Control of Nitrate Pollution using Optimization Techniques in Combination with Numerical Models

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Abstract: The over-exploitation of subsurface water, the non-rational use of fertilizers from the farmers and the continuous use of surface water conduce in the deterioration of the quality of fresh water that is used for potable and irrigation purposes. A declining quality of marine sediment is also reported in coastal regions due to a large number of uncontrolled pollutant sources. In the present work the mathematics of groundwater management are presented and, based on these, a developed methodology was applied to a heavily cultivated coastal aquifer in Korithian Gulf. First, the physical system is simulated using a 3-D numerical simulator for groundwater flow and mass transport and specifically in this work the Princeton Transport Code (PTC), was employed. Second, the numerical simulator is combined with the Outer Approximation Method in order to determine the optimal design of a groundwater management problem, related to the movement of the nitrate plume.

Key-Words: Nitrate pollution, Subsurface flow, Numerical Simulation, Optimization Methodology

1 Introduction

In the early ’50s numerical simulation models were presented in an attempt to obtain solutions for large problems of oil reservoirs. This effort was later expanded to address subsurface management problems related to groundwater ‘quality’ and “quantity”. These models couple and solve simultaneously the governing equations of groundwater flow, mass transport and chemical reaction.

The main objective of such models is to “predict” the groundwater movement and the contaminant transport through a subsurface system. In many cases these problems are very complicated and difficult to describe mathematically. The accurate description of the physical system, necessary for an optimal prediction to be obtained, requires a large volume of data. In addition, analytical solutions cannot be used due to the inhomogeneities, irregularities and uncertainties of the physical system. Therefore, numerical simulation must be employed. In the past, several numerical simulator models of groundwater flow and transport have been presented based on the theories of finite elements and finite differences (Sutra, Modflow, MD3d, PTC, FEMWATER, etc).

In the early ’70s groundwater numerical simulation models were combined with optimization techniques [1] and became a powerful tool for solving groundwater management problems. The motivation of the attempt to combine simulation with optimization was the desire to determine the ‘best’ solution (among several feasible solutions) that could be applied to a groundwater management problem. As indicated by Gorelick et al. [2], simulation models are often inadequate because the problems of aquifer management do not involve prediction alone. Rather, they involve both simulation, for prediction, and optimization. The role of optimization is to determine the best operating policy for a particular objective, taking into account the restrictions that exist on a site-specific basis. The combination of groundwater simulation and optimization techniques can be thought of as organized and methodical trial-and-error methods. However, in contrast to most trial-and-error approaches, the objective, constraints and solution search strategies are clearly specified. An optimization problem is formulated mathematically as a problem that minimizes or maximizes an objective function, subject to a set of constraints that are based on physical, economic, technical or social restrictions.

In the present work, first the mathematics of the groundwater management problem are presented followed by the proposed optimization technique. The numerical simulation model of the area of interest, where the proposed management methodology is applied, is also presented.

2 The Mathematics of Groundwater Management Problems

Groundwater management problems can be very simple or very complicated. This depends on the formulation of the problem. A groundwater management problem with a linear objective function and a linear set of constraints is characterized as a simple problem and is relatively easy to solve. Problems where the decision variables do not appear in any power and/or in a product form have linear behavior. The geometric representation of a linear objective function or constraint is a straight line for problems with one decision variable (one-dimensional problems, 1-D), a plane for 2-D problems, or a hyperplane for multi-dimensional problems (Fig. 1).

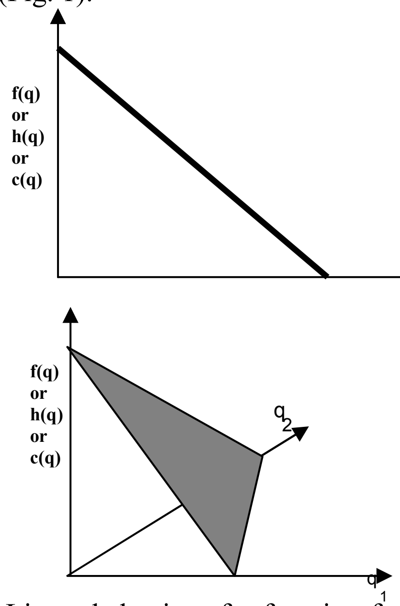

Figure 1: Linear behavior of a function for 1-D and 2-D problems

The most complicated form of groundwater management problems appears when either the objective function or any of the constraints are nonlinear. Typical examples for 1-D and 2-D problems are shown in Fig. 2.

In most practical cases, hydraulic head and hydraulic gradient constraints have linear behavior with respect to the pumping rate. If the objective function is also linear, the management problem is characterized as linear. Linear problems involve only flow equations in the numerical simulation. It should be noted that, in order for the above constraints to exhibit linear behavior, the aquifer has to be in steady state (no changes with time). These problems can be solved using classical linear programming techniques (simplex method). Several software packages exist to solve problems in this category (Lindo, Minos, Modman).

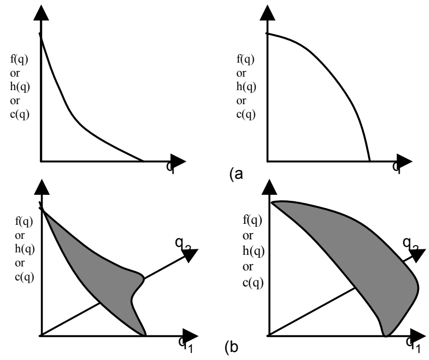

Figure 2: Nonlinear behavior of a function for 1-D (a) and 2-D (b) problems

Groundwater management problems that involve concentration constraints are nonlinear problems (since the mass transport equation has a nonlinear behavior) and are known as "*groundwater quality management problems*". In this case the objective function can be either linear or nonlinear. This kind of problems is more difficult to solve due to the nonlinear behavior. Several methodologies for the solution of nonlinear groundwater management problems that have been developed in the past few years will be presented in a later section. The degree of difficulty in solving nonlinear groundwater management problems using optimization techniques is mostly dependent on the behavior of the objective and constraint functions. Regarding the objective function, the mathematical formulation can be either minimization (e.g., minimization of the total pumping cost) or maximization (e.g., maximization of the total pumping) of the function. The objective function can be linear or non-linear. A nonlinear function can be continuous or discontinuous, convex or non-convex (concave), monotonic or non-monotonic. Some typical examples are presented in Fig. 3.

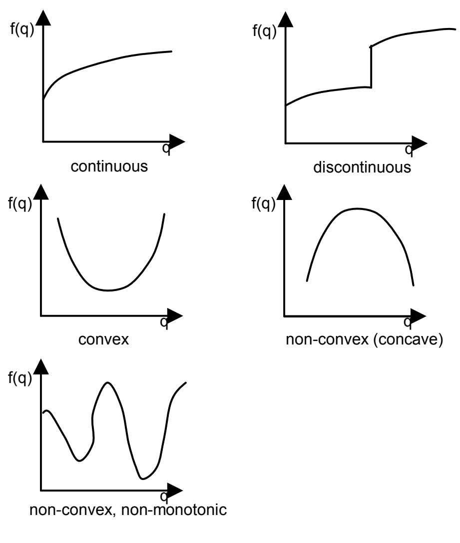

Figure 3: Typical behaviors of an objective function

The most complicated case is the non-convex, non-monotonic function where most of the optimization techniques have difficulties to determine the "global optimal" and, instead, terminate the process at a local optimal. Fig. 4 illustrates the concept of local and global optima.

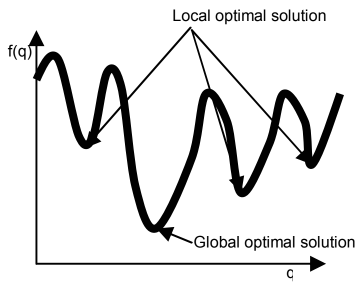

Figure 4: The concept of local and global optimal in a minimization problem

The constraint functions can also be linear or non-linear, convex or non-convex. The geometric representation of the constraint functions is illustrated in Fig. 5.

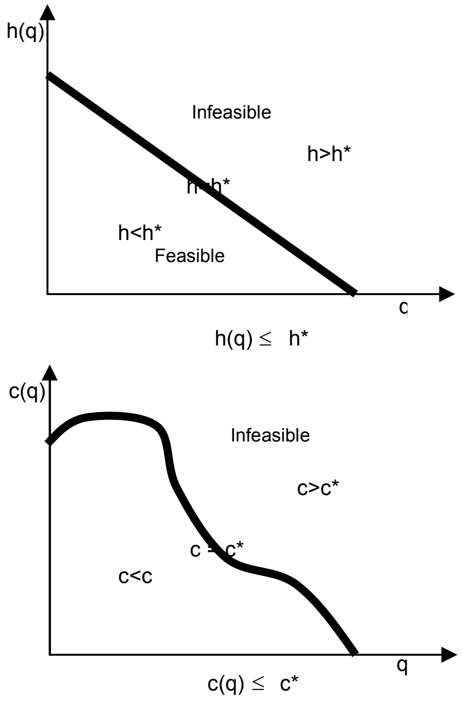

Figure 5: Geometrical representation of the constraints

In case that the problem has several constraints the *feasible region* is defined as the intersection of all the constraints. The objective function is imposed over the feasible region defined by the set of constraints. The optimal solution must be either inside the feasible region or along the perimeter of this region (Fig. 6).

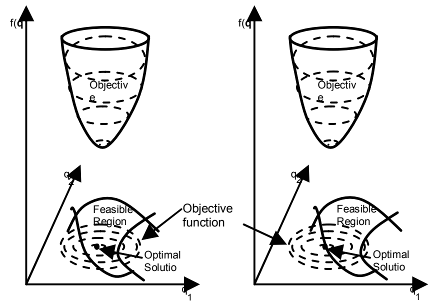

Figure 6: Geometric representation of the objective function, feasible region and optimal solution for a 2-D minimization problem.

Several optimization techniques using linear and non-linear programming theory have been presented in the past to solve this kind of problems. The optimization techniques are combined with groundwater numerical models of groundwater flow and mass transport.

In the present work the Outer Approximation Method, first presented by Karatzas and Pinder ([3] and [4]) has been used in combination with the Princeton Transport Code [5] for the simulation of the groundwater flow and the contaminant transport.

3 The Optimization Method of the Outer Approximation

The optimization model employed in this work is the Outer Approximation Method, first presented by Karatzas and Pinder ([3] and [4]). This methodology has been expanded by Karatzas et al. [6] and Papadopoulou et al. ([7] and [8]) concerning time-varying multiperiod and post remediation design. The method is a global minimization technique that uses a cutting plane approach to determine the optimal solution. The algorithm starts by determining a polytope that encloses the feasible region, which is defined by a set of vertices. The feasible region is determined as the space where all the constraints are satisfied.

The objective function, the function to be minimized, is formulated as a concave function. Based on the characteristic property of concave functions, that the minimum always occurs at one of the most outer points of the feasible region, the algorithm determines the vertex of the enclosing polytope that minimizes the objective function. Next, it examines if the selected vertex is feasible. If all constraints are satisfied, it declares this vertex as the optimal solution. Otherwise, a cutting plane is introduced that eliminates this vertex and its surroundings, creates a new enclosing polytope that is a better approximation of the feasible region and the process is repeated. The goal of this process is not to determine the best approximation of the feasible region but rather to determine the most extreme point of the feasible region without eliminating any part of it (Fig. 7).

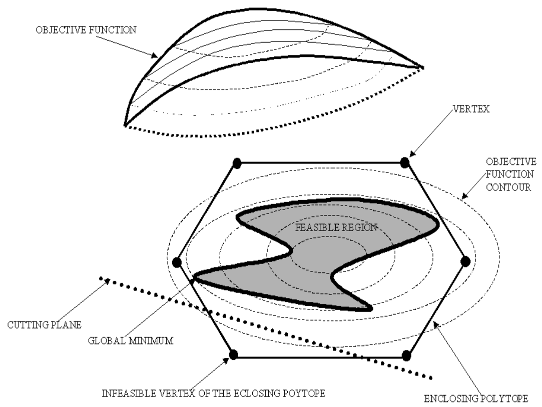

Figure 7: The concept of the Outer Approximation Method

The Outer Approximation method takes advantage of the concave shape of the objective function that ensures that the minimum of such a function over a compact convex or non-convex set (feasible region) occurs always at the boundary of the feasible region. The problem has the following formulation:

$$\mathbf{min}\ \ f(\mathbf{x}) \quad such \quad that \ \ \mathbf{x} \in D, \mathbf{x} \geq 0 \tag{1}$$

where

x: the vector of decision variables,

f: $R^n \rightarrow R$ a real-valued continuous concave function defined throughout R^n,

D: A closed non-convex subset of R^n defined by a set of m constraints of the following form:

$$g_i(\mathbf{x}) \leq 0 \qquad i = 1,\ldots, m \tag{2}$$

where

$g_i(\mathbf{x})$: continuous convex or non-convex real-valued functions.

The Princeton Transport Code (PTC) is a three-dimensional groundwater flow and contaminant transport simulator which can use both finite-element and finite-difference discretization. It can create and process up to 2000 elements. PTC is written in FORTRAN 77, thus can be easily applied in combination with Argus ONE, in a user-friendly Windows environment ([9] and [10]). PTC uses the following system of partial differential equations to represent the groundwater flow described by hydraulic head h, the groundwater velocity components, and contaminant transport described by concentration C.

$$\nabla \bullet (K \bullet \nabla h) - S\frac{\partial h}{\partial t} - Q_i = 0 \tag{3}$$

$$q + K \bullet \nabla h = 0 \tag{4}$$

$$\theta R_f \frac{\partial c}{\partial t} + q \bullet \nabla c - \nabla \bullet (D \bullet \nabla c) - Q_i (c - c_o) = 0 \tag{5}$$

where $\boldsymbol{K}$ hydraulic conductivity tensor [LT^{-1}], h hydraulic head [L], S specific storage coefficient [L^{-1}], Q_i source/sink term at location i [L^3T^{-1}], q groundwater velocity (Darcy's) [LT^{-1}], θ effective porosity, R_f retardation coefficient, c concentration of contaminant at location (x,y,z) at time t [M/L^3], $\boldsymbol{D}$ dispersion tensor.

PTC employs a unique splitting algorithm for solving the fully three-dimensional equations, which reduces the computational burden significantly. The algorithm involves discretizing the domain into approximately parallel horizontal layers. Within each layer a finite element discretization is used allowing for accurate representation of irregular domains. The layers are connected vertically by a finite difference discretization. This kind of approximation of the domain, in two different directions (vertical and horizontal), has a lot of advantages, since it significantly reduces the number and the size of the calculations needed. [5]

4 Field Application

4.1 Model setup

The area of the present study covers the majority of the coastal zone of the Corinthian Prefecture (an area of 60 Km^2, approximately). The boundaries of the area are defined by the sea to the North and by a fault zone to the South, which coincides with the Old National Road from Lexeon to Asopos River. The Corinthian basin contains alluvial deposits of mixed fluvial, lacustrine and terrestrial origin [11].

There are several pumping wells shown in Fig.9 (the squares).

Figure 8: Geological characteristics of modeled area

The hydraulic head distribution, shown in Fig. 9, represents the flow field in October 2002 and is based on field measurements, performed during the period October 2000 and March 2001. The extended use of fertilizers contaminated the modeled aquifer at three main locations. The aquifer situation regarding nitrate mass distribution prior to any management plan is shown in Fig. 10. At areas where the nitrate concentration is higher than 50ppm, the groundwater is unsuitable for drinking and irrigation purposes [12].

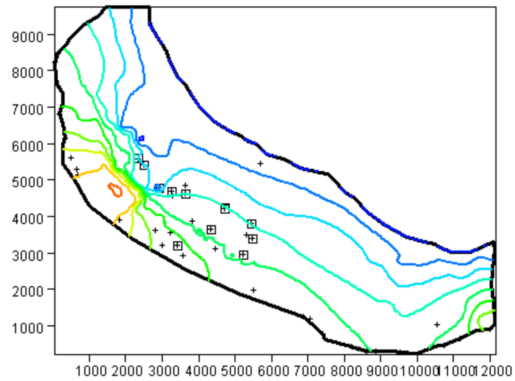

Figure 9: Hydraulic head distribution in October 2002

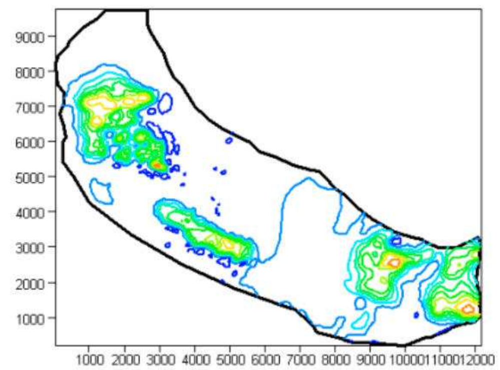

Figure 10: Nitrate mass distribution prior to any management plan

4.2 Results[1]

In this paper, a management strategy for the optimal operation of the 7 extraction (e1-e7) and 5 injection (in1-in5) wells is proposed using the above methodology, in order to prevent further spreading of the nitrate plume towards the inland pumping locations. For these purposes, a series of constraints are imposed at 7 observation locations (o1-o7) where the nitrate concentration should not exceed a pre-specified value (Fig. 11). The aim of these observation locations was to protect the existing municipal pumping wells, assuming that during the two-year remediation period there is not any additional nitrate load into the aquifer.

The aim of the proposed remediation design is the containment of the plume at the October 2002 levels, preventing further spread of the plume. The proposed remediation design activates 3 out of 12 remediation wells at the southeastern plume (Fig. 12).

The proposed remediation design requires activation of the extraction well # 7 (429.6 m^3/day) and the injection wells # 4 (2826.3 m^3/day) and #5 (2000 m^3/day). The activation of these three is due to the hydraulic gradient at this area that is more severe and dominates the movement of the plume [13].

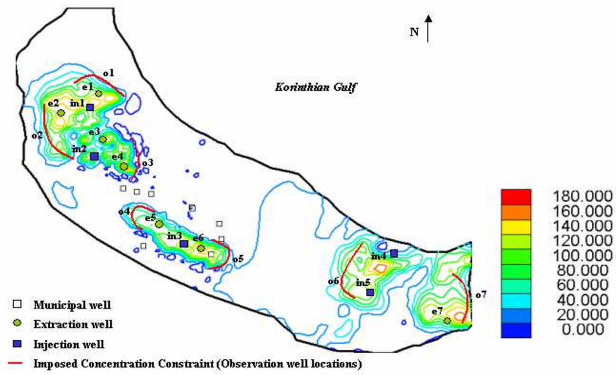

Figure 11: Remediation design

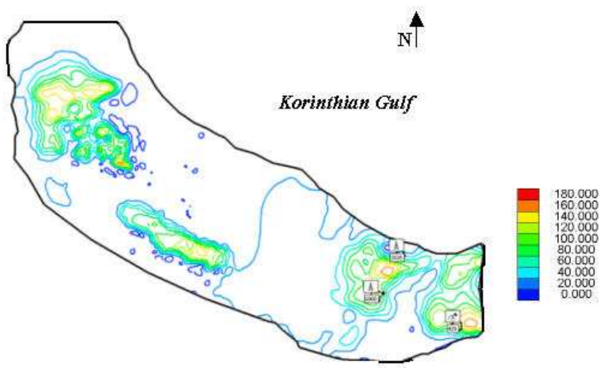

Figure 12: Locations of the active remediation wells

5 Conclusions

By applying the proposed methodology, a remediation design that prevents further spreading of the existing three major nitrate plumes, without deteriorating the subsurface water quality at areas that have not been contaminated until the October of 2002, has been achieved. However the proposed design lead only to the anticipation of further contamination of the aquifer, assuming that any use of chemical fertilizers has been eliminated, and not to the restoration of the aquifer.

The development of methodologies that ensure the rational and optimal management of the subsurface water resources, will allow the containment of the nitrate pollution in aquifers that are heavily cultivated. A remediation design that will propose an integrated management strategy for all the municipal and remediation wells is necessary in order to obtain improvement of the subsurface water quality.

References:

[1] Deninger R A., Systems analysis of water supply systems. *Water Resour. Bull.* 6: 573–579, 1970.

[2] Gorelick, S.M., R.A. Freeze, D. Donohue, and J.F. Keely. *Groundwater Contamination: Optimal capture and containment,* Lewis Publishers, Chelsea, Michigan, 385 p., 1993.

[3] Karatzas G. P. and G.F. Pinder, Groundwater management using numerical simulation and the outer approximation method for global optimization, *Water Resoures Research*, 29(10), 3371–3378, 1993.

[4] Karatzas G. P. and G.F. Pinder, The solution of groundwater quality management problems with a nonconvex feasible region using a cutting plane optimization technique, *Water Resources Research*, 32(4), 1091– 1100, 1996.

[5] Babu D.K. and G.F. Pinder, A Finite Element–Finite Difference Alternating Direction Algorithm for 3-Dimensional Groundwater Transport, *Advances in Water Resources*, 7(3), 116-119, 1984.

[6] Karatzas, G.P., Spiliotopoulos, A.A., Pinder, G.F., A multiperiod approach for the solution of groundwater management problems using the outer aoximation method, *Proceedings of the North American Water and Environment Congress '96 American Society of Civil Engineers*, CD-ROM, 1996.

[7] Papadopoulou, M.P., Pinder, G.F., Karatzas, G.P., Enhancement of the outer approximation method for the solution of concentration-constrained optimal-design ground-water-remediation problems *Water Resources Research*, 39 (7), 1185 doi: 10.1029/2002WR001541, 2003.

[8] Papadopoulou, M.P., Pinder, G.F., Karatzas, G.P., Flexible Time-Varying Optimization Methodology for the Solution of Groundwater Management Problems, *European Journal of Operational Research*, Vol. 180, No. 2, pg. 770-785, doi: 10.1016/j.ejor.2006.02.041, 2007.

[9] Babu D.K., G.F. Pinder, A. Niemi, D.P. Ahlfeld, and S.A. Stothoff, Chemical Transport by Three-Dimensional Groundwater Flows, Princeton University, 84-WR-3, USA, 1997.

[10] Pinder G.F., *Groundwater Modelling using Geographical Information Systems*, John Willey & Sons, Inc., New York, 2002.

[11] Psarropoulou, E. and G.P. Karatzas, Field Studies of Nitrate Mass transfer in the Coastal Aquifer of Corinth, Greece, *Conference Proceedings*, Syros, September 2001.

[12] Dokou Z, A. Mouskeftara A., and D. Pagkalou , *Groundwater Flow and Nitrate Transport in the Korinthian Gulf Aquifer,* undergraduate Thesis, Dept. of Environmental Engineering, Technical University of Crete, 2002 (in Greek).

[13] Mirasgedis D., *Groundwater Remediation using Combination of Numerical Simulation and Optimization – A Field Application*, undergraduate Thesis, Dept. of Environmental Engineering, Technical University of Crete, 2003 (in Greek).