Groundwater clean-up: the optimization perspective

M. da Conceição Cunha

Instituto Superior de Engenharia de Coimbra
Quinta da Nora - 3000 Coimbra - Portugal

Abstract

There are many sources of groundwater petroleum hydrocarbon contamination. When groundwater is to be used for drinking purposes, irrigation, etc. it is necessary to evaluate the extent of contamination. The design of monitoring networks to provide initial detection of groundwater contamination is therefore very important. Nevertheless, in many situations it is also necessary to use clean-up techniques to restore the quality of groundwater. How to design a monitoring network and a remediation system are two problems addressed in many research studies published in the literature. Optimization methods play an important role in finding the best decisions regarding the two problems. This paper presents a synthesis of the optimization models reported in the literature on this subject. Through this presentation, both the mathematical characteristics of these models, and the adequacy of the optimization methods employed, which range from classical mathematical programming to modern heuristics are discussed.

1 Introduction

Contamination of groundwater resources is becoming a serious environmental problem. Regarding the petroleum hydrocarbon, there are many sources of contamination: underground or above-ground storage tanks, tanker trucks, transfer terminals, pipelines, refineries, etc. When groundwater is to be used for drinking purposes, irrigation, etc. it is necessary to evaluate the extent of contamination and to use appropriate remediation techniques. An important aspect of groundwater protection is the implementation of monitoring networks designed to detect the earliest stages of contamination, thus reducing the costs of subsequent remediation. Huge investments are usually needed to establish the monitoring networks, and, indeed, to contain or to clean up contaminated
groundwater. It is therefore important that the measures employed to achieve these ends have been developed by means of tools that can properly identify the most cost-effective ones. Optimization techniques can obviously play an important role here. The literature shows that during the last fifteen years a great deal of work has been done on this subject. The application of optimization techniques to reduce remediation costs has become an area of active research, and much progress has been made in the development of mathematical optimization models for groundwater management and remediation. This paper presents a synthesis of the optimization models reported in the literature on this subject, and discusses both their mathematical characteristics and their suitability.

2 Model formulation

The decisions to be taken regarding groundwater protection and clean-up involve the location, size and operation of the infrastructures needed to evaluate the extent of the contamination and/or to implement a remediation programme. A contamination problem may consider different strategies (Morgan et al.): isolation of the contaminated plume, physical removal of the contaminated water and soil, in situ treatment of contaminants in the aquifer, hydraulic removal of the polluted water, etc.

A general formulation for an optimization model aiming at finding the best decisions to implement in this field can be written as:

\[
\text{Min } C_f + \sum_{t=1}^{T} C_{vf}(Q_t, H_t, CN_t)
\]

- \(C_f\): capital/fixed costs of well installation and/or treatment plants
- \(C_{vf}\): operation/variable costs of remediation strategy during management period \(t\)
- \(Q_t\): pumping rates during management period \(t\)
- \(H_t\): hydraulic heads in period \(t\)
- \(CN_t\): concentration level in period \(t\)
- \(T\): total number of management periods.

subject to:

\[
L_f(Q_t, H_t, CN_t) \leq 0, \quad t = 1, \ldots, T
\]

The constraints on the optimization problem \(L_f\) usually concern water quality, hydraulic head and pumping rates, and so flow and mass transport equations should be considered. The objective function usually representing cost minimization incorporates different types of costs, namely, drilling and installation costs, plus those involving extracting and treating the contaminated groundwater, and, finally, the costs of treatment plants. In general, the model defined above is non-linear mixed-integer. The resolution of such a model is extremely complicated because of its mathematical nature and the dimensions.
encountered in real-world models. Coupling the simulation model for evaluating heads and concentrations with the optimization model still is a subject of research. Flow and mass transport equations do not have analytical solutions for most real-world problems. Therefore it is necessary to resort to numerical models. Methods such as the embedding approach and response matrix approach have been used to incorporate physical aquifer behaviour into the decision models. Remediation strategies can be determined considering either steady state or time-varying policies. The model size for each case will be quite different and will have consequences on computational effort. The way the capital costs are handled also has a strong impact on the choice of the solution method. In the past, the capital costs were sometimes ignored to simplify the optimization models. But capital costs are a significant portion of the total costs, especially for remediation over a shorter number of periods. Aspects like uncertainty relative to aquifer parameters can also give rise to different kinds of models.

3 Literature review

Already mentioned, many factors may influence the resolution of optimization models for remediation purposes, which is why many different optimization methods have been tried. This section comprises a literature review, with emphasis on the mathematical characteristics of the models, as well as the capabilities of the optimization methods employed. Methods ranging from classical mathematical programming (linear, nonlinear, dynamic programming, optimal control, etc.) to those of modern heuristics (genetic, simulated annealing, tabu search, and neural networks algorithms) are analysed.

3.1 Classical methods

Wagner and Gorelick\cite{Wagner1990} and Ahlfeld et al.\cite{Ahlfeld1989} used nonlinear programming to minimize the pumping rates in a remediation problem. This objective was assumed to represent the minimization of the total operating costs, as well as the implicit minimization of the capacity of the treatment plant. However it cannot represent the capital costs of wells, because drilling costs can be much more important than costs related to pump size.

Sawyer and Ahlfeld\cite{Sawyer1993, Sawyer1996} developed a mixed integer linear programming model that considered a simplified version of the cost function of extraction and/or injection strategy, including the linear costs of well installation and operation. Sawyer and Lin\cite{Sawyer1995} extended this model to incorporate both uncertainty in groundwater simulation models and in the cost coefficients used in the objective function. Chance-constrained programming was applied, and the model thus became a nonlinear mixed-integer model. Those results are compared with the results of deterministic linear (where capital costs are neglected) and integer formulations. The use of a linear model produces an optimal solution where five wells are used instead of the one or two wells encountered in the other models. It is the result of not considering capital costs. Taking into account reliability increases the amount of water to be pumped. Morgan et al.\cite{Morgan1998} developed a mixed-integer-linear-chance-constrained programming method in order to find the globally optimal trade-off curve for maximum reliability versus a minimum
pumping objective in a pump-and-treat scheme. The uncertainty of the physical aspects (hydraulic conductivity) was incorporated through the coefficients of the constraints for a steady-state case. The remediation costs were only dependent on the total pumping rates at the wells. In linear models, constraints regarding contaminant concentrations cannot be considered directly because the inclusion of this physical aspect into an optimization model implies the formulation of a nonlinear model.

Many dynamic programming models define optimal policies over a set of management periods, only taking into account operating costs. In fact, dynamic programming requires the separability of the objective function between management periods, because the decisions in each period are obtained relative to the state at the beginning of the period, paying no heed to decisions in other management periods. That is the reason for the difficulties of incorporating capital costs in this approach. An important group of papers (Andricevic and Kitanidis, Chang et al., Culver and Shoemaker for pump-and-treat problems; Minsker and Minsker and Shoemaker for bioremediation problems) uses a variant of differential dynamic programming called successive approximation linear quadratic regulator (SALQR). It is a two-phase iterative optimization method that enables different time periods to be considered. In the first phase the algorithm runs the finite-element groundwater simulation model. The second phase, taking into account the effects of the pumping strategy obtained in the first phase, determines the derivatives of the objective function and transition equations to improve that strategy. The iterative procedure stops once the convergence to an optimal pumping strategy occurs (for more details of this algorithm see Culver and Shoemaker). The conclusions reveal that time-varying policies are more cost-effective than time-invariant policies. However, these models only examine operating costs of pumping and treatment. While in steady state models the minimization of operating costs may implicitly minimize the capital costs concerning the treatment plant, if the capital costs of treatment plants are not taken into account in the decision models for time varying policies using dynamic programming, this could define a shorter remediation period with the need for large treatment plant capacity. Mansfield and Shoemaker explored the sparsity of a finite-element model within an optimization model using the SALQR approach, in order to reduce the computational effort. Mansfield and Shoemaker present exact derivative equations and the corresponding computationally-efficient approximations regarding unconfined aquifers. This type of aquifer is much more complex due to its nonlinear flow dynamics than the confined aquifers previously studied by these authors. Culver and Shoemaker described a model to determine dynamic policies using a control theory algorithm, quasi-Newton differential dynamic programming (QNDDP), in conjunction with a finite-element groundwater simulation model. Even if some capital costs were included (the treatment facility costs as a function of the peak operating rate), costs related to the well field could not be incorporated into the decision model. The conclusions show that for short time-varying policies (about six months or less), the consideration of treatment plant capital costs has a tremendous impact on the optimal policies selected. For large management periods the consideration of such costs only had a slight effect. Yoon and Shoemaker compared three major classes of algorithms
Oil and Hydrocarbon Spills II: Modelling, Analysis and Control 133

(evolutionary algorithms, direct search methods and derivative-based optimization methods) that can be used to identify the most cost-effective policy for bioremediation problems. Their results make it apparent that SALQR was the fastest algorithm, but one of the evolutionary algorithms tried (using a derandomized evolutionary strategy) yielded a very good combination of both speed and accuracy.

Lee and Kitanidis\textsuperscript{14} included the capital costs of treatment in a dynamic control model by using regression equations to predict the annualized capital costs as a function of total pumping rates.

Some works include capital costs of well installation in steady-state remediation problems. This entails representing the discontinuous fixed cost function by a continuous function containing the fixed cost multiplied by a penalty. That penalty coefficient will be zero or one, depending on whether the well is to be built or not. McKinney and Lin\textsuperscript{19} used a polynomial penalty coefficient. Karatzas and Pinder\textsuperscript{12,13} used an outer approximation method to solve a concave non-linear remediation model where they considered a continuous cost function with an exponential penalty coefficient. McKinney and Lin\textsuperscript{21} compared the polynomial penalty coefficient method and the exponential penalty coefficient method. They noticed that the first method gave less expensive designs and was less time consuming than the second one. It should be emphasized that the consideration of capital costs for the well field and for the treatment process have a significant impact on the design achieved. In fact, the costs obtained were less in comparison with those given by other models that do not include capital costs. This reduction is due to the characteristics of the design obtained (fewer wells but larger flow rates). McKinney and Lin\textsuperscript{22} proposed the penalty coefficient method as a means to incorporate the capital costs into a nonlinear model, for homogeneous and heterogeneous conditions. The consideration of heterogeneity produced different well locations and pumping rates. Even if these methods could accommodate capital costs, their use to define time-varying policies would require an important extra computational effort.

3.2 Modern heuristics

The methods considered in this context (simulated annealing, genetic algorithms, tabu search and artificial neural network) can very easily explicitly include capital costs. In fact they do not require derivatives with respect to decision variables as is needed in nonlinear programming. Discrete variables representing capital costs can therefore be included in the decision models.

Simulated annealing is inspired by the physical annealing process. The randomized nature of the procedure permits asymptotic convergence to optimal solutions under mild conditions (Aarts and Korts\textsuperscript{1}, Reeves\textsuperscript{3}, Aarts \textit{et al.}\textsuperscript{2}). Dougherty and Marryott\textsuperscript{8} used simulated annealing to find the optimal design, considering constant capital costs for well installation and linear cost for the operation. The approach has been applied to several hypothetical scenarios and its ability to handle multiple technologies has been demonstrated. Marryott \textit{et al.}\textsuperscript{18} presented the application of the same approach to a real-world problem. Meyer \textit{et al.}\textsuperscript{23} described a multiobjective model, taking uncertainty into account, to design a monitoring network aiming to minimize the number of monitoring
wells, to maximize the probability of detecting a contaminating leak and to minimize the expected area of contamination once detected. The model was solved by a simulated annealing algorithm that performed well when dealing with the large number of realizations considered in the Monte Carlo simulation of groundwater flow and contaminant transport. A clear trade-off among the three objectives was observed.

Genetic algorithms use concepts from population genetics and evolution theory. They also are randomized algorithms, but convergence is supported by empirical evidence only (Goldberg\textsuperscript{10}, Reeves\textsuperscript{31}, Mühlenbein\textsuperscript{28}). Genetic algorithms were used by Ritzel \textit{et al.}\textsuperscript{32} for solving a multiobjective groundwater contamination problem in steady-state context, considering well installation costs. Using genetic algorithms, McKinney and Lin\textsuperscript{20} included capital costs regarding the treatment facility, as well as well installation cost to define a steady-state policy in a pump-and-treat problem. The results were found to be as, good as or better than, those determined by linear or nonlinear programming.

Tabu search is inspired by the human memory process. It combines a deterministic iterative improvement procedure with a possibility of overruling the requirement for strict improvement (Reeves\textsuperscript{31}, Hertz \textit{et al.}\textsuperscript{11}, Glover and Laguna\textsuperscript{9}). Zheng and Wang\textsuperscript{39} used tabu search coupled with linear programming to solve a remediation design problem. Well installation costs were considered. They found that the maximum number of wells allowed has an important impact on the final costs. Lee and Ellis\textsuperscript{15} compared eight heuristic algorithms used to define the optimal design of a groundwater monitoring network. They tested heuristics of two kinds: modern heuristics (simulated annealing, genetic algorithms and tabu search) and conventional heuristics (involving sequential exchange search algorithms). They further evaluated a Nelder and Mead's downhill simplex method. In their conclusions they pointed out the superior performance of the simulated annealing and the tabu search heuristics.

Artificial neural networks (Peterson and Soderberg\textsuperscript{29}) are derived from the structure of biological neural networks. The optimal solutions are not obtained by the full or partial evaluation of the solution space, but by using a statistical interpretation of the results, which in a fuzzy manner will point the way to good solutions. Rogers and Dowla\textsuperscript{33} solved a model including the capital costs of pipes connecting the wells to the treatment facility by means of artificial neural networks (a hybrid artificial neural network genetic algorithm). Ranjithan \textit{et al.}\textsuperscript{30}, kept in mind the fact that the uncertainty due to groundwater parameters should be considered when designing groundwater remediation strategies. They described a neural network-based approach for reducing the computational effort needed to establish a reliable design by identifying the critical realizations that would have the most influence on the final solution.

4 Conclusions

Concern about groundwater pollution problems has led to the development of many research studies aiming at finding the least-cost strategies for remediation purposes. The variety of methods used to solve the corresponding optimization models is proof of the complexity of such problems. Simplifications have sometimes been introduced in such models to make it possible to apply various
mathematical programming techniques. In some cases the capital costs for well installation and treatment plants were ignored and the nonlinear or linear programming (if the operating costs functions were linear) was used. Other studies take into account the capital costs but consider a linear version of the cost functions, and so linear mixed-integer programming was the method applied. Optimal control permits the determination of dynamic policies over a set of remediation periods, but has some difficulties in accommodating capital costs. Even if modern heuristics present some difficulties in solving time-varying optimization models, because of the increased of the computational effort, yet they can easily handle the incorporation of all kinds of costs, whether they are capital or operation costs.

The developments achieved through the research carried out in these last few years indicates the big effort made towards finding global optimal solution of models that incorporate all the aspects present in remediation groundwater problems (uncertainty, realistic cost functions, time-varying strategies, etc.)

References


