Desalination and Water Treatment
www.deswater.com

doi: 10.5004/dwt.2017.20993

86 (2017) 297–304
August

Coupling groundwater simulation and optimization models, using MODFLOW and Harmony Search Algorithm

M. Antoniou, N. Theodossiou*, D. Karakatsanis

Division of Hydraulics and Environmental Engineering, Department of Civil Engineering, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece, Tel. +302310995660; emails: margarca@civil.auth.gr (M. Antoniou), niktheod@civil.auth.gr (N. Theodossiou), diamontkarakat@gmail.com (D. Karakatsanis)

Received 10 January 2017; Accepted 19 May 2017

ABSTRACT

In this paper, a groundwater management model for which the solution is obtained through a coupled application of simulation and optimization models is analyzed. The most widely used numerical groundwater flow model, MODFLOW, which is a three-dimensional (3-D) model using the finite differences method for solving the governing groundwater flow equations, is used as the flow-simulation model. This model is then connected to the Harmony Search Algorithm, one of the most emerging and successful metaheuristic optimization techniques, which simulates the quest for perfect harmony in music. In this paper, this technique is applied to a classic, theoretical example found in the manual of MODFLOW for comparison purposes, by examining the optimization of its aquifer system in terms of minimizing the pumping cost. For this application, a specially designed computer software programme was developed in MATLAB environment. This software, apart from coupling the simulation and optimization models, provides 2-D and 3-D graphical representations of the results allowing users to have a visual image of the piezometric surface in the whole aquifer system area. More specifically, in the specific management problem, the positions and the total required water demand for the pumping wells from the three aquifers system are pre-defined, while the optimal distribution of the pumping rates is determined through the proposed methodology. The results show that coupling flow-simulation and optimization models could be a very useful procedure when solving complex groundwater management problems.

Keywords: Groundwater resources management; Groundwater flow-simulation models; MODFLOW; Harmony Search Algorithm; Optimization

1. Introduction

Since groundwater aquifers constitute one of the main sources of water for domestic and agricultural use, intense measures for ensuring good quality and sufficient quantity are needed. For this reason, it is of most importance to develop suitable simulation and optimization models for the determination of the optimal operation of pumping wells, thus ensuring the maximum coverage of the demand while at the same time, keeping the operational and maintenance cost of the system to a minimum and protecting the environment.

Groundwater mathematical flow-simulation models, are considered to be absolutely necessary tools for ensuring rational water resources management [1]. These models, which are usually non-linear, are often combined with optimization algorithms in order to determine the optimal policy among a number of potential alternatives. Huang and Mayer [2] presented a pump-and-treat optimization application using well location and pumping rates as decision variables, in which genetic algorithms were used as an optimization tool combined with the groundwater flow simulator MODFLOW. Genetic algorithms were also used as an optimization tool in the investigation of the optimal extraction of groundwater in Gaza coastal aquifer [3], where CODES-3D hydrological

---

* Corresponding author.

Presented at the 13th International Conference on Protection and Restoration of the Environment (PRE-XIII), 3–8 July 2016, Mykonos, Greece.

model was used to simulate the physical model. Ayvaz [4] applied Harmony Search algorithm, a metaheuristic optimization algorithm introduced by Geem et al. [5], combined with the groundwater flow-simulation model MODFLOW. He concluded that this optimization algorithm can successfully converge to at least the same, and in some cases, to better solutions than those derived from the application of other methods that were used for the solution of the specific problem in the past. To demonstrate his approach, Ayvaz used a simplified unconfined aquifer example with 10 pumping wells, using three different objective functions, the maximization of total pumping, the minimization of the total pumping cost, and the minimization of total pumping cost for multiple management periods.

In another paper by Luo et al. [6], a multi-objective fast harmony search (MOFHS) was coupled with MODFLOW and applied to both a two-dimensional (2-D) hypothetical test problem and a three-dimensional (3-D) field problem in Indiana (USA), and compared with other methods proved to give successful results. One of the authors, Theodossiou [7], also presented a coupled groundwater flow-simulation model with MINOS [8] a non-linear optimization model, to solve a complex non-linear case-study problem with more than 400 pumping wells, aiming at the minimization of the pumping cost. The coupling of the models was achieved through the response matrix technique.

The main target of the present paper is the development and presentation of a groundwater management tool that couples the 3-D flow-simulation model MODFLOW with the Harmony Search Algorithm in a general multi-layered aquifer. For this reason, a theoretical problem with a known solution, in order to test the results, was used. The software combining the simulation and the optimization models was developed under the MATLAB environment.

The applications of the proposed methodology are not restricted to the optimization of groundwater flow-simulation problems. This methodology, with some adjustments, can also be used to couple optimization models with other simulation models as well. The authors provide the codes used to solve significant problems that might arise in the formulation of such a coupling software, extending in this way, the applicability of the proposed methodology. At the same time, the software presented in this paper not only couples the two models but also produces graphical representations of the water-level distribution in the form of 2-D and 3-D graphs.

2. Methodological approach

2.1. Harmony Search Algorithm

The Harmony Search Algorithm (HSA) is a metaheuristic optimization method inspired by music harmony. It was first introduced by Geem [9] in his PhD thesis. This algorithm is based on a stochastic random search technique whose natural corresponding system is the process for the search of a better harmony by musicians. The simplicity, the fast convergence and the ease of programming of the algorithm have contributed in the spreading of the applications of HSA in various fields. HSA applies the three following procedures in every iteration. Procedure "b" is used (in a percentage) only if procedure "a" is activated. Option "c" is applied every time procedure "a" is not selected:

- HS is choosing any value from HS memory. This process is defined as Memory Consideration and it is very important because it ensures that good harmonies (values that give good results) will be considered through the solution. Moreover, these "good" harmonies will be the material (similar with parents in Genetic Algorithms) for the creation of new, even better harmonies. In order to use this process effectively, Harmony Memory Considering Rate (HMCR) was defined. This index will specify the probability that a new harmony will include a value from the historic values that are stored in the Harmony Memory. If this rate is too low, only few elite harmonies will be selected. As a result, HSA will converge slowly. Moreover, an HMCR value of 1.0 is not recommended because the exploration of the entire feasible range will be obstructed and optimization will fail. Typical values of HMCR are always greater than 70%.
- Every component of the new harmony chosen from HM is likely to be pitch-adjusted. For example, a pitch adjusting rate (PAR) of 10% indicates that algorithm will choose neighboring values for the 10% of the harmonies chosen from HM. The new harmony will include the value x_i^{new} which will be:

  $x_i^{\text{new}} = x_i \pm \text{Random}\cdot\text{bw}$,

  where x_i is the existing pitch stored in HM, random is a random number between 0 and 1, and bw is the bandwidth of the adjustment.
- The third choice is to select a totally random value from the possible value range. Randomization occurs with probability (100-HMCR)% and increases the diversity of the solutions. Although pitch adjustment has a similar role, it is limited in a local area. Randomization can drive the algorithm to explore the whole range and attain the global optimality.

The contribution of the authors of this paper to the development of the Harmony Search Algorithm as a widely recognized, highly credible optimization method for the solution of hydraulic engineering related problems, is significant as expressed through a number of publications [10–14].

2.2. MODFLOW

MODFLOW (modular 3-D finite difference ground water flow model) developed by United States Geological Survey is one of the most widely used groundwater flow-simulation models. MODFLOW is an open source program written in FORTRAN using a deterministic finite differences numerical scheme.

The governing 3-D flow equation used by MODFLOW [15,16] combines the Darcy law with the conservation of mass principle through the following equation:

$$Ss\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) - W \tag{1}$$

where K_{xx}, K_{yy}, K_{zz} are the values of the hydraulic conductivity along the three axes x, y, and z (L/T) considered to be parallel to the main directions of flow, h the hydraulic head (L), W represents the sources and sinks (T^{-1}), S_s is the storativity coefficient (L^{-1}) and t the time (T).

3. Case study

The application used in order to demonstrate the proposed methodology was introduced by McDonald and Harbaugh [15] in the tutorial of MODFLOW and it is still considered to be a prototype for the formulation of the input and output files of the software. This is why the problem is relatively simple but at the same time comprises several complex elements in order to demonstrate to users the multi-dimensional possibilities of MODFLOW and the way they are introduced in the formulation of the input and output files and the processes for the discretization of the grid.

This application comprises three permeable layers separated from each other by impermeable ones. The boundary conditions include a constant head boundary to the east simulating an existing lake. The aquifer system is replenished by infiltrating precipitation which is added to the first permeable layer. Outflows are a result of underground drains distributed across the first layer in different depths, of 15 pumping wells and of the proximity to the lake. Fig. 1 presents the characteristics of the aquifer system. All layers are considered to be horizontal. The flow is steady-state, the aquifer is considered homogeneous and isotropic. Fig. 2 presents the exact positions of the drains and the pumping wells. According to the reference status, the quantity of water pumped from each pumping well is considered to be 5 ft^3/s (=141.58 L/s).

The optimization problem incorporated within the management model calls for the optimal re-distribution of the amount of water pumped from each one of these 15 pumping wells. The number of wells and their position are considered to be pre-defined. The decision variables of the optimization model are the pumping rate of each well, considering that they lie within pre-defined boundaries. The objective function of the optimization model is defined as the pumping cost expressed as the product of the pumping rate and the water-level drop at each well location (Eq. (2)).

$$z = \min\left\{\sum_{i=1}^{N} s_i * Q_i\right\} \tag{2}$$

The constraints of the optimization model are as follows:

- The total amount of water abstracted from these wells must be at least equal to the total demand, as expressed by the current practices.

$$\sum_{i=1}^{N} Q_i \geq \widetilde{Q} \tag{3}$$

where $\tilde{Q}$ = 75 ft^3/s (=2 123.76 L/s).

- The pumping rate of each well must lie within a pre-defined range in order to avoid dewatering of the aquifer.

$$Q_{\min} \leq Q_i \leq Q_{\max} \tag{4}$$

$$0 \leq Q_i \leq 10 \ \text{ft}^3/\text{s} \ (= 283.17 \ \text{l/s}) \tag{5}$$

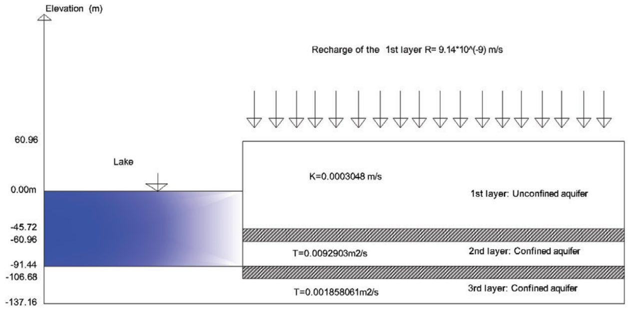

Fig. 1. Side view of the aquifer system.

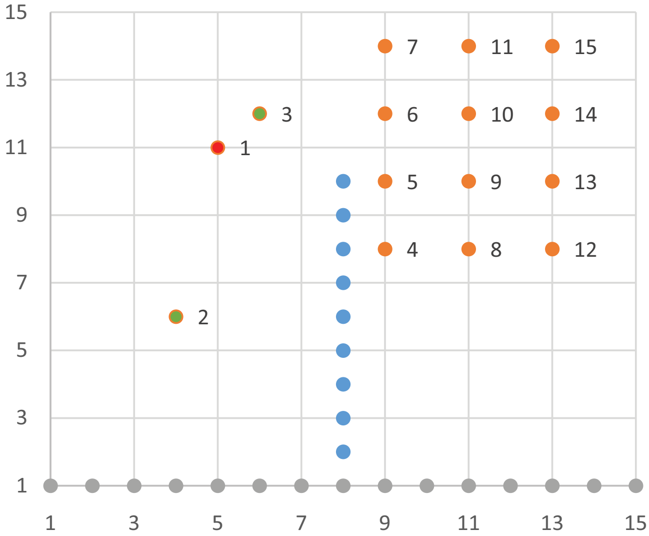

Fig. 2. Plan view of the aquifer system. Active wells pumping from the first layer are represented in orange, those from the second layer, in green and those from the third layer, in red. Blue dots represent the drains while grey ones, the constant head boundary.

4. Combined use of simulation and optimization models

A special software was developed using the MATLAB environment aiming at the combined use of the flow-simulation model (MODFLOW) and the optimization technique (HS algorithm). In the flow chart presented in Fig. 3, the proposed methodology is graphically demonstrated through the structure of the developed software.

The general steps of the program are the following.

Step 1: The problem is initialized and the parameters, which minimize the objective function, are selected. Moreover, the parameters of the Harmony Search Algorithm are defined. These parameters are the size of the harmonic memory (HMS) – the probability for HSA to choose a value from Harmony Memory, defined as Memory Consideration (HMCR) – whose values range from 0.7 to 0.95, the Pitch Adjusting Rate (PAR), which takes values between 0.1 and 0.6 and the maximum

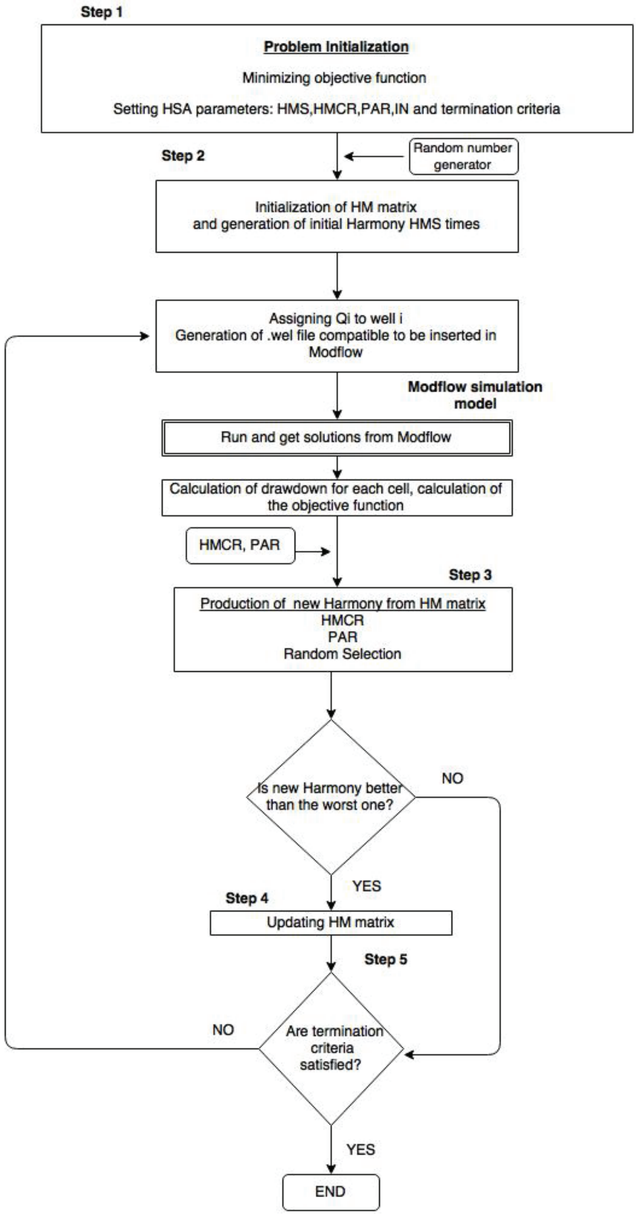

Fig. 3. Flow chart of the proposed methodology as described by the special software developed to combine the use of the simulation and optimization models.

number of iterations IN, with values usually up to 100,000. These values are suggested from the literature, since HS algorithm seems to perform better under these combinations. The execution of the program was tested with several parameter combinations in order to achieve optimum convergence.

Step 2: After the creation of the harmony memory HM, the resulting pumping rates Q_i correspond to the actual wells *i*. The input files for MODFLOW are then created and the simulation model is executed. A function was specifically developed for the connection of the MATLAB environment and the simulation program. More specifically, the function reads and creates .wel files in the appropriate format, then calls MODFLOW as a subroutine and inputs MODFLOW results. In the same way, functions and subroutines can be created for the other packages of MODFLOW as well. The function that has as input the HM table and number of HAS is presented in the following code:

```
function [head_layer_1,head_layer_2,
   head_layer_3, well_coordinates]=
   modflow(HM,a)
```

The .wel file is processed by the program. The data are then corresponded to a table (twri table). This table is structured in four columns. The first column corresponds to the layer in which the well is located, the second and third columns represent the coordinates of the well, while the fourth column is the pumping rate of each well. It also creates a separate table with the positions of the wells.

```
[x,y,z,x1]=textread(‘twri.wel’,’%s %s
   %s %s’, 17);
   twri=[x,y,z,Q];
   q=num2str(HM(1:15,a));
   q1=cellstr(q);
   well_coordinates=[str2double(x(3:17)),
                     str2double(y(3:17)),
                     str2double(z(3:17))];
```

Matching algorithm data .wel file appeared to be challenging, as MODFLOW is written in Fortran and the input and output files need to follow a strict format. Following a trial and error procedure, the proper commands that extract the correct format in MATLAB were identified. Particular attention was given to the blank characters that exist between the tables so they can be read correctly from the MODFLOW.

```
for i=3:17
   twri{i,4}=HM(i-2,a);
end
   fileID = fopen(‘twri.wel’,’w’);
   [nrows,ncols] = size(twri);
   fprintf(fileID,’%s\n’,
         ‘   15    0    MXWELL,IWELBD’);
   fprintf(fileID,’%s\n’,
         ‘   15    ITMP (NWELLS)’);
for i=3:nrows
   fprintf(fileID,’%10s %9s %9s %10f\n’,
          twri{i,:});
end
   fclose(fileID);
```

A twri.nam file should be created for the new .wel file to run. It should be noted that all files with the executable mf2005.exe file must be located in the same folder and must necessarily have the same name.

```
fname = ‘twri.nam’;
system([‘mf2005.exe’ fname]);
%run executable with content of
   fname as inputs
```

Then, once MODFLOW runs and provides results in .lst in the respective file, the data are processed by the program.

```
[x1,x2,x3,x4,x5,x6,x7] = textread
   (‘twri.lst’,’%s %s %s %s %s %s %s’,
   510);lst=[x1 x2 x3 x4 x5 x6 x7];
```

Within the output files, the important data are those representing the hydraulic head of the grid in all layers. It is of great importance to emphasize that the output file has no fixed form, but it changes according to the initial data. What remains constant, though, is the relative position of the printed messages and the results. Therefore, the way to find the effects of stresses in .lst files as the ones used in this application is the following: the word HEAD needs first to be detected within the file in order to identify the exact position where the results are printed. The number of columns and rows that represent head values are constant for each problem. The part of the corresponding code for the implementation of this procedure is the following:

```
[x1,x2,x3,x4,x5,x6,x7] = textread
   (‘twri.lst’,’%s %s %s %s %s %s
   %s’, 510);
   lst=[x1 x2 x3 x4 x5 x6 x7];
   index = find(strcmp(lst, ‘HEAD’));
   head_1 = lst(index(5,1):
            (index(5,1)+52),1:7);
   head_2 = lst(index(6,1):
            (index(6,1)+52),1:7);
   head_3 = lst(index(7,1):
            (index(7,1)+52),1:7);
```

The hydraulic heads at the positions of the wells are then calculated and the differences to the initial ones (for each one of the aquifers) are recorded as the water-level drop. The pumping cost as expressed by Eq. (2) defines the objective function of the optimization model.

Step 3: New harmony is produced by HM table. Depending on HMCR and PAR, values are selected from the initial harmonic memory or new solutions are randomly created. Then the impact of the new solution is estimated, again by calling the MODFLOW function, and if it is better than the worst one stored in HM, the program proceeds to *Step* 4, otherwise it proceeds to *Step* 5.

Step 4: HM table is updated.

Step 5: Termination criterion is tested. If it is satisfied, then the program is terminated, otherwise it returns to *Step* 2.

The results of the program are all stored in an excel file. A suitable macro is created in Microsoft Excel, in order to format the results in easy-to-read matrices while some of the 3-D graphs and charts are also created there.

5. Results

The program was executed for two alternatives of the example, in the second of which the drains have been removed. The best solution for the first alternative was accomplished using the combination HMS = 50, HMCR = 0.7, PAR = 0.5 and IN = 40,000, while for the second alternative, the optimal combination was HMS = 10, HMCR = 0.7, PAR = 0.45, IN = 3,000 (Figs. 4 and 5). The solution for the second, less complicated alternative was obtained in much less iterations [17].

These solutions result to a pumping cost and a total water-level drop 18% and 14% lower than the ones corresponding to the reference status for the first alternative, while the percentage for the second alternative are 8% and 9%, respectively. In Table 1, the pumping rates of the wells for the optimal solution of the first alternative case are presented, as well as their respective water-level drops.

The coupling software, developed by the authors, was programmed so that it can also produce graphical representations of the water-level distribution in the form of 3-D graphs (Figs. 6 and 7 for the first alternative). This representation is also available for the underlying layers (Fig. 8) and for the top layer in the form of a 2-D graph (Fig. 9). The same information is also presented for the second alternative respectively. Figs. 10 and 11 represent the 3-D graphs, Fig. 12, the underlying layers and Fig. 13, the 2-D distribution of the top layer.

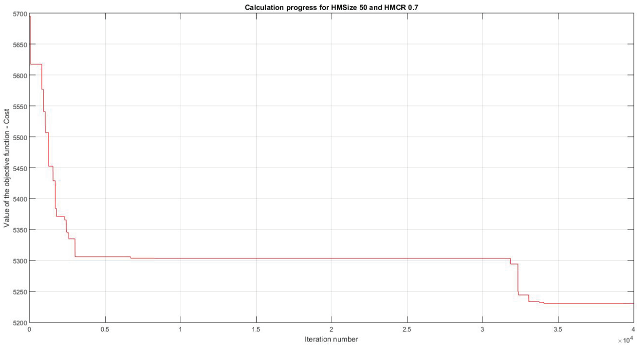

Fig. 4. Convergence to the optimal solution for the first alternative of the example.

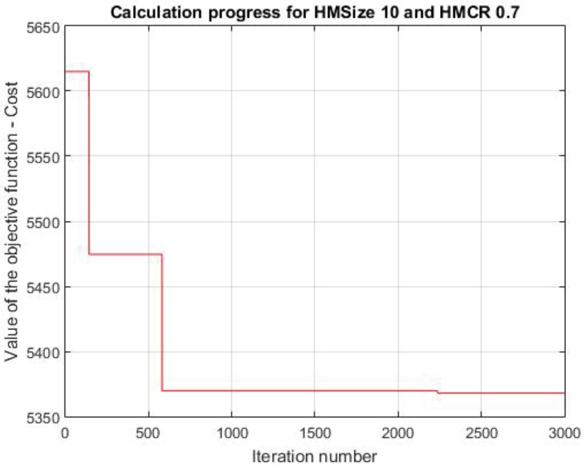

Fig. 5. Convergence to the optimal solution for the second alternative of the example (without drains).

Table 1
Locations of wells, their pumping rates and their respective water-level drops for the proposed solution of the first alternative of the example

Well	Layer	*x*	*y*	Q (L/s)	S (m)
1	3	5	11	−109.73	20.18
2	2	4	6	−234.94	15.18
3	2	6	12	−172.17	21.04
4	1	9	8	−273.34	14.74
5	1	9	10	−278.13	19.46
6	1	9	12	−179.67	22.13
7	1	9	14	−37.89	20.87
8	1	11	8	−216.6	19.67
9	1	11	10	−138.43	22.61
10	1	11	12	−96.54	23.30
11	1	11	14	−78.15	22.80
12	1	13	8	−32.69	17.90
13	1	13	10	−192.78	23.50
14	1	13	12	−76.06	23.14
15	1	13	14	−9.62	22.12
Sum				−2,126.9	308.7

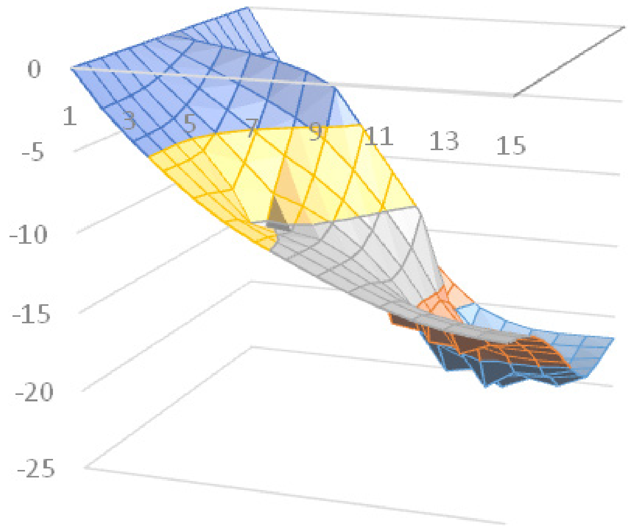

Fig. 6. 3-D representation of water-level drop for the top aquifer under operating pumping wells conditions (m) for first alternative.

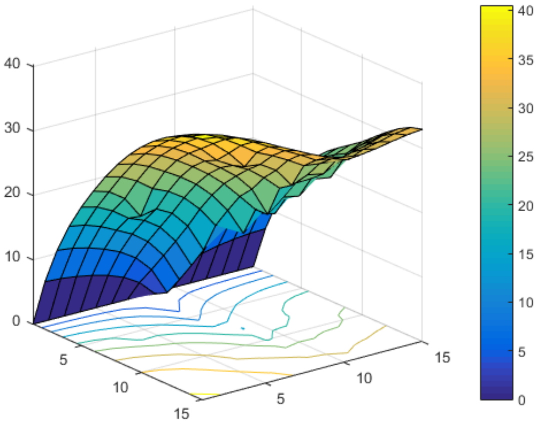

Fig. 7. 3-D representation of the hydraulic head distribution for the top layer under operating pumping wells conditions for the first alternative (m).

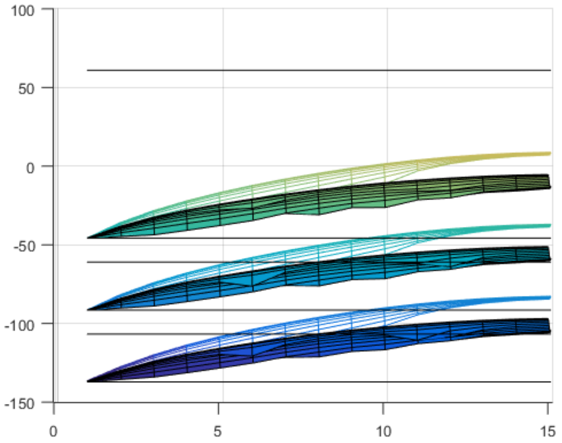

Fig. 8. Side view of the hydraulic head distribution before the operation of the wells (transparent grid) and during the operation of the wells (colored grid) for first alternative.

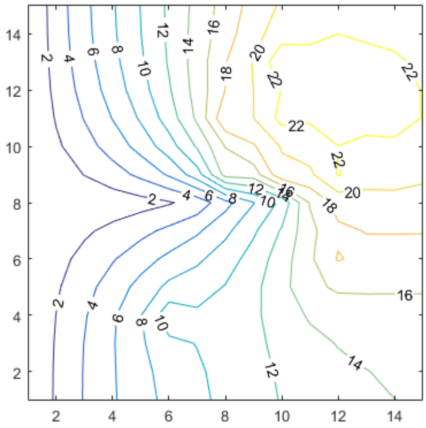

Fig. 9. Contours demonstrating equal water-level drop for the top aquifer under operating pumping wells conditions for first alternative.

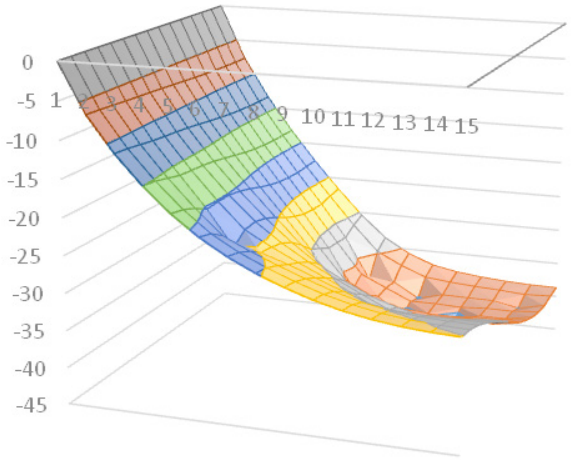

Fig. 10. 3-D representation of water-level drop for the top aquifer under operating pumping wells conditions (m) for the second alternative.

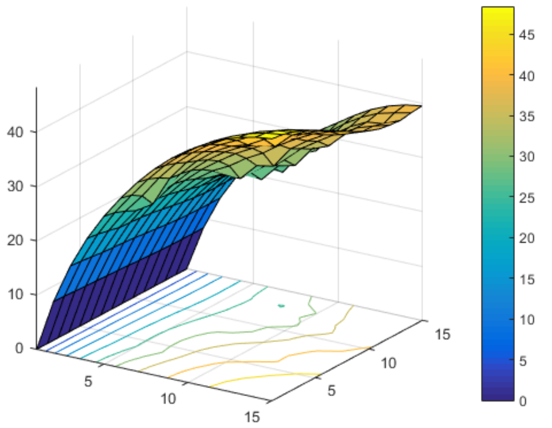

Fig. 11. 3-D representation of the hydraulic head distribution for the top layer under operating pumping wells conditions (m) for the second alternative.

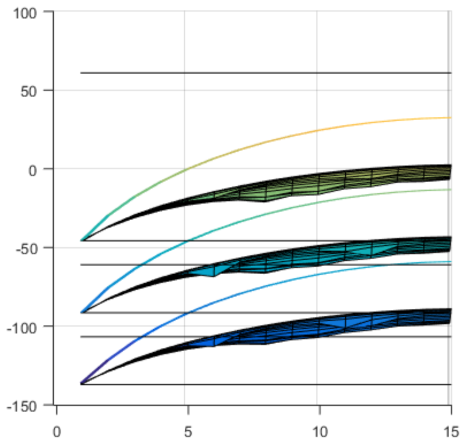

Fig. 12. Side view of the hydraulic head distribution before the operation of the wells (transparent grid) and during the operation of the wells (colored grid) for the second alternative (without the drains).

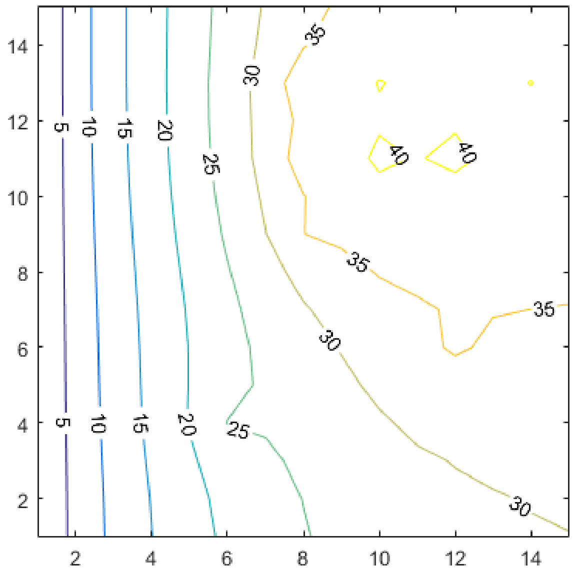

Fig. 13. Contours demonstrating equal water-level drop for the top aquifer under operating pumping wells conditions for the second alternative (without the drains).

6. Conclusions

In this paper, a methodology is presented for the combined use of a flow-simulation model with an optimization algorithm aiming at the rational and optimal management of groundwater aquifer systems. One of the most widely used and most efficient 3-D flow-simulation models, MODFLOW is used combined with the Harmony Search Algorithm, one of the novel metaheuristic optimization techniques. These two models are combined with a specially designed software developed under the MATLAB environment, formulating a powerful, user friendly and effective management tool.

In order to investigate the efficiency of the developed combining software and the proposed methodology, a classic example of the application of MODFLOW was used and executed in two alternative cases. This example was optimized using the operational cost as the objective function. A logical number of iterations were needed for the achievement of the optimal solution encouraging the use of the proposed methodology in similar problems.

The results of the presented methodology demonstrate that the combined use of a groundwater flow-simulation model like MODFLOW with an efficient optimization technique like HS algorithm can formulate a very effective management tool. The graphical representation of the outputs, as provided by the developed software, offers the user a visualization of the results of alternative solutions, thus assisting the understanding of the impacts of the application of complex management policies.

The applications of the proposed methodology are not restricted to the optimization of groundwater flow-simulation problems. This methodology, with some adjustments, can also be used to couple optimization models with other simulation models emphasizing, for example, on water quality, energy production, protection and restoration and many others.

Acknowledgment

An initial shorter version of the paper has been presented in the International Conference on Protection and Restoration of the Environment XIII, Mykonos, 2016.

References

[1] N. Theodossiou, Optimization Techniques in Groundwater Resources Management, Lecture Notes, Department of Civil Engineering Aristotle University of Thessaloniki (in Greek), 2000.

[2] C. Huang, A.S. Mayer, Pump-and-treat optimization using well locations and pumping rates as decision variables, Water Resour. Res., 33 (1997) 1001–1012.

[3] K. Qahman, A. Larabi, D. Ouazar, N.A.J.I. Ahmed, H.D.C. Alexander, Optimal extraction of groundwater in Gaza coastal aquifer, J. Water Resour. Prot., 1 (2009) 249.

[4] M.T. Ayvaz, Application of Harmony Search Algorithm to the solution of groundwater management models, Adv. Water Resour., 32 (2009) 916–924.

[5] Z.W. Geem, J.-H. Kim, G.V. Loganathan, A new heuristic optimization algorithm: harmony search, Simulation, 76 (2001) 60–68.

[6] Q. Luo, J. Wu, X. Sun, Y. Yang, J. Wu, Optimal design of groundwater remediation systems using a multi-objective fast Harmony Search Algorithm, Hydrogeol. J., 20 (2012) 1497–1510.

[7] N. Theodossiou, Application of non-linear simulation and optimisation models in groundwater aquifer management, Water Resour. Manage., 18 (2004) 125–141.

[8] B.A. Murtagh, M.A. Saunders, MINOS 5.1 User's Guide, Technical Report SOL 83-20R, Department of Operations Research, Stanford University, Stanford California, 1987.

[9] Z. Geem, Optimal Design of Water Distribution Networks Using Harmony Search, PhD Thesis, Korea University, Seoul South Korea, 2000.

[10] I. Kougias, L. Katsifarakis, N. Theodossiou, Medley multiobjective Harmony Search Algorithm. Application on a water resources management problem, Eur. Water, 39 (2012) 41–52.

[11] I. Kougias, N. Theodossiou, Multiobjective pump scheduling optimization using Harmony Search Algorithm (HSA) and polyphonic HSA, Water Resour. Manage., 27 (2013) 1249–1261.

[12] I. Kougias, T. Patsialis, N. Theodossiou, J. Ganoulis, Hydropower Projects Within a Municipal Water Supply System, Optimum Allocation and Management Using Harmony Search, Exploring Innovative and Successful Applications of Soft Computing, IGI Global, Chapter 4, doi: 10.4018/978-1-4666-4785-5.ch004, 2014, pp. 59–75.

[13] N. Theodossiou, D. Karakatsanis, E. Fotopoulou, Introducing Novel Optimization Techniques in Irrigation Pipe Network Applications, 2nd EWaS International Conference, Chania, Crete, Greece, 2016.

[14] I. Kougias, D. Karakatsanis, A. Malatras, F. Monforti-Ferrario, N. Theodossiou, Renewable energy production management with a new harmony search optimization toolkit, Clean Technol. Environ. Policy, 18 (2016) 2603–2612. doi: 10.1007/s10098-016-1173-4.

[15] M.G. McDonald, A.W. Harbaugh, A Modular Three-dimensional Finite-Difference Ground-Water Flow Model, U.S. Geological Survey Techniques of Water-Resources Investigations, Book 6, Chapter A1, 1988.

[16] A.W. Harbaugh, E.R. Banta, M.C. Hill, M.G. McDonald, MODFLOW-2000, the U.S. Geological Survey Modular Ground-Water Model – User Guide to Modularization Concepts and the Ground-Water Flow Process, U.S. Geological Survey Open-File Report 00-92, 2000.

[17] M. Antoniou, N. Theodossiou, D. Karakatsanis, Groundwater Management Optimization with Combined Use of Harmony Search Algorithm and Modular Finite-Difference Flow Model ModFlow, International Conference on Protection and Restoration of the Environment XIII, Mykonos, 2016.