Stochastic Optimization and Numerical Simulation for Pumping Management of the Hersonissos Freshwater Coastal Aquifer in Crete

P. N. Stratis[‡], Z. A. Dokou[†], G. P. Karatzas[†], E. P. Papadopoulou[*] and Y.G. Saridakis[‡]

Abstract—In the present study, the well known Princeton Transport Code (PTC), a groundwater flow and contaminant transport simulator, is being used to simulate the dynamics of the freshwater coastal aquifer located in Hersonissos area of the Greek island of Crete, and guided by the Algorithm of Pattern Extraction (ALOPEX), a real time stochastic optimization method, to optimally manage area's main pumping activities and prevent saltwater contamination. Main objective of this hybrid coupling of the PTC's finite-element (FE)/finite-difference (FD) routines to the ALOPEX stochastic optimization technique, is to create an optimal pumping management plan, for the Hersonissos aquifer, that maximizes the total extracted freshwater volume from the aquifer and, at the same time, keeps all pumping locations safe from saltwater intrusion. For this, we utilize the recently adopted version of the ALOPEX unconstrained optimization algorithm accompanied by an efficient penalty system designed for the aquifer pumping management problem. The numerical simulations conducted led to summer and winter pumping plans that considerably improve the total extracted freshwater volume from the aquifer while the active pumping locations remain safe from seawater even if a 2% increase of the proposed pumping plan is applied.

Keywords—ALOPEX stochastic optimization, penalty system, PTC code, finite elements, coastal aquifers, saltwater intrusion, pumping management.

I. Introduction

SALTWATER intrusion is a phenomenon that poses a significant threat to the quality of groundwater reserves in coastal aquifers. This phenomenon is mainly affected by unrestrained groundwater withdrawals that disturb the natural balance of freshwater - saltwater in groundwater systems. To protect groundwater reserves and design a sustainable water management strategy in coastal aquifers, researchers have been focused on the combined use of mathematical models, numerical simulations and optimization algorithms.

The objective of this work is to assess the saltwater intrusion and then extend and provide sustainable management alternatives for the Hersonissos aquifer, located in Crete, Greece. The saltwater intrusion phenomenon at this aquifer has been studied previously by a number of researchers. In [15] (see also [16]), the finite difference MODFLOW and the finite element PTC models are employed to simulate saltwater intrusion and compare the numerical results to the ones obtained by geostatistical techniques (Kriging). In [10] the PTC simulator is coupled by a differential evolution (DE) algorithm to maximize the total extracted freshwater volume from five preselected pumping locations (production wells) while satisfying minimum hydraulic head constraints at specified locations, ensuring no further intrusion of seawater. The same approach was followed in [4] using sequential linearization in order to reduce the computational cost. The Hersonissos aquifer has been also studied in [20] by making use of geostatistical techniques (Kriging and Ordinary Kriging).

ALOPEX stochastic unconstrained optimization originates at the area of neurophysiology (cf. [8]) and, since then, has been applied with success in many real time applications (see for example [21] and the references therein). Recently, in [18], the dynamics of the algorithm were studied in depth for the problem of saltwater intrusion of coastal aquifers. The determination of the algorithm's feedback and noise amplitudes and the introduction of an effective penalty system, to enforce problem's constraints, revealed its potential to successfully treat the problem of pumping management in coastal aquifers.

The approach employed, thus, here is to combine the groundwater simulation model PTC with the newly introduced constrained version of the ALOPEX stochastic optimization technique. The objective is to maximize groundwater withdrawal in the existing pumping well network while precluding saltwater to enter a safe zone around the active wells in the region.

II. Methodology

A. Groundwater simulation model - PTC

PTC (Princeton Transport Code [3]) is a well known three-dimensional groundwater flow and contaminant transport simulator that uses a combination of finite element and finite difference methods to solve the groundwater flow Boussinesq equation which, for the heterogeneous isotropic unconfined case, takes the form (cf. [7])

$$\nabla \cdot (Kh\nabla h) + W = S_y \frac{\partial h}{\partial t} \tag{1}$$

where h denotes the hydraulic head, K is the hydraulic conductivity (considered to be heterogeneous and isotropic), W is the volumetric flux per unit volume representing sources and/or sinks of water, S_y is the specific yield and t denotes time.

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PTC employs a hybrid splitting algorithm for solving the fully three-dimensional system. The domain is discretized into approximately parallel horizontal layers, within each of which a finite element discretization is employed allowing accurate representation of irregular domains. The vertical connection of the layers is represented by finite differences. This hybrid finite element and finite difference coupling provides the opportunity to divide the computations into two steps during a given time iteration (splitting algorithm). In the first step, all horizontal equations are solved while in the second step, the vertical equations which connect the layers are solved (cf. [3]).

B. Sharp interface approach

In this work, the PTC model is used in conjunction with the sharp interface approach and the Ghyben-Herztberg approximation in order to estimate the saltwater intrusion extent. The sharp interface is a hydraulic approach, thus only the hydraulic head values on the model domain are needed in order to approximate the saltwater intrusion extent, as opposed to other approaches that utilize chloride or electrical conductivity measurements. The main assumption is that the mixing zone between the two immiscible fluids (fresh and saline water), that have different densities, is limited into an interface of a small finite width. The location of the sharp interface between the two fluids is determined by the difference between the hydraulic heads of the saline and fresh water and the volume of freshwater flowing towards the shoreline from inland (cf. [19]). The location of the seawater intrusion front is approximated using the Ghyben-Herzberg relationship:

$$\xi = \frac{\rho_f}{\rho_s - \rho_f} h_\xi \approx 40 h_f, \tag{2}$$

where, ξ is the interface depth below the sea level, h_f the hydraulic head of the freshwater above the sea level, ρ_f =1000 kg/m^3 the density of freshwater and ρ_s =1025 kg/m^3 the density of saline water. This approach has been applied and extended by many researchers in the literature (e.g. [1], [10], [11], [12], [16] among many others).

C. Study area and numerical model development

The study area of Hersonissos aquifer is located on the north coast of Crete, 25 km from the city of Heraklion in Crete, Greece. The Hersonissos basin covers an area of about 18 km^2, and stretches for 3.8 km in W - E direction and almost 4.7 km in N - S direction. During the summer period water demand is high due to extensive touristic and agricultural activities, leading to significant drawdown in the area, intensifying the problem of seawater intrusion. The region of interest has five pumping wells that are active all year, especially during the dry period, in order to meet the irrigation needs and the increased population during the summer period due to tourism.

The basin is covered mainly with karstified limestones of variable hydraulic conductivity and marls, whereas along the coastal line alluvial deposits with high permeability can be found (cf. [15]). The hydraulic conductivity values used for each geologic formation were 12.96 m/d for limestones and dolomitic limestones, 5.2 m/d for bioclastic limestones, 0.15 m/d for marl formations, 0.6 m/d for clay and 430 for alluvial deposits located near the coastline (cf. [10]).

Initially, a six month groundwater flow simulation, representing the dry season, when saltwater intrusion is more intense, was implemented. This was followed, in the sequel, by a six month wet season simulation in order to study the aquifer's response to saltwater intrusion during conditions of increased fresh water inflow to the basin. A Dirichlet boundary condition of fixed head equal to 100 m was applied along the coastline to simulate the sea boundary, assuming a change in the reference level from the sea level to the bottom of the aquifer (the aquifer bottom elevation was set to zero thus the sea level was set to 100 m). Various Neumann conditions were applied at the southern boundary of the region during the calibration process, in order to simulate groundwater inflow from connecting basins and match the measured hydraulic head values at the wells (see Fig. 1).

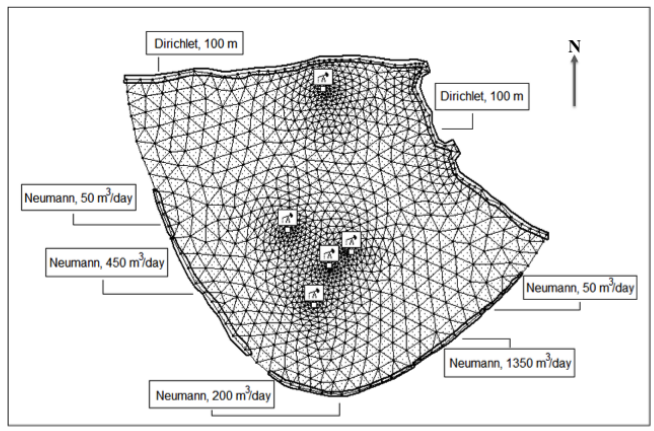


Fig. 1. Hersonissos aquifer. Sideways water recharge values.

Regarding the saltwater intrusion toe location, according to the Ghyben-Herzberg relationship, h_f was estimated at 2.5 m, given that the depth of the studied aquifer is about 100 m (based on Boring Log information). Thus, the contour of 100+2.5 = 102.5 m represents the hydraulic head isolevel limit below which a zone is considered intruded by saltwater.

D. Pumping management

To fix notation, let M be the number of active wells in the region and let the vector $\boldsymbol{Q}$ be defined by

$$\boldsymbol{Q} = (Q_1 \ , \ \cdots \ , \ Q_M) \tag{3}$$

where $Q_i \ , \ i = 1, \ldots, M$ denotes the pumping rate of the i-th active well with coordinates (x_i, y_i). The objective, to maximize groundwater withdrawal while precluding saltwater to enter a safe zone around all active wells, may then be described by the following nonlinear optimization problem (cf.

[18]):

$$\begin{aligned} &maximize: \quad P \equiv P(\boldsymbol{Q}) = e^{-\left[S(\overline{\boldsymbol{Q}})-S(\boldsymbol{Q})\right]^2/S^2(\overline{\boldsymbol{Q}})} \in [0,1] \\ &under\ the\ constraints: \quad 0 \le \underline{Q_i} \le Q_i \le \overline{Q_i} < Q_A, \\ &\qquad\qquad S(\boldsymbol{Q}) = \sum_{i=1}^{M} Q_i \le Q_A \qquad (4) \\ &\qquad\qquad x_{\tau,i} \le x_i - d_s,\ i \in \{1,..,M\}, \end{aligned}$$

where P denotes the profit (objective) function, $\underline{Q_i}$ and $\overline{Q_i}$ are the minimum and maximum, respectively, pumping capabilities of the i-th well, Q_A is the total discharge capability of the aquifer, $x_{\tau,i}$ is the x-coordinate of the saltwater's front in the neighborhood of the i-th well and d_s is a pre-specified safety distance (set equal to 180m in the present implementation).

E. Constrained ALOPEX for pumping management

For the solution of the nonlinear optimization problem (4), described in the previous section, we employ ALOPEX stochastic optimization algorithm coupled by a penalty system to enforce problem's constraints.

To be more specific, in each iteration step, ALOPEX updates simultaneously the values of all control variables Q_i , $i = 1, \ldots, M$ by means of the following vector rule:

$$\mathbf{Q}^{(k)} = \mathbf{Q}^{(k-1)} + c_k \Delta\mathbf{Q}^{(k-1)} \Delta P^{(k-1)} + \mathbf{g}^{(k)}, \qquad (5)$$

with

$$\begin{aligned} \Delta\boldsymbol{Q}^{(k)} &= \boldsymbol{Q}^{(k)} - \boldsymbol{Q}^{(k-1)} \\ \Delta P^{(k)} &= P(\boldsymbol{Q}^{(k)}) - P(\boldsymbol{Q}^{(k-1)}) \end{aligned} \qquad (6)$$

where c_k is a real parameter controlling the amplitude of the feedback term, while $\mathbf{g}^{(k)}$ is the noise vector, with values uniformly distributed in an appropriately chosen interval, in order to provide the necessary agitation needed to drive the process to global extrema avoiding local problems. The methodology for determining a near optimal set of values for c_k and $\mathbf{g}^{(k)}$ is thoroughly discussed in [18].

In each ALOPEX iteration step all control variables Q_i , $i = 1, \ldots, M$ are being rectified, if needed, via a two-phase penalty system. Phase one refers to the enforcement of the first two constraints described in (4), and precedes PTC's implementation, while phase two refers to the enforcement of the third *toe-constraint* described in (4), needs the trace of the saltwater interface and, thus, follows PTC's implementation. While the algorithms of implementing said penalty system are described in detail in [18], it is worthwhile to point out that:

- In both penalty phases, the values of those Q_i needed to be rectified, are being, ultimately, reduced or increased by a percentage, which in our implementation (as in [18]) has been set to 5%.
- In phase two, the enforcement of the toe-constraint is being achieved in two cycles. In cycle one only the pumping rates of the active wells at risk are being rectified, while, if necessary, in cycle two the pumping rates of all active wells that affect the endangered wells are being rectified.
- The efficiency of the standard-deviation/mean-value stopping criterion, introduced in [18], is also reported in the present work through all numerical simulations included in the next section.

Finally, in Fig. 2 that follows, the whole ALOPEX/PTC pumping management methodology, described in the above paragraphs, is being depicted via the flow chart of the whole process.

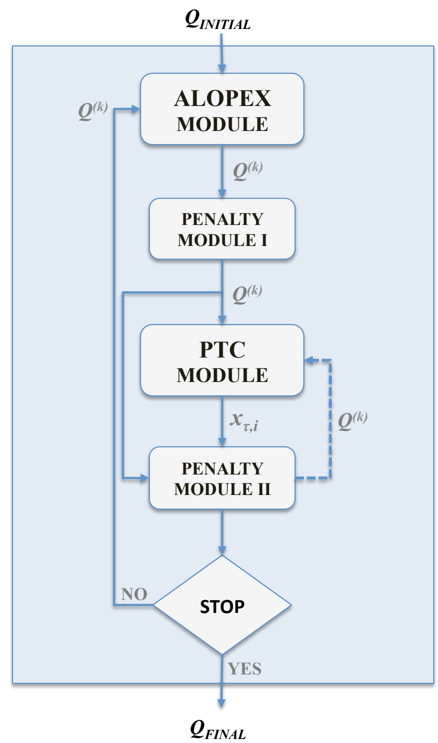


Fig. 2. Flow chart of the ALOPEX/PTC pumping management methodology.

III. Numerical simulations

In this section we include the results from characteristic numerical simulations performed for the freshwater aquifer located at Hersonissos, Crete, Greece.

To characterize the simulation profiles included, recall the main governing flow equation from (1) and let the volumetric flux W satisfy

$$W = N - Q$$

where N denotes the recharge rate distributed over the surface of the aquifer and Q denotes the discharge rate distributed over the active pumping area. Then, the simulations included refer to a *dry case* scenario as well as to a *wet case* scenario characterized by

- *Dry Case*: $N = 0$ mm/year, while the sideways (subsurface) recharge, characterized by the Neumann boundary conditions, is as defined in Fig. 1,
- *Wet Case*: $N = 500$ mm/year with percentage of infiltration set at 30%, while the sideways recharge is as described in Fig. 1 increased by 20%.

Both case scenarios consider five active public pumping locations, the coordinates of which (see Fig. 1) have been assigned via a geographical information system. From the five active wells the top one, located close to the north coastline of the aquifer (see Fig. 1), is always flooded by seawater, independently from the pumping activities in the region. This is due to the fact that the *natural* saltwater intrusion, namely the hydraulic head isolevel at 102.5m when $Q = 0$ (the thin light-blue contour line included in all figures that follow), is far beyond the well's location. The water extracted from this location is always unsuitable for human consumption or land irrigation and, therefore, may as well considered to be inactive. Nevertheless, to comprise with relevant results in the literature, we consider active all five pumping locations despite the fact that we are able to protect only four of them from saltwater intrusion.

In Table I we have included the maximum $\overline{Q}_i$ pumping capabilities of all five active locations, while the corresponding minimum ones have been set to satisfy $\underline{Q}_i = 0.3 * \overline{Q}_i$.

TABLE I
PUMPING CAPABILITIES (m^3/d) OF ACTIVE LOCATIONS

i	1	2	3	4	5
$\overline{Q}_i$	1850	2550	600	2550	200
$\underline{Q}_i$	555	765	180	765	60

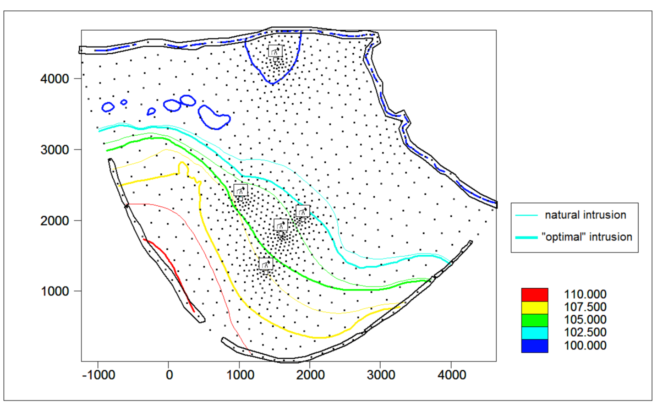
Finally, we note that in all numerical simulations the pumping rates Q_i , $i = 1, \ldots, M$ are considered to be numbered in a top-to-bottom fashion, namely $y_1 \geq \ldots \geq y_M$.

A. Dry Case

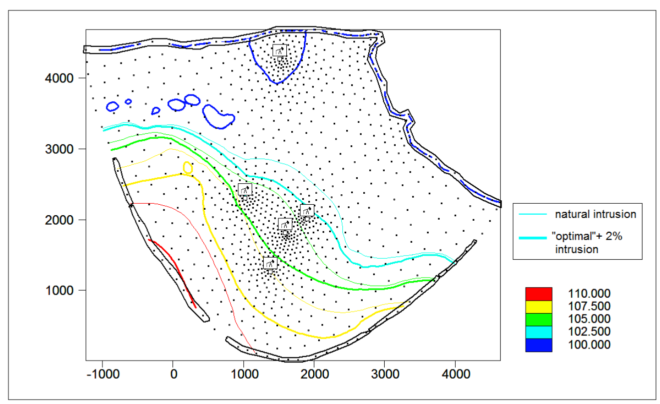
All results, pertaining to the dry (summer) case ($N = 0$) scenario, from the ALOPEX/PTC pumping management performance, during a typical cycle of 500 iterations, are summarized in Table II and Fig. 3 that follow.

TABLE II
ALOPEX/PTC PERFORMANCE: DRY CASE

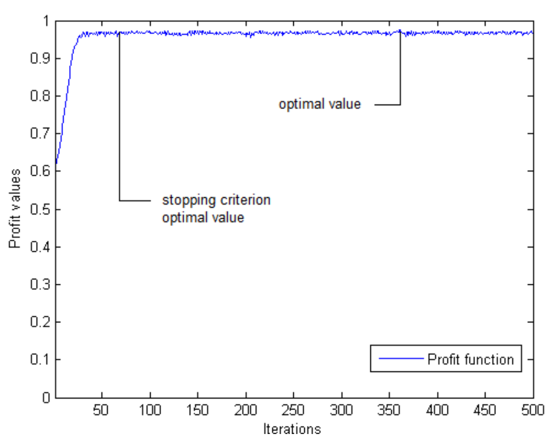
Problem Parameters	*Total Optimal Values*	*Stopping Criterion Optimal Values*
k (# *iter.*)	362	59
$P(\boldsymbol{Q}^{(k)})$	0.97424	0.97033
$Q_1^{(k)}$	1839.06	1783.77
$Q_2^{(k)}$	1375.14	1338.24
$Q_3^{(k)}$	558.96	546.16
$Q_4^{(k)}$	2525.95	2539.59
$Q_5^{(k)}$	198.78	197.14
$S(\boldsymbol{Q}^{(k)})$	6497.89	6404.90



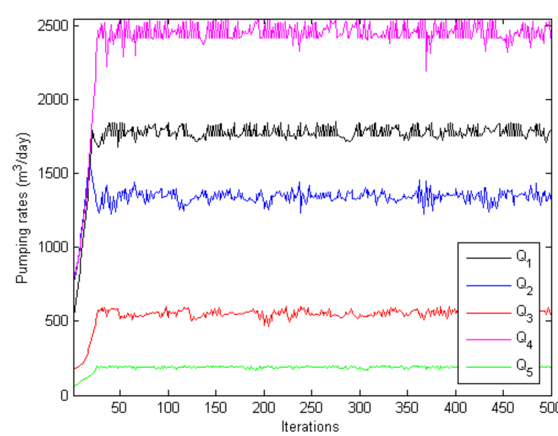
(a) Hydraulic head isolevel curves using the optimal pumping rates. The countour line at 102.5m denotes the saltwater interface.



(b) Hydraulic head isolevel curves using the optimal pumping rates increased by 2%. The countour line at 102.5m denotes the saltwater interface.



(c) Values of $P(\boldsymbol{Q}^{(k)})$ during a cycle of $k = 500$ iterations.



(d) Pumping rates Q_i during a cycle of $k = 500$ iterations.

Fig. 3. *Dry Case*: ALOPEX/PTC performance for five (5) active pumping locations in a typical run of 500 iterations

Inspecting, now, Fig. 3a it can be easily verified that all pumping locations, except naturally the top one, remain safe from saltwater intrusion, since we kept the saltwater interface (contour line at $h = 102.5$m) at a distance of at least d_s=180m away from all protected active locations. It is also significant that, as Fig. 3b suggests, increments of 2% - 5% on all optimal pumping rates Q_i (reported in Table II) do not expose the protected active pumping locations to saltwater intrusion due to the carefully chosen value of the safety distance d_s. As it pertains now to the ALOPEX performance notice that (see figure 3c) the algorithm drives the objective function to a narrow neighborhood of its constrained maximum in less than 50 iterations and remains close to it, for the rest of the process, within relatively small amplitude fluctuations. Similar behavior may be observed, in Fig. 3d, for the process's control variables Q_i.

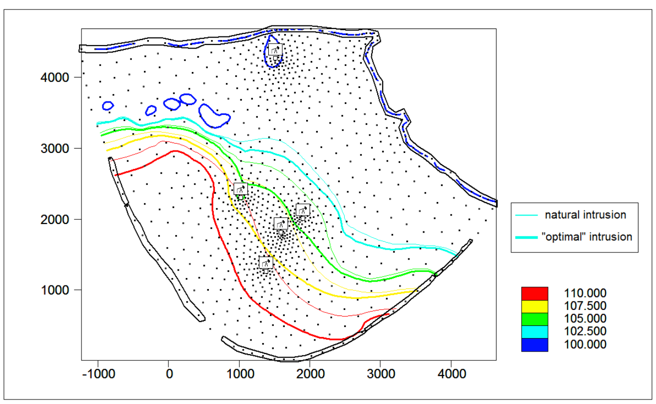
B. Wet Case

All results, pertaining to the wet (winter) case ($N = 500$) scenario, from the ALOPEX/PTC pumping management performance, during a typical cycle of 500 iterations, are summarized in Table III and Fig. 4 that follow. By inspection only of the reported results one may easily verify that this is an untroubled case in the sense that the active pumping locations may perform at maximum pumping rates without any threat from saltwater intrusion.

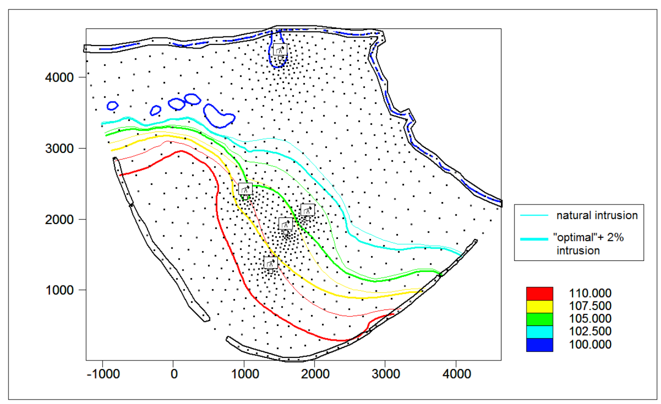
TABLE III
ALOPEX/PTC PERFORMANCE: WET CASE

Problem Parameters	*Total Optimal Values*	*Stopping Criterion Optimal Values*
k (*# iter.*)	476	59
$P(\boldsymbol{Q}^{(k)})$	0.97424	0.97033
$Q_1^{(k)}$	1807.49	1683.33
$Q_2^{(k)}$	2539.68	2537.39
$Q_3^{(k)}$	598.70	578.29
$Q_4^{(k)}$	2545.65	2534.73
$Q_5^{(k)}$	193.98	186.96
$S(\boldsymbol{Q}^{(k)})$	7682.40	7520.70

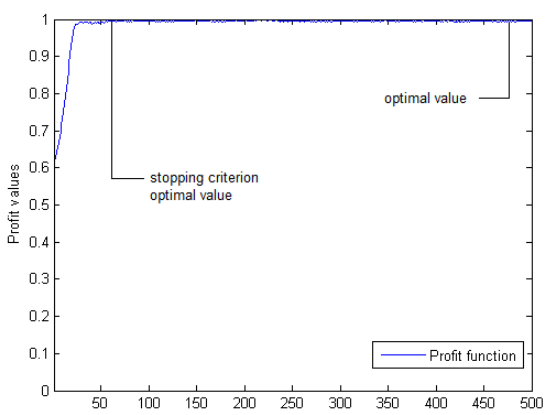
Indeed, as both Figs. 4a and 4b suggest, all pumping locations, except naturally the top one, remain safe from saltwater intrusion, since the saltwater interface (contour line at $h = 102.5$m) is not even close to the safety distance of d_s=180m from all protected active locations. ALOPEX drives in less than 50 iterations (see figure 4c) the objective function to its global maximum and remains close to it, for



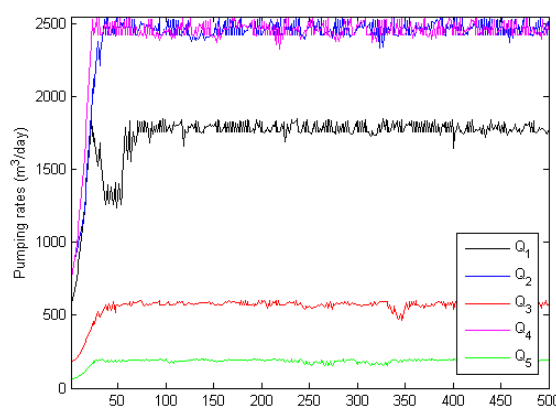
(a) Hydraulic head isolevel curves using the optimal pumping rates. The countour line at 102.5m denotes the saltwater interface.



(b) Hydraulic head isolevel curves using the optimal pumping rates increased by 2%. The countour line at 102.5m denotes the saltwater interface.



(c) Values of $P(\boldsymbol{Q}^{(k)})$ during a cycle of $k = 500$ iterations.



(d) Pumping rates Q_i during a cycle of $k = 500$ iterations.

Fig. 4. *Wet Case*: ALOPEX/PTC performance for five (5) active pumping locations in a typical run of 500 iterations.

the rest of the process, within very small amplitude fluctuations. Similarly, inspecting Fig. 4d, it can be noticed that all control variables Q_i reach within a few iterations maximum performance.

IV. Conclusion

In this study, we combined the PTC groundwater simulation model with the newly introduced constrained version of the ALOPEX stochastic optimization technique, in an attempt to maximize groundwater withdrawal in the existing pumping well network while avoiding saltwater to enter a safe zone around the active wells in the region. The results, for both dry and wet case scenarios considered, revealed that the recently introduced constrained version of the ALOPEX stochastic optimization method cooperates effectively with PTC and, operating on pumping locations in both local and global range, is capable to produce considerably improved results. We strongly believe that the reported results justify and encourage further investigation on the performance of the method.

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