{1ij}.A_j / \eta_1 + X_{2ij}.A_j / \eta_2\right) - \beta_3 \text{Pompa} j_i - \beta_4 P_i A\right] \leq GW_{\text{total}} \tag{11}$$

$$\text{demand}_{ij} = TW_{ij} = X_{1ij} + X_{2ij} \tag{12}$$

Constraints (8) and (9) are related to planting area of crops where A_j is the optimal planting area of crop j, A_{total} is the total agricultural area. Constraints (10) and (11) are related to water resources, where η_1 and η_2 is the water use efficiency of surface water and groundwater, SW_{total} is the total of available surface water in agricultural section, $Pompaj_i$ is the volume of groundwater extracted in municipal and industry section, P_i is the precipitation in month i, β_2 and β_3 is the leakage loss of agricultural return flow and absorption wells, β_4 is the percolation coefficient of precipitation, GW_{total} is the groundwater exploitation quantity. Constraint (12) represent the total of available water must be equal to the gross water demand during month i for crop j.

2.3 Study Area

The study area is Najaf Abad plain, a part of Zayanderood river basin located in west-central Iran. The plain area is approximately 1720 km^2 while the Najaf Abad aquifer area is about 1065 km^2. The region has a predominately semi-arid climate. Average annual precipitation is only 135 mm, most of which occurs over the winter season from November to April. During the summer, there is no major rainfall event. A part of the Zayanderood River passes through the western side of the plain and recharges the aquifer (Fig. 2).

Generally, there is a two-season cropping pattern (summer- winter crops) in Najaf Abad irrigation system. Also, there are a number of annual and perennial crops including orchards and alfalfa. Table (1) shows cropping pattern in Najaf Abad irrigation system.

In Najaf Abad plain, in spite of water supply plans in Zayanderood Basin, surface water continues to shrink because of recent droughts in main tributary subbasins compounded with growing water withdrawals in upstream areas. In recent years, groundwater level declined
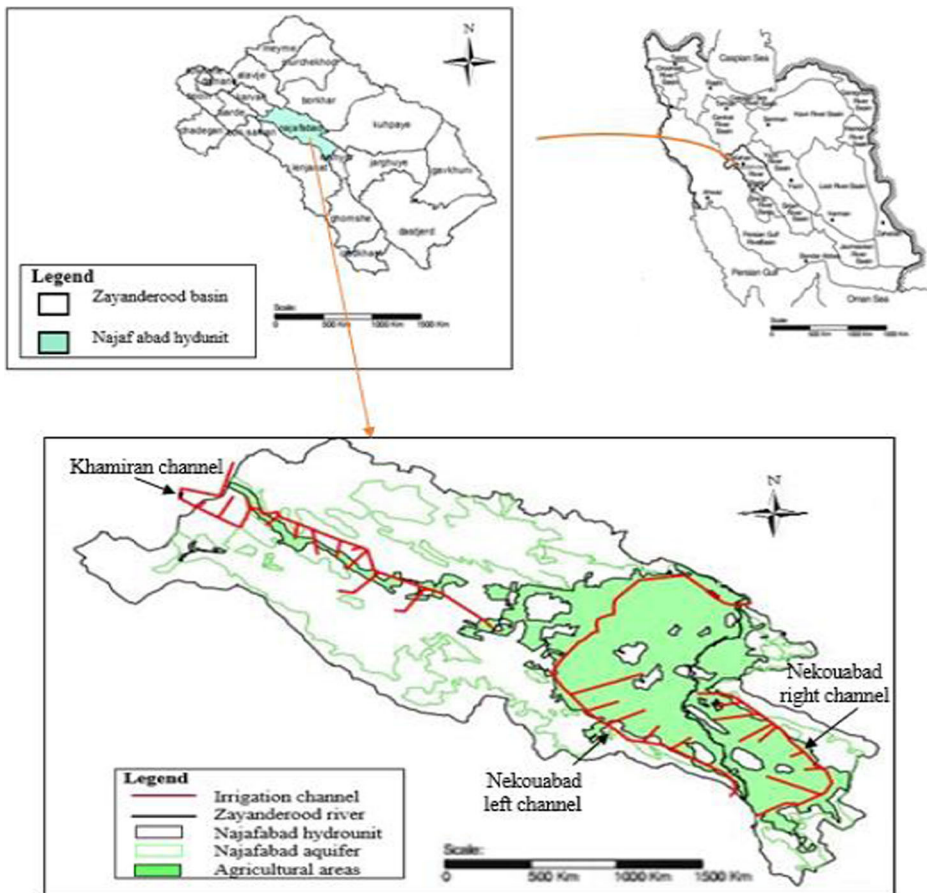

Fig. 2 Zayanderood River and irrigation channels (Safavi et al. 2010)

Table 1 Typical crop calendar in Najafabad plain (Organization of Jahad Agriculture Isfahan 2009)

Crop	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
Wheat		*	*	*	*	*	*	*	*			
Barley	*	*	*	*	*	*	*	*				
Potato							*	*	*	*	*	
Onion	*	*	*	*	*	*	*	*	*	*		
Sugar beet	*							*	*	*	*	*
Rice	*							*	*	*	*	*
Alfalfa	*	*	*				*	*	*	*	*	*
Orchards	*	*					*	*	*	*	*	*

substantially because of irregular extraction from alluvial aquifer by means of numerous pumping wells. Also industrial wastewater in the region and use of excessive pesticides led to groundwater contamination which significantly affected the quality of agricultural products in the region. Degradation of groundwater quality and quantity as well as reduction in surface water quantity demands conjunctive management of both resources so as to minimize negative consequences in water supply in the region.

3 Results

3.1 Groundwater Flow Simulation

In this study, groundwater flow was simulated by MODFLOW model. A three-dimensional grid was overlaid on the aquifer boundary that had 106 rows and 149 columns with a size of 500 m. Here, in addition to enforcing the river boundary conditions in the corresponding cells, another boundary condition was considered as General Head Boundary (GHB) in the location of aquifer connection with adjacent aquifers in northwest, southeast, and central parts of the study area.

Calibrating under steady state was carried out using groundwater hydraulic head in 29 observation wells during 2009–2010 period. In this calibration stage, changes were made on recharge and hydraulic conductivity parameters using PEST tool in GMS software. The hydraulic conductivity and recharge values after calibration varied between 0.6–1.1 m/day and 1.18E-4-0.0021 m/day respectively. Moreover, validation of the model was performed using groundwater level data during 2010–2011 period and the average of mean absolute error and R^2 values turned out to be 0.9 m and 0.99 in this stage.

In transient state calibration aimed to determine aquifer storage coefficient, calibrated parameters under steady state calibration were used as a first approximation. The period of simulation in transient state was one year while the length of each stress period was equal to one month. The storage coefficient after calibration varied between 0.05–0.085. Validation was performed for one year time period in four time steps of three month in transient state over 2010–2011. The average of mean absolute error turned out to be 1.8 m. The coefficient of determination of 0.97 in validation stage indicates the flow model is acceptable in simulation of the groundwater level.

3.2 Solute Transport Simulation

The transport model MT3DMS requires flow data in grid cells as input, which is generated by the MODFLOW model. For indirect calibration of parameters, trial and error method was adopted to estimate the longitudinal dispersivity coefficient. The longitudinal dispersivity coefficient after calibration varied between 7.2–16.3 m. The average of mean absolute error was equal to 2.6 mg/lit in calibration while the coefficient of correlation of 0.97 in validation stage shows acceptable performance of transport model in simulation of the TDS concentration.

3.3 Water Resources Allocation Model

As shown in Fig. 1a. the proposed water allocation model in this study consists of two main components: surrogate simulation models and multi-objective optimization model. The performance of these components are presented in this section.

3.3.1 Surrogate Models

Surrogate models were used to replace the numerical models in order to reduce the computational effort of the water allocation model. For training the surrogate models, the aquifer area was divided into seven regions based on a set of criteria such as the location of the agriculture zones, the rate of discharge and recharge, distance to the river and etc. Generally speaking, to select the best reference monitoring wells in the area, the aquifer was divided based on the most important indicators that impact the groundwater head and quality. Then, one reference observation well for groundwater head and quality was selected in each region.

The groundwater level in each reference observation well was simulated by ANNs. The neural network models have a pre-defined network structure. Here, we adopted a single hidden layer within a standard back-propagation feed-forward ANN model. The input layer had five neurons with a tansigmoidal transfer function whereas the output layer had one neuron with a pure linear transfer function. The hidden layer involved five neurons after training.

Input variables included pumping rate, stream discharge, recharge and rainfall while the output variable was groundwater level in each observation well. For training and testing, 384 strategies were inputted into the MODFLOW and the model outputs were recorded. Then, the training of ANN models was performed. All ANN models were well trained in a single stage and there was no need to retrain the models. Table (2) shows the goodness of fit (R^2) and mean squared error (MSE) values in ANN model training for each observation well. The table indicates that the developed ANN models mimics the MODFLOW model very well and uses as a surrogate model in connection with the NSGA-II optimization model.

In this study, GP and ANN models were used for simulation of the TDS concentration. The selection of appropriate architecture for each ANN was performed by trial and error procedure. Eventually, feed-forward ANN models with 8–7-1 architecture within a standard back-propagation algorithm was found to perform relatively well for TDS concentration at each location.

The GP models were also developed for TDS concentration prediction. GP model is free from the pre-set structure and uses any combination of the input with the set of functions and operators. The best values of GP adjustment parameters after sensitivity analysis turned out to be: mutation probability (P_{mutate}) 0.044, crossover probability (P_{cross}) 0.3, population size 30,

Table 2 Performance of groundwater level simulation using ANN and simulation of TDS concentration by GP model

Obs. wells	ANN				Obs wells	GP			
	training		testing			training		testing	
	R^2	MSE (m)	R^2	MSE (m)		R^2	MSE (mg/lit)	R^2	MSE (mg/lit)
W1	0.98	0.08	0.96	0.18	C1	0.99	0.53	0.98	0.75
W2	0.97	0.11	0.96	0.19	C2	0.98	0.69	0.97	0.82
W3	0.98	0.12	0.94	0.22	C3	0.98	0.84	0.97	0.92
W4	0.97	0.1	0.94	0.19	C4	0.98	0.94	0.98	1.13
W5	0.97	0.05	0.95	0.13	C5	0.99	0.71	0.98	1.07
W6	0.98	0.06	0.94	0.19	C6	0.99	1.21	0.98	1.37
W7	0.97	0.11	0.95	0.23	C7	0.98	1.08	0.97	1.11

number of genes 3 and constants per gene 2. Root relative squared error (RRSE) was selected as fitness function.

In order to form a single training pattern, input variables included pumping rate in the entire aquifer, stream diversions, artificial recharge, rainfall, groundwater level at the observation well and the TDS concentration in hydrometric stations. The output variable involves the TDS concentration in the observation wells. For training and testing, 384 strategies were inputted into the MT3DMS and the outputs were recorded.

At this stage of model development, the results showed the GP models' predictions were better than those of the ANN models. Also the average training time for each ANN and GP model with similar input-output patterns was approximately 50 min and 40 min, respectively. The maximum number of model parameters applied in all GP models were limited to 42 whereas, each of the ANN models had 71 weights. Furthermore, flexible model structure of GP enables it to express the relations between inputs and output in terms of mathematical formulas, instead of voluminous coded meta-models. This significantly decreases the SO model run time.

Overall, the GP models were found to be superior compared to the ANN models for predicting the TDS concentration, thereby increasing the efficiency and speed of the SO model and decreasing the uncertainty involved in the model prediction due to the less number of parameters in the model structure.

At last stage, GP models were trained based on different combinations of input data and the best pattern was identified. Results showed that the pattern wherein TDS concentration was a function of groundwater level was the most efficient pattern. Performance of GP model in simulating TDS concentration in comparison with MT3DMS is shown in Table (2). The table shows the appropriate performance of GP model in simulation of TDS concentration.

3.3.2 Parameterization of NSGA-II Optimization Model

NSGA-II optimization algorithm is one of the main components of the optimal allocation model User inputs' include population size, the number of generation, crossover and mutation operators. The best values of these parameters after sensitivity analysis included Uniform function with rate 0.01 for mutation, Intermediate function with ratio 1 for crossover operator

and the number of generation equal to 30,000. Also for determining an optimum population size, Mahfoud (1995) proposed the following equation to compute a lower bound on population size in NSGA:

$$\text{Population size lower bound} = \ln\left(1-\gamma^{1/G}/c\right)/\ln(c-r/c) \tag{13}$$

Where G is the number of generations, c is the number of niches (peaks), γ is the level of confidence to maintain c niches for at least G generation, and r is the minimum fitness/maximum fitness ($0 \leq r \leq 1$). In this study, Mahfoud's proposed relationship will be adopted in determining the population size in NSGA-II algorithm.

Population size was selected by assuming $\gamma = 0.95$ and $r = 0.5$. A test was implemented by solving the multiobjective optimization algorithm NSGA-II and comparing the convergence of the objective functions 1 and 2 to investigate the accuracy of Eq. 13 for selecting the population size. Using 25,000 generations and 100 peaks, Eq. (13) yields 3531 population size. Fig. 3a. shows the optimization results using 1000, 2000, 3000, 5000 and 6000 and 3531 population sizes. The results for population sizes over 3531 were slightly better but consumed a large CPU time. Thus, Eq. 13 is used to select the population size for solving the optimal conjunctive use problem.
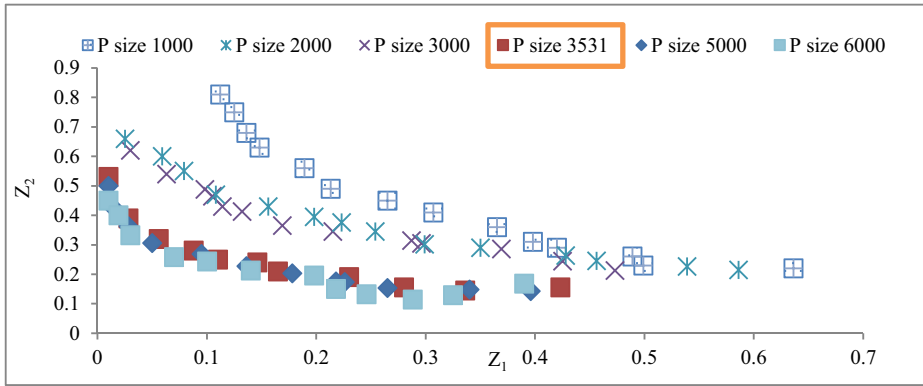
3.4 Simulation-Optimization Results

ANN-GP-MOGA framework was applied to the case study region. The results of the model application are presented and discussed as follows. Fig. 3b. shows the trade-off curve for solutions in front 1 based on 30,000 generations and 3567 population size.

The results for one of non-dominated solutions in the pareto front 1 (point 5) as shown in Table (3) indicates that the optimal planting area in summer subject to high water demanding crops such as rice, sugar beet, potato, alfalfa and orchards crops decreased relative to the current condition. This is while optimal planting area of wheat, barely, and onion increased relative to the current cropping pattern. Table (3) shows that the largest reduction in planting area by 30 % corresponds to rice which, in comparison with other crops, is more water demanding. One reason for reduction in planting area in summer crops is shortage of surface water resources and limitations in pumping extra water from the aquifer. Furthermore, the results show that the highest relative shortage belongs to rice crop and the lowest relative water shortage is associated with barely crop.

The performance of the water resources allocation model to supply the water demand of agricultural products was further investigated by three criteria consisting of reliability, resiliency and vulnerability. Considering the gross water requirement of each product as the threshold (X^T), the amounts of monthly optimal water allocation for each product (x_t) was divided into two categories: satisfactory state ($X^T < = x_t$) and unsatisfactory state ($X^T > x_t$).

Reliability is defined as the number of occurrences in satisfactory state divided by the total number of occurrences in the time series. Table (3) shows barley crop enjoys the highest reliability, because the crop water demand is fully met during the growing season and there is no unsatisfactory state. Sugar beet and rice crops have the least amount of reliability.

Resiliency is defined as the probability that even if a system is in unsatisfactory state, its next state is satisfactory. Orchards have the highest resiliency. If there is no unsatisfactory state in a time series, resiliency criteria cannot be determined. That is the case for barley crop in this study.

(a)
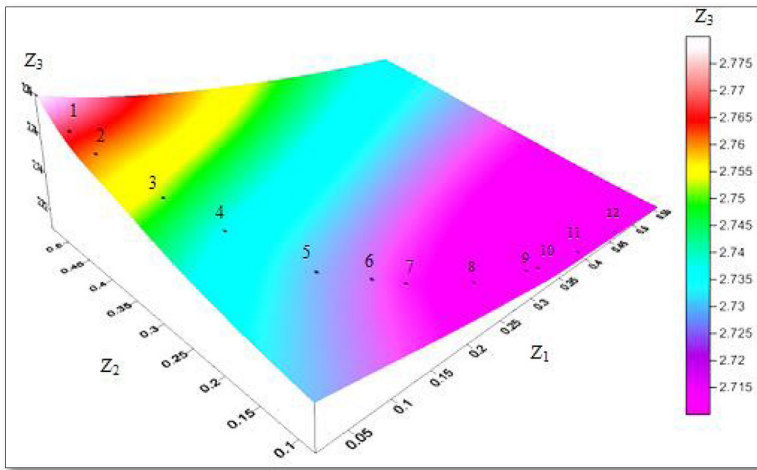
(b)

Fig. 3 **a** Validating Mahfoud's equation using 25,000 generations for NSGA-II, **b** Pareto surface simulated by the NSGA-II

**Table 3** Optimized results of the multiobjective model

Crop	Change in Planting area[a] (%)	Relative water deficit (%)	Reliability	Resiliency	Vulnerability
Wheat	3.11	0.5	0.67	0.00	1.33
Barley	2.89	0	1.00	-	0.00
Rice	−32.3	4.3	0.17	0.00	5.92
Potato	−18.3	1.7	0.40	0.00	3.04
Onion	0.65	0.6	0.60	0.25	0.45
Sugar beet	−15	1.4	0.17	0.00	1.40
Alfalfa	−0.42	2.1	0.56	0.00	2.56
orchards	−17.5	2.3	0.50	0.50	2.41

[a] Negative coefficients indicate the reduction in the planting area of crops compared to the existing condition

Vulnerability shows the extent of the difference between the amount of threshold and the amount of unsatisfactory in the time series. Table (3) shows that the rice crop is most and barley crop is least vulnerable crops, respectively. Least vulnerable crops have the ability to maintain the steady and satisfactory state and are flexible in coping with unsatisfactory conditions.

Optimal allocated irrigation surface and groundwater volume and monthly crop water demands are shown in Fig.4a. The percentage of water supply to crops from surface water and groundwater resources are also shown in Fig. 4b. Results indicate that during spring and summer when surface water availability is limited, the rate of extracted groundwater is higher than the allocated surface water. In these two seasons, an average of 84 % from groundwater resources and 16 % from surface water resources were allocated. Also over autumn and winter seasons, because of availability to surface water resources, an average of 71 % of water demand is provided from surface water while the remaining 29 % comes from the groundwater resources.

To assess aquifer state under optimal water allocation, optimal strategies were used as inputs to MODFLOW and MT3DMS models. Simulation results of monthly changes of relative water shortage values, groundwater level, and TDS concentration in optimal conditions are shown in Fig.5. The results indicate that the highest water shortage occur in late spring until early autumn while during October to January, there is no water shortage.
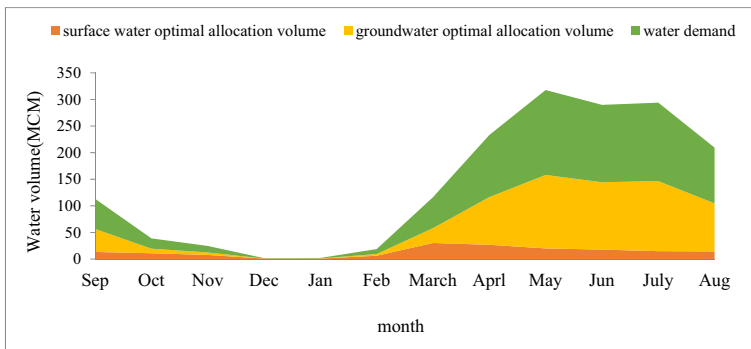
(a)
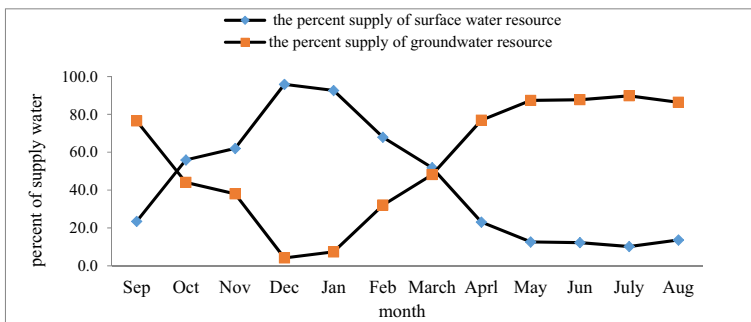
(b)

Fig. 4 a Total water demand and optimal irrigation water allocation, **b** Optimal water supply from different resource
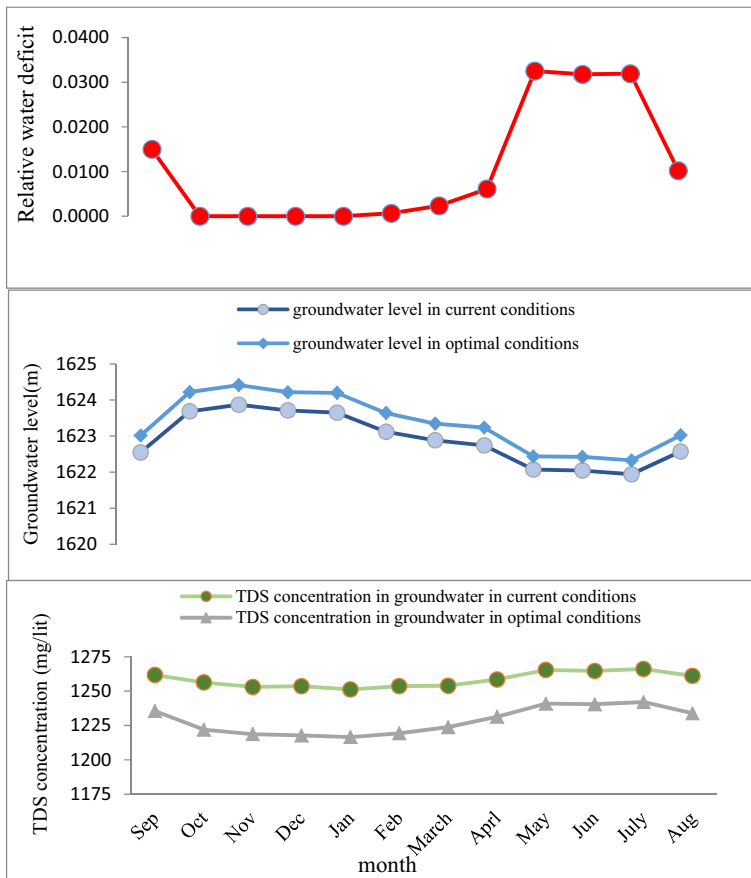
Fig. 5 Time series of water deficit, groundwater level and TDS concentration

Moreover, the lowest changes in groundwater level and TDS concentration in optimal condition in comparison to the existing condition corresponds to May, June, and July. Groundwater level and TDS concentration in Najaf Abad aquifer over 2009–2010 and also quality and quantity changes in the aquifer under optimal allocation pattern relative to the existing condition is shown in Fig. 6.

As shown in Fig. 6b. in optimal pattern, groundwater level increases over the entire Najaf Abad aquifer relative to the existing condition. In central and southeast parts of the study area where the dominant agricultural areas exist, the impact of the optimal pattern to improve the groundwater level is more pronounced. The optimal pattern in these areas rises the groundwater level by 77 % relative to the existing condition. Furthermore, Fig. 6d. indicates that by implementing the optimal pattern in the region, TDS concentration in groundwater decreases significantly relative to the existing condition. TDS concentration in central and southeastern parts of the region decreases by 36 mg/lit relative to the existing condition.

Generally speaking, the average of groundwater level drawdown in the optimal condition is equal to 0.18 m. Thus groundwater level drawdown in the optimal pattern could reduce the
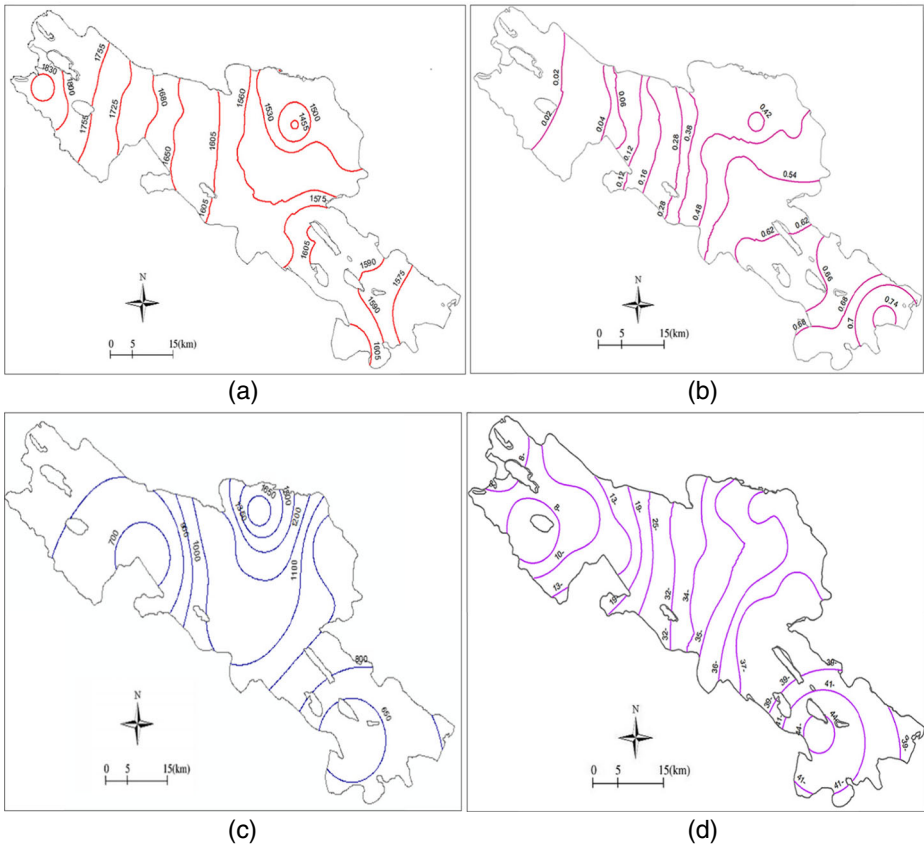
Fig. 6 **a** Groundwater level (m), **b** Groundwater level changes (m) in optimal relative to existing condition, **c** Solute concentration (mg/lit) and **d** TDS concentration changes in optimal relative to existing condition (mg/lit) in Najaf Abad aquifer over 2009–2010

existing rate by 2/3. Monthly average of TDS concentration also decreases from 1257 to 1229 mg/lit under the optimal plan.

4 Conclusions

In this study, a multi-objective simulation-optimization model was developed to derive a set of optimal conjunctive use of surface and groundwater resources in an arid and semi-arid region considering the water quality and quantity issues. The proposed simulation-optimization approach was developed using NSGA-II multi-objective algorithm coupled with surrogate models trained based on the input-output sets of scenario-simulated MODFLOW and MT3DMS models.

Given the large number of monitoring locations in the study area, the training of the individual surrogate models at each location led to increased computational burden and complexity in the SO model. Thus the aquifer area was divided into seven regions based on the physical properties of the aquifer and the water withdrawal points. Then, one reference

observation well for groundwater level and TDS concentration was chosen in each zone. This approach is also effective in reducing the computational time and the number of required training patterns compared to a global meta-model which predicts the groundwater level or TDS concentration simultaneously at all the monitoring locations.

The study relied on Artificial Neural Networks (ANNs) and Genetic Programing (GP) as efficient surrogate models for prediction of groundwater level and TDS concentration, respectively, within the SO framework. Here, for increasing the prediction accuracy of the surrogate models, inputs were selected similar to those of basic inputs in the conceptual simulation model. Although large number of inputs in the surrogate models increased the training computational complexity, adopting a surrogate model structure nearly similar to the conceptual simulation model proved successful in simulation of groundwater level and TDS concentration. Moreover, the post-optimization evaluation of surrogate model capability showed that the SO model determined feasible strategies that would not breach the constraints of the optimization problem. Thus, the trained surrogate models developed are simple and fast models to predict the aquifer response compared with complex and hard-to-handle numerical flow and solute transport models.

Once the surrogate simulation model were developed, the NSGA-II optimization algorithm were then coupled with the trained meta-models to determine the optimal management strategy. The application of ANN-GP-NSGA-II model in the Najafabad plain showed that the proposed model satisfactorily generates well distributed solutions to improve the quality and quantity conditions of the aquifer. Results showed the optimal pattern reduced the water shortage and rose the groundwater level by 77 % relative to the existing condition while the TDS concentration in the groundwater decreased significantly. Moreover, the developed model was able to support the decision maker to optimize the temporal and spatial distribution of conjunctive water use and water extraction to ensure water resources sustainability in an arid and semi-arid region.

It is to be emphasized that the proposed model is not a flawless model due to structural and parametric uncertainty involved in both simulation and optimization models. As a result, the uncertainty analysis may provide better decision making based on the reliability analysis of the complex groundwater and surface water systems.

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