Combining Stochastic Optimization and Numerical Methods-Software for the Pumping Management of Coastal Aquifers: Case Study of a Rectangular Homogeneous Aquifer

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***Abstract*—The advantages of using the Algorithm of Pattern Extraction (ALOPEX) stochastic optimization technique in combination with both analytical models as well as 3D numerical simulators have been recently studied in detail in [23]–[25]. In this work, we present some preliminary results from the coupling of the Collocation method and the FEniCS open source modules to the ALOPEX algorithm as an effective pumping management process of 2D aquifer approximation models. The results refer to a test case of a homogeneous rectangular aquifer that approximates the freshwater coastal aquifer at Vathi area in the Greek island of Kalymnos. The objective is, on the one hand, to provide an optimal pumping management plan for the aquifer that would maximumize the total freshwater volume pumped from the aquifer and, on the other, to keep all pumping active locations safe from saltwater intrusion. For this we adapt and use the ALOPEX parameter configuration and the efficient penalty system introduced in [25] with guard points around the pumping locations. Our numerical simulations indicate that our pumping management results using the Collocation and FEniCS methods strongly compete the results obtained by using the analytical representation of the flow potential, known for this type of aquifers. Therefore, both Collocation and FEniCS methods can be effectively used to investigate the problem of optimal pumping management in heterogeneous aquifers with complex geometry boundaries and in general, aquifers where the analytical representation of the flow potential is unavailable.**

***Index Terms*—Collocation, FEniCS, finite elements, ALOPEX stochastic optimization, guard points, penalty system, coastal aquifers, saltwater intrusion, pumping management.**

I. INTRODUCTION

SALINIZATION of freshwater is the direct result from saltwater intrusion into a freshwater coastal aquifer. It is mainly due to unrestrained groundwater withdrawals that disturb the natural balance of freshwater - saltwater in groundwater systems. The uncontrolled progress of the phenomenon implies the decrease of freshwater storage in the aquifer, and in some cases, the abandonment of the supply wells. It is clear, that saltwater intrusion poses a significant threat to the quality of groundwater reserves in coastal aquifers, thus an efficient management strategy that protects groundwater reserves is required. In the name of the design of 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 saltwater intrusion phenomenon has been thoroughly studied in the past. In [19] (see also [20]), 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 [12] 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 taken in [6] using sequential linearization in order to reduce the computational cost. Finally, in the recent work of [25], where a detailed analysis of the ALOPEX algorithm was presented and a complete penalty system system was devised, the performance, stability and sensitivity analysis performed for the ALOPEX algorithm, as it pertains to the analytical flow potential model described in [16], revealed the effectiveness of the method. Different recharging and pumping scenarios were examined, and in each case, ALOPEX created an optimal pumping plan, where the freshwater pumping volume was maximized, while all the wells were kept safe from saltwater intrusion.

FEniCS is an open source automated programming environment, that provides automated solution for differential equations by the Finite Element Method, and is licensed under the GNU GPL. FEniCS has recently been acknowledged as a mainstream scientific computing tool and continues to build its reputation as user-friendly, open source software comprising a large number of scientific computing tools. The solution of a physical problem, like the saltwater intrusion problem in this study, in FEniCS consists of a number of discrete steps, after the PDE and the boundary conditions have been identified.

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Specifically, the user has to reformulate the PDE problem as a variational problem, and then, make a Python program where the formulas in the variational problem are coded, along with definitions of the input data. FEniCS thereafter, automatically generates basis functions, evaluates the variational forms and assembles the finite elements.

Furthermore, for comparison reasons, we used the Hermite Collocation Method (HC) for the numerical treatment of the PDE model. HC is a fourth order spatial discretization method for BVPs that requires no numerical integration unlike other finite element methods. In some of our recent work (cf. [1], [2]) we used the HC method, coupled with third order Diagonally Implicit and Strong Stability Preserving Runge-Kutta (RK) schemes, for the numerical investigation of a general class of parabolic PDEs for medical and biological applications. Therefore, the high accuracy and stability of the HC-RK, were the reasons that prompted us to implement the method in large-scale steady state models like the saltwater intrusion.

The approach in this study is to efficiently couple a Collocation or a FEniCS module, that would deal with the PDE arising from the physical problem, with the latest ALOPEX version introduced in [25]. In this hybrid coupling, an extended guarding system will be used in order to create a control zone around the pumping locations. The ultimate objective is the development of an open source simulation model coupled with a stochastic optimization algorithm, that could provide an efficient pumping management strategy.

II. Methodology

A. Simulation model

The governing Struck's flow potential equation, is expressed as

$$\nabla \cdot (K \nabla \phi) + N - Q = 0 \tag{1}$$

where ϕ denotes the flow potential, K is the hydraulic conductivity, N is the recharge distributed over the surface of the aquifer and Q is the discharge rate over the active pumping area.

B. Model assumptions

The above model equation is valid inside the aquifer under the following two common simplifications:

- the sharp interface assumption, where the no mixing zone is assumed between the fresh and salt water, and
- 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, $\rho_f = 1000\ kg/m^3$ the density of freshwater and $\rho_s = 1025\ kg/m^3$ the density of saline water. Assuming steady state conditions, this equation is used to estimate the position of the saltwater interface inside the aquifer.

This approach has been applied and extended by many researchers in the literature (e.g. [3], [12], [13], [16], [20] among many others), while a discussion about the validity of use of this approach was conducted in the work of [14].

FEniCS

The FEniCS implementation presupposes the formulation of the variational problem, by the multiplication of the equation by a test function v and then integrating by parts. The bilinear and the linear form are introduced then as

$$a(u,v) = \int_D K \nabla u \nabla v dx \tag{3}$$

$$L(v) = \int_D d \cdot v dx + \int_{\partial D} q \cdot v dx \tag{4}$$

respectively [15]. FEniCS automatically assembles the linear system of the equations, using the proper boundary conditions, solves and provides the flow potential ϕ of the aquifer.

Hermite Collocation

Let us consider a uniform partition into $N_x \times N_y$ squares of length h. The HC method seeks approximate solutions $u(x,y) \sim \phi(x,y)$ in the form:

$$u(x,t) = \sum_{i=1}^{2N_x+2} \sum_{j=1}^{2N_y+2} \alpha_{ij} \Phi_{ij}(x,y) \tag{5}$$

where $\Phi_{ij}(x,y) = \Phi_i(x)\Phi_j(y)$ are the bicubic hermite polynomials centered at node (x_i, y_j). For the evaluation of the unknowns $\alpha_{ij} \equiv \alpha_{ij}(t)$, $i = 1, \ldots, N_x + 1$ and $j = 1, \ldots, N_y + 1$ the Collocation method produces a system of ordinary differential equations by forcing the approximate solution $u(x,t)$ to vanish at $(2N_x+2) \times (2N_y+2)$ interior and boundary collocation points. The needed interior collocation points, known as Gauss Points, arise from the roots of Legendre Polynomial in each element $I_{ij} = [x_i, x_{i+1}] \times [y_j, y_{j+1}]$ are given by

$$\sigma^x_{2i-1} = \frac{x_i + x_{i+1}}{2} - \frac{h}{2\sqrt{3}} \quad , \quad \sigma^x_{2i} = \frac{x_i + x_{i+1}}{2} + \frac{h}{2\sqrt{3}}$$
$$\sigma^y_{2j-1} = \frac{y_j + y_{j+1}}{2} - \frac{h}{2\sqrt{3}} \quad , \quad \sigma^y_{2j} = \frac{y_j + y_{j+1}}{2} + \frac{h}{2\sqrt{3}}$$

Substituting, now, the approximate solution u(x,y) of (5) into the PDE (1), observing that each element has 16 degrees of freedom and assuming that K is scalar, the elemental equations may be written as:

$$K \sum_{k=2i-1}^{2i+2} \sum_{l=2j-1}^{2j+2} \alpha_{kl} \frac{\partial^2 \Phi_{kl}}{\partial x^2}(\sigma^x_K, \sigma^y_L) + \\ + K \sum_{k=2i-1}^{2i+2} \sum_{l=2j-1}^{2j+2} \alpha_{kl} \frac{\partial^2 \Phi_{kl}}{\partial y^2}(\sigma^x_K, \sigma^y_L) = (Q-N)(\sigma^x_K, \sigma^y_L) \tag{6}$$

for $K = 2i-1, 2i$ and $L = 2j-1, 2j$. Working as in [2] the elemental equations are expressed in the matrix form:

$$\sum_{k=2i-1}^{2i+2} \sum_{l=2j-1}^{2j+2} \alpha_{kl} \frac{\partial^2 \Phi_{kl}}{\partial x^2}(\sigma^x_K, \sigma^y_L) = \left(C^{(2)}_i \otimes C^{(0)}_j \right) \boldsymbol{\alpha_{ij}} \tag{7}$$

and equivalently,

$$\sum_{k=2i-1}^{2i+2} \sum_{l=2j-1}^{2j+2} \alpha_{kl} \frac{\partial^2 \Phi_{kl}}{\partial y^2}(\sigma^x_K, \sigma^y_L) = \left(C^{(0)}_i \otimes C^{(2)}_j \right) \boldsymbol{\alpha_{ij}} \tag{8}$$

where, $C_i^{(0),(2)}$, $C_j^{(0),(2)}$ are well defined in [1], [2] and $\boldsymbol{\alpha_{ij}} = \boldsymbol{\alpha_i} \otimes \boldsymbol{\alpha_j}$ for

$$\boldsymbol{\alpha_i} = [\alpha_{2i-1}(t)\ \alpha_{2i}(t)\ \alpha_{2i+1}(t)\ \alpha_{2i+2}(t)]^T \tag{9}$$

and

$$\boldsymbol{\alpha_j} = [\alpha_{2j-1}(t)\ \alpha_{2j}(t)\ \alpha_{2j+1}(t)\ \alpha_{2j+2}(t)]^T \tag{10}$$

Furthermore, the combination of the well known properties of hermite and the Boundary Conditions yields the relations:

$$\boldsymbol{\alpha_{1j}}(t) = \boldsymbol{\alpha_{(2N_x+2)j}}(t) = \boldsymbol{\alpha_{i2}}(t) = \boldsymbol{\alpha_{i(2N_y+2)}}(t) = 0 \tag{11}$$

Finally, the above elemental and boundary collocation equations lead to linear system of the form:

$$K\left(C^{(2)} \otimes C^{(0)}\right)\boldsymbol{\alpha} + K\left(C^{(0)} \otimes C^{(2)}\right)\boldsymbol{\alpha} = \boldsymbol{f} \tag{12}$$

where, of course,

$$\boldsymbol{f} = \left[f(\sigma_1^x, \sigma^y),\ f(\sigma_2^x, \sigma^y), \ldots, f(\sigma_{2N_x+2}^x, \sigma^y)\right]$$

for $f(x,y) = (Q-N)(x,y)$ and $\sigma^y = \left[\sigma_1^y,\ \sigma_2^y, \ldots, \sigma_{2N_y+2}^y\right]$.

C. Study area and numerical model development

The test area of this study is an homogeneous (in terms of hydraulic parameter values), almost rectangular aquifer, located at the area of Vathy, in the Greek island of Kalymnos. The aquifer is 7 km long ($L = 7000\ m$) and 3 km wide ($W = 3000\ m$) and is characterized by the following properties: $K = 100\ m/day$, $d = 25\ m$, $N = 30\ mm/year$, $Q_A = 20000\ m^3/day$, $(\underline{Q_i}, \overline{Q_i}) = (200, 2500)\ m^3/day$. In the aquifer area there are 5 active pumping wells located in the following spots: $x_i = (2640, 3340, 3920, 4620, 4860)\ m$, $y_i = (1560, 2200, 960, 2460, 1580)\ m$.

The well with the higher impact in the pumping procedure is the well No 1, the closest one to the saltwater interface, as it moves inward the aquifer. This is the critical well of the optimization procedure, as most of the ALOPEX's implied penalties will be on this active pumping location. So, the protection of this well is of the highest importance, because this way, we can automatically protect all the other wells of the aquifer. We note here, that for reasons explained in [25], we choose a guard point in front of every well (see Fig. 1), in a safety distance of $d_s = 400\ m$, preserving that way the stagnation points in front of all the wells and thus, creating stable pumping solutions.

As far as the boundaries are concerned, a Dirichlet boundary condition of fixed head equal to 0 m were applied along the coastline, at the left side of the aquifer, to simulate the sea boundary. On the upper, lower and right side of the aquifer, Neumann conditions where applied.

D. Pumping management

The objective in this study, is to maximize the groundwater withdrawal, while avoiding saltwater front entering into safe zones around all active wells. This task can be achieved by the following nonlinear optimization problem (cf. [25]):

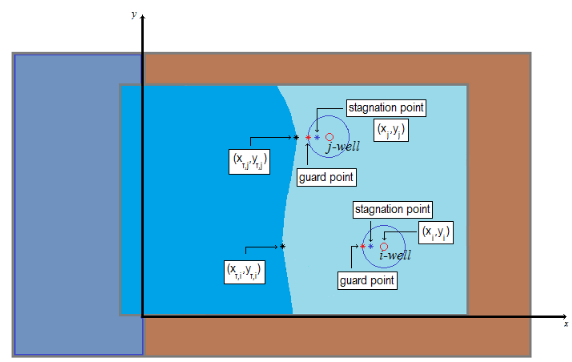

Fig. 1. Guard and stagnation points in front of an aquifer well.

$$\begin{aligned} maximize:\quad & P \equiv P(\boldsymbol{Q}) = e^{-\left[S(\overline{\boldsymbol{Q}})-S(\boldsymbol{Q})\right]^2/S^2(\overline{\boldsymbol{Q}})} \in [0,1] \\ s.t:\quad & 0 \le \underline{Q_i} \le Q_i \le \overline{Q_i} < Q_A, \\ & S(\boldsymbol{Q}) = \sum_{i=1}^{M} Q_i \le Q_A \\ & x_{\tau,i} \le x_i - d_s,\ i \in \{1,..,M\}, \end{aligned} \tag{13}$$

where Q_i , $i = 1,\ldots,M$ denotes the pumping rate of the i^{th} active well with coordinates (x_i, y_i), P is 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 recharge capabilities of the aquifer, $x_{\tau,i}$ is the x-coordinate of the saltwater's front in the neighborhood i^{th} well, d_s is a pre-specified safety distance (set equal to $400m$ in the present implementation) and M is the number of active wells in the region.

E. Constrained ALOPEX for pumping management

For the solution of the nonlinear optimization problem (13), described in the previous section, we employ the following ALOPEX V stochastic optimization algorithm coupled by a penalty system to enforce problem's constraints.

$$\mathbf{Q}^{(k)} = \mathbf{Q}^{(k-1)} + c_k \Delta\mathbf{Q}^{(k-1)} \Delta P^{(k-1)} + \mathbf{g}^{(k)}, \tag{14}$$

with

$$\begin{aligned} \Delta\boldsymbol{Q}^{(k)} &= \boldsymbol{Q}^{(k)} - \boldsymbol{Q}^{(k-1)} \\ \Delta P^{(k)} &= P(\boldsymbol{Q}^{(k)}) - P(\boldsymbol{Q}^{(k-1)}) \end{aligned} \tag{15}$$

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 [25].

F. The penalties management

In each ALOPEX V iteration step all control variables Q_i, $i = 1,\ldots,M$ are being rectified, if needed, via a two-phase penalty system, that is described in [25]. Phase one refers to the enforcement of the first two constraints described in (13), and precedes the Collocation or FEniCS's implementation, while phase two refers to the enforcement of the third *toe-constraint* described in (13), needs the trace of the saltwater interface and, thus, follows the Collocation or FeniCS's implementation. A 5% correction policy is also used here, to create the necessary agitation in every ALOPEX step, in order to help the algorithm to propose an new pumping solution, that is better than the one of the previous step and at same time within the predefined constraints of the problem.

III. Numerical simulations

In this section we present the results of the Collocation/ALOPEX and FEniCS/ALOPEX procedures in a typical run of 500 iterations, side by side with the analytical/ALOPEX approach, presented in our previous works [23], [24] and [25], for comparison reasons. We note that in all numerical simulations the wells numbering is considered to be numbered in a left-to-right fashion, namely $x_1 \leq \ldots \leq x_M$.

TABLE I
ANALYTICAL, COLLOCATION AND FENICS (IN COOPERATION WITH ALOPEX) PERFORMANCES:

Problem Parameters	*Analytical solution optimal values*	*Collocation optimal values*	*FEniCS optimal values*
k (*# iter.*)	161	383	446
$P(\boldsymbol{Q}^{(k)})$	0.62716	0.63195	0.63211
$Q_1^{(k)}$	209.75	201.16	202.62
$Q_2^{(k)}$	1089.32	317.34	695.46
$Q_3^{(k)}$	1069.24	1101.93	1303.02
$Q_4^{(k)}$	306.39	1342.76	376.06
$Q_5^{(k)}$	1287.18	1068.57	1457.01
$S(\boldsymbol{Q}^{(k)})$	3961.88	4031.76	4034.18

As it can be observed in Fig. 2, the proposed optimal solution in each case, corresponds to a set of pumping rates, that keeps all active pumping locations safe from saltwater intrusion. The saltwater front cannot infiltrate the safety zone created around every well, due to the activation of the constrains of the pumping procedure. The objective (profit) function in less than 50 iterations in all three cases (see Fig. 2c, 2d and 2e), reaches its maximum value, corresponding to an optimal pumping solution. Then, for the rest of the optimization procedure, it examines alternative but equivalent sets of optimal solutions, in order to find the global maximum of the profit function. Finally, we should comment that the ALOPEX is a stochastic optimization procedure, following every time a different path in order to find its optimal value, explaining that way the differences in the optimal pumping plans presented in the Table I above.

IV. Conclusion

In this study, we combined the Collocation and the FEniCS PDE solver modules with the latest constrained version of the ALOPEX stochastic optimization technique, in an attempt to maximize groundwater withdrawal, in the existing pumping well network in a coastal aquifer at the Greek island of Kalymnos. At the same time, we created a safe zone around every active well in the region, in order to create stable optimal solutions, as they are described in [25], and of course to protect the pumping locations from the saltwater intrusion phenomenon. The application of the Collocation and FEniCS modules successfully replaced the part of the analytical solution of the flow potential ϕ in our optimization algorithm, estimating the position of the saltwater front in every iteration step. This, ultimately, provides the option of the future examination of aquifers with more complex geometry, hydraulic parameters with spatial variability and in general, cases where the analytical solution of the flow potential is unknown. In summary, the numerical results presented in this work, shall well be considered as an encouraging first step to further investigation on the performance of the combination of the presented methods.

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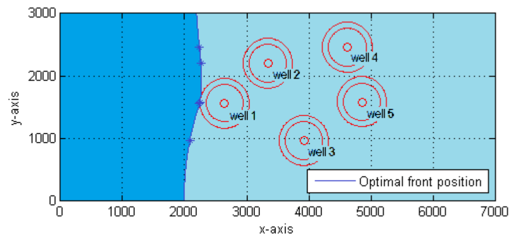
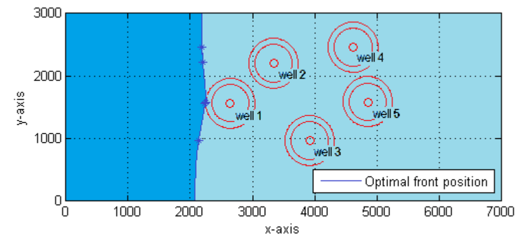
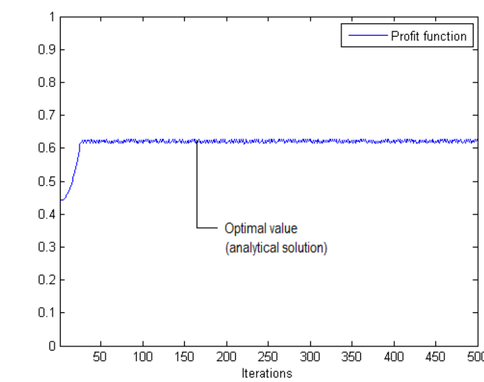


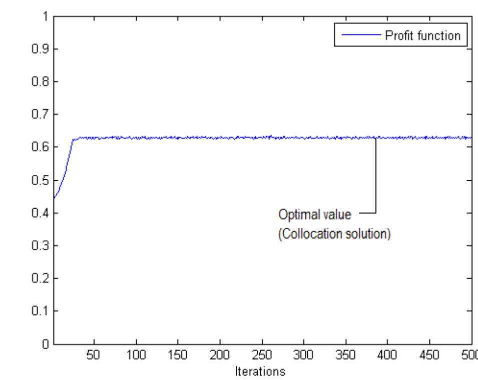
(a) Saltwater front using the analytical solution and the optimal pumping rates. All wells are kept safe from saltwater intrusion.



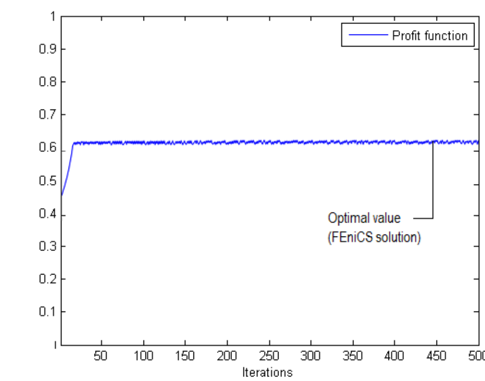
(b) Common saltwater front using the Collocation and the FEniCS methods, equipped with the optimal pumping rates. All wells are kept safe from saltwater intrusion.



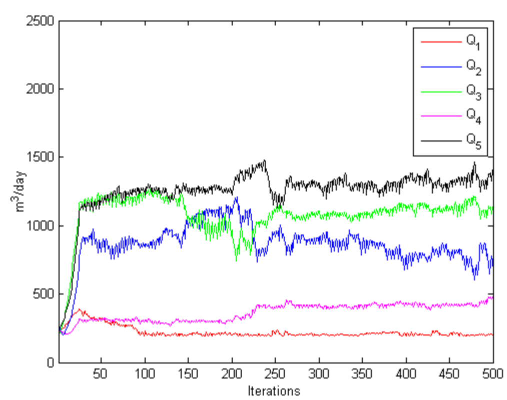
(c) Values of the profit function $P(\boldsymbol{Q}^{(k)})$, using the analytical solution.



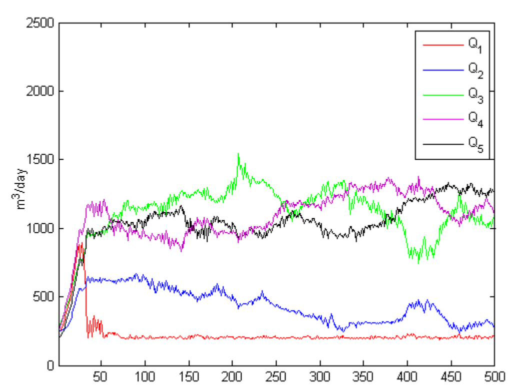
(d) Values of the profit function $P(\boldsymbol{Q}^{(k)})$, using the Collocation method.



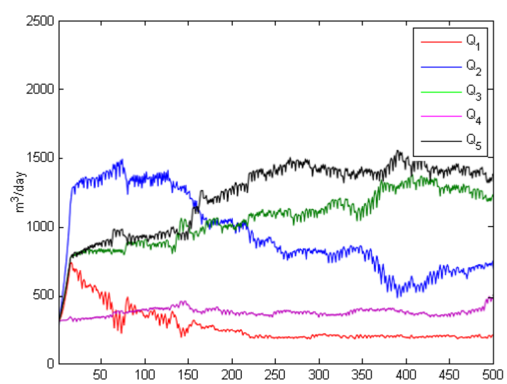
(e) Values of the profit function $P(\boldsymbol{Q}^{(k)})$, using the FEniCS method.



(f) Pumping rates Q_i, using the analytical solution.



(g) Pumping rates Q_i, using the Collocation method.



(h) Pumping rates Q_i, using the FEniCS method.

Fig. 2. Analytical solution and Collocation and FEniCS methods, in cooperation with the ALOPEX optimization algorithm performance, for the test case of Kalymnos aquifer with five active pumping locations in a typical run of 500 iterations.

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