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EMPLOYING EVOLUTIONARY ALGORITHMS FOR OPTIMIZING FREE PHASE LNAPL RECOVERY

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Summary. A non-linear, multi-objective optimization method is presented that seeks to maximize free product recovery of light non-aqueous phase liquids (LNAPLs) while minimizing operation cost. This approach combines FEHM (Finite Element Heat and Mass transfer code), a groundwater model that can simulate LNAPL transport in the subsurface, with two evolutionary algorithms: the genetic algorithm (GA) and the differential evolution (DE) algorithm. The proposed optimal free phase recovery algorithm is tested using data from a field site contaminated with LNAPLs, located near Athens, Greece. The results obtained using the two evolutionary algorithms (GA and DE) are presented and discussed.

1 INTRODUCTION

Numerous industrial sites worldwide have been contaminated by light non-aqueous phase liquids (LNAPLs) such as petroleum hydrocarbons (oil, gasoline, diesel etc) and organic solvents. LNAPL migration is a complex process that is affected by various parameters such as: gravity forces (vertical migration), capillary forces (horizontal spreading), aquifer heterogeneity, type of spill and the presence of fractures[1]. During the vertical migration of LNAPL some will remain behind, trapped in the vadose zone (residual saturation). When LNAPL reaches the capillary zone it accumulates, creating an oil table that rests directly above the water table, often causing a depression on the water table due to its weight[2]. Finally, some of the LNAPL partitions into the groundwater through dissolution causing long-term groundwater contamination[1].

Successful remediation of the contaminated sites can prove to be a costly and time consuming task. To this end, researchers have directed their efforts on developing tools that can improve the time-efficiency and cost-effectiveness of groundwater remediation strategies. Such tools are algorithms that couple groundwater contaminant transport simulation models with optimization techniques. Since LNAPL remediation process involves different tasks, such as cleanup of residual LNAPL phase, free-product recovery and removal of the dissolved phase, various techniques have been developed to accomplish the optimization of each task. In recent years, most researchers focused on optimizing the removal of LNAPLs dissolved in groundwater using the pump and treat method that has been the most commonly used remediation strategy[3-16]. A number of studies were also devoted to optimizing bioremediation designs[17-22]. Others optimized different remediation techniques like bioslurping[23], bioventing[24] and soil vapor extraction (SVE) method[25].

There are a few studies that attempted to optimize free product recovery of LNAPLs. Specifically, Cooper et al. [26] presented a methodology for optimizing free product recovery from a single well that combines simulation, nonlinear regression and optimization (using MINOS), neglecting the economical aspects of the problem was proposed. Qin et al.[27] also coupled numerical modeling, a multivariate regression method and a genetic algorithm to optimize a vacuum enhanced free product recovery (VFPR) process. Their method included environmental and economical effects and provided a means to analyze the tradeoffs between them. A related work by Qin et al.[28] optimized a similar process namely the dual phase vacuum extraction (DPVE) using a multiphase flow simulator and cluster analysis in conjunction with a genetic algorithm to solve a multiobjective optimization problem. An extensive literature review of the recent developments associated with optimization techniques applied to site remediation is available by Mayer et al. [29] and Qin et al.[30].

As a continuation of the work performed previously, the focus of this paper is to develop a simulation-optimization model that couples a multiphase flow simulation model with two evolutionary algorithms: the genetic algorithm (GA) and the differential evolution (DE) algorithm, taking into account both the environmental and economical aspects of the remediation problem. More specifically, the goal is to achieve maximum LNAPL free product removal at least cost. The performance of the proposed optimal free phase recovery algorithms (GA and DE) is compared using data from a field site contaminated with LNAPLs, located near Athens, Greece.

2 METHODOLOGY

2.1 Multiphase flow simulator

For the purpose of simulating the LNAPL transport in the subsurface, FEHM (Finite Element Heat and Mass transfer code), a model developed by the Los Alamos National Laboratory, was used. Its purpose is to simulate mass transfer for multiphase flow within porous and permeable media, and noncondensible gas flow within porous and permeable media[31]. In this work, isothermal NAPL-water transport was assumed. This assumption is generally valid for shallow subsurface transport, where pressure is practically constant and physicochemical properties are not affected significantly by temperature fluctuations[32]. The model uses a pressure formulation and solves two conservation equations; one for liquid (free phase) NAPL and one for liquid water:

$$\phi \frac{\partial S_l(\mathbf{x},t)}{\partial t} + \nabla \cdot \mathbf{q}_l(\mathbf{x},t) = F_l(\mathbf{x},t) \tag{1}$$

$$\mathbf{q}_l(\mathbf{x},t) = -\lambda_l(\mathbf{x},t)\left[\nabla \cdot P_l(\mathbf{x},t) + \rho_l g\right], \quad \text{with: } \lambda_l(\mathbf{x},t) = \frac{k(\mathbf{x})k_{rl}S_l}{\mu_l} \tag{2}$$

The above equations are subject to the following initial conditions:

$$P_l(\mathbf{x},0) = P_{l0}(\mathbf{x}) \ , \ x \in \Omega \ ; \ P_l(\mathbf{x},t) = P_{lt}(\mathbf{x},t) \ , \ x \in \Gamma_A \ ; \ \mathbf{q}_l(\mathbf{x},t) \cdot \mathbf{n}(\mathbf{x}) = Q_l(\mathbf{x},t) \ , \ x \in \Gamma_B \tag{3}$$

where l denotes liquids (l=w for water and l=n for NAPL), S_l are the liquid saturations, with $S_w+S_n=1$, $q_l(x, t)$ are the liquid fluxes, $F_l(x, t)$ is a source or sink term, $\lambda_l(x, t)$ is liquid mobility, $P_l(x, t)$ is the fluid pressure, ρ_l is fluid density, k(x) is the intrinsic permeability of the porous media, k_{rl} is the water or NAPL relative permeability, μ_l is the liquid dynamic viscosity; $P_{l0}(x)$ is the initial pressure in the domain, $P_{lt}(x, t)$ and $Q_l(x, t)$ are the prescribed pressure and fluid fluxes across boundary segments Γ_A and Γ_B, n(x) is the outward unit vector normal to the boundary Γ_B and ϕ is the porosity[32]. The input to the model consists of an initial description of the fluid pressure as well as media properties. The output consists of the final fluid pressure and the volume fraction of water-NAPL[31].

2.2 Optimization problem formulation

The objective of the proposed optimization algorithm is twofold: maximizing the remediation efficiency (LNAPL free product removal) while minimizing operation cost. The well locations and number are assumed fixed, thus, the capital cost associated with their construction will not be included in the objective function. The length of the pumping period to ensure successful remediation is also assumed fixed. Consequently, the decision variables are the LNAPL pumping rates for each well.

The first objective is associated with the economical aspect of the problem, in this case the pumping wells operation cost and the second objective involves the environmental considerations of the problem that in this work are represented by the maximization of free product removal or equivalently the minimization of the NAPL free phase product that remains in the aquifer after the end of the remediation period. This is measured by the LNAPL head at observation locations. The two objectives are combined into one objective function equation using weights whose selection depends on their relative importance:

$$\min \ w_1 t c_1 \sum_{i=1}^{n} Q_i + w_2 \sum_{i=1}^{n} H_i + w_3 \tag{5}$$

where t is the remediation period, c_1 is the unit cost of operation, n is the number of existing pumping wells, Q_i the pumping rate of each well, H_i is the LNAPL head at each observation well, w_1 and w_2 are weights that define the relative importance of the two terms of the fitness function and w_3 is an additional penalty term imposed whenever the second objective is less than or equal to a prespecified small value.

2.2 Solution algorithms

Classical optimization algorithms are not convenient when dealing with multiobjective problems. Evolutionary algorithms on the other hand, are highly effective in finding multiple solutions in a single simulation run due to their population based approach, making them an ideal choice when trying to solve such multiobjective problems[33]. Therefore, the optimization problem formulated above was solved using two evolutionary algorithms: the genetic algorithm (GA) and the differential evolution (DE) algorithm. Evolutionary algorithms are stochastic search methods inspired by natural biological evolution. A fixed size population of potential solutions is required to initialize the process. In most cases, the initial population is created randomly. The next step involves the evolution of the population using genetic operators such as crossover and mutation in order to find better solutions. The newly created population is then used in the next iteration (generation) of the algorithm until a stopping criterion terminates the process. The stopping criterion can be either in the form of maximum number of generations or a satisfactory fitness level. If the algorithm has terminated due to a maximum number of generations a satisfactory solution cannot be guaranteed[30].

The difference between genetic and differential evolution algorithms lies in the process of generating a new population. In GAs, during each iteration individuals from the previous population are selected using some selection scheme, and are combined (crossover) in order to form a new population. Some of those individuals will undergo mutation, which is a random change in one or more of their chromosomes. The number of individuals that will be combined and/or mutated is determined by the crossover and mutation probabilities respectively. The rest of the individuals will enter the new population unchanged[34].

In DEs, new individuals are created by adding the weighted difference between two individuals to a third, called mutated vector (mutation). The mutated vector is combined with a randomly chosen individual of the population, called target vector, in order to produce a trial vector (crossover). Then, the fitness of the trial vector is compared to that of the target vector and if it is greater, the trial vector replaces the target vector in the next generation (selection). In each iteration, each of the individual has to serve once as the target vector[35].

Traditional genetic algorithms are binary coded. Nevertheless, when applied to real world problems, real-coded evolutionary algorithms have proved more computationally efficient and easier to implement[36]. For this reason, a real-coded genetic algorithm was used in this work.

3 FIELD APPLICATION AND RESULTS

The applicability of the proposed strategy and the relative effectiveness of the two evolutionary algorithms were demonstrated through a field application in an industrial area located near Athens, Greece. The environmental assessment performed at the site detected significant hydrocarbon contamination in all three phases (free phase product, soil vapor and groundwater solutes). The main geological formation encountered in the area is limestone consisting of a fractured upper part that extends 1-6 m below the ground surface. This fractured part constitutes a confined aquifer which was vertically discretized in 2 numerical layers. The horizontal discretization of the study area was implemented using a quadrilateral finite element mesh consisting of 902 nodes and 832 elements. The initial hydraulic head distribution for each layer was obtained by interpolation of field measurements (corrected for the effect the floating oil product). The calibration of the flow field was also performed using field measurements (Figure 1a).

An initial hydrocarbon free phase distribution was created by interpolating existing LNAPL thickness field measurements (Figure 1b). There are 10 pumping wells on site. Those locations plus 10 other points serve as observation wells i.e. locations where LNAPL thickness needs to be minimized. The length of the remediation period was set to one year.

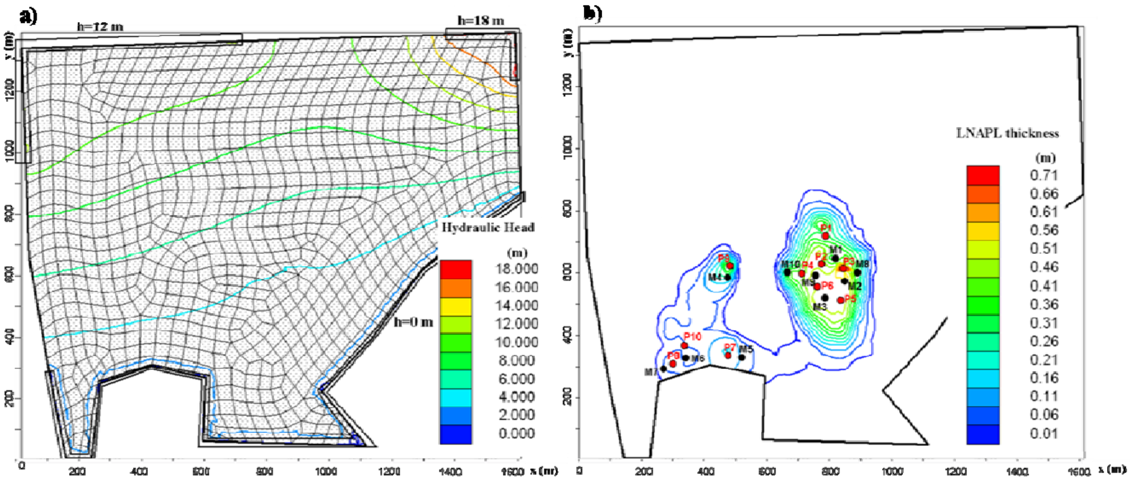

Figure 1: a) Finite element mesh, boundary conditions and hydraulic head distribution, b) Initial LNAPL distribution and location of pumping (red circles) and monitoring (black circles) wells

The hydraulic conductivity field of the model area is considered heterogeneous. The main model area has a hydraulic conductivity of 2×10^{-3} m/s and additionally there exist three lenses with hydraulic conductivities of 3.1×10^{-4}, 1.9×10^{-4} and 4.3×10^{-4} m/s around wells M9, M10 and P9 respectively and one with a value of 1.1×10^{-4} m/s north of well M10 that were determined using pumping tests. The porosity is 0.03, the hydrocarbon density and viscosity are 878.7 kg/m^3 and 6.04×10^{-4} Pa·s and the residual liquid saturation is 0.05.

As mentioned before, the optimization problem of this work was solved using a genetic algorithm and a differential evolution algorithm. For both algorithms a population of 30 individuals was used in each generation and a maximum number of 500 iterations were defined as the stopping criteria in both cases. This corresponds to 15,000 calls to the simulation model. The weights used in this optimization problem were 0.01, 1 and 10 respectively and were experimentally defined trying to make sure that the first two terms of the objective function have similar orders of magnitude. For the GA, the crossover (P_c) and mutation probabilities (P_m) were 0.8 and 0.1 respectively while for the DE, the crossover (Cr) and scaling parameters (F) were set to 0.8 and 0.5. These parameters were adjusted for optimal performance by the two algorithms, starting with initial values taken from the literature[34,35]. The optimization parameters and optimal solutions obtained from the two optimization methods are summarized in Tables 1 and 2.

In Figure 2, the final LNAPL thickness distribution after implementing the optimal pumping strategy of the GA is presented. The LNAPL thickness is reduced to zero in all 10 pumping wells. Regarding wells M1-M3 and M8-M10 the reduction in LNAPL thickness is

17.7%, 48%, 47.5%, 6.3%, 44.8% and 8.3%, respectively. For wells M4-M7, while the initial product thickness was relatively low, now it has been increased. This is due to the fact that using the existing number and location of pumping wells, the contamination cannot be contained and LNAPL escapes moving towards the sea.

Parameter	**Value**	**GA parameters**	
Population number	30	Crossover probability: Pc	0.8
Max. number of iterations	500	Mutation probability: Pm	0.1
Pumping rate bounds: Q_{min}, Q_{max}	0 kg/s , 0.002 kg/s		
Minimum LNAPL head: H_{min}	0.005 m	**DE parameters**	
Cost coefficient: c_l	0.001 €/kg	Crossover parameter: Cr	0.8
Weights: w_1 , w_2 , w_3	0.01 , 1 , 10	Scaling parameter: F	0.5

Table 1: Parameters used by the optimization algorithms (GA and DE)

Pumping well	**Q_{GA} (kg/s)**	**Q_{DE} (kg/s)**	**Pumping well**	**Q_{GA} (kg/s)**	**Q_{DE} (kg/s)**
P1	1.45×10^{-4}	1.41×10^{-4}	P6	2.46×10^{-4}	2.38×10^{-4}
P2	2.64×10^{-4}	2.51×10^{-4}	P7	4.54×10^{-4}	4.49×10^{-4}
P3	1.94×10^{-4}	1.92×10^{-4}	P8	2.36×10^{-4}	2.03×10^{-4}
P4	2.05×10^{-4}	1.92×10^{-4}	P9	1.61×10^{-4}	1.44×10^{-4}
P5	3.80×10^{-4}	3.75×10^{-4}	P10	1.04×10^{-4}	3.35×10^{-4}
Objective value	13.38	13.42			

Table 2: Optimal pumping strategies for GA and DE

This is also evident when comparing the initial and final LNAPL distributions (Figures 1b and 2); while the maximum LNAPL thickness has been reduced, the plume's extent has been increased. The optimal objective function values for the two algorithms are very similar with that of the GA being slightly better. One the other hand, the DE converges much faster to a nearly optimal solution, as can be observed in Figure 3.

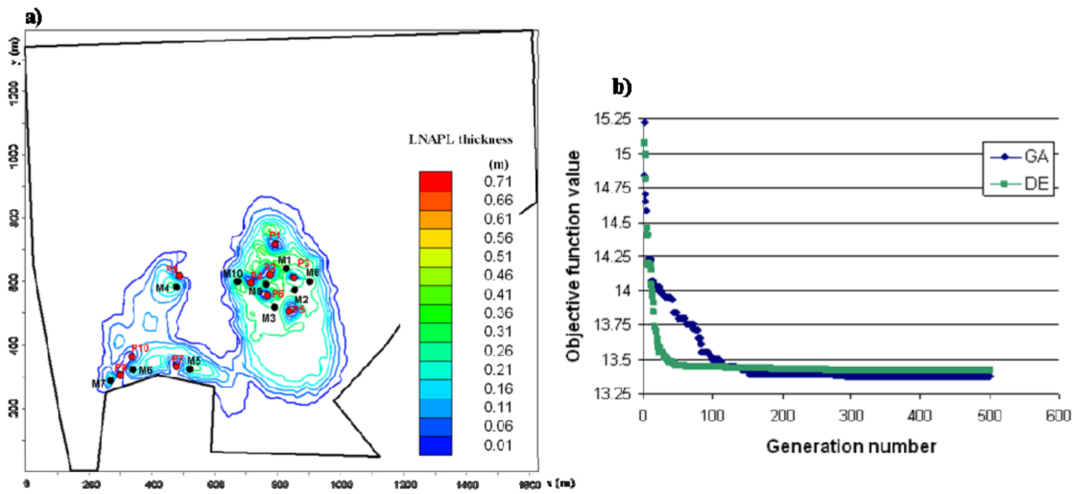

Figure 2: a) Final LNAPL thickness distribution, b) Convergence rate of GA and DE algorithms

4 CONCLUSIONS

The solutions obtained using the two optimization algorithms are very similar, concerning the pumping rates, the optimal objective function values and the computation time needed to perform the same number of algorithm iterations. The genetic algorithm converges to a slightly smaller objective value (13.38 for the GA and 13.42 for the DE); this difference is considered negligible. However, as can be observed in Figure 3 the DE converges to a nearly optimal solution much faster than the GA (around 50th generation in comparison to the GA which converges around the 145th generation). Thus, it can be said that if a convergence stopping criterion was used instead of allowing the algorithms to run a fixed number of iterations, then the computation time needed by the DE in order to find a satisfactory solution would be much smaller than the GA.

The results indicate that the existing number and location of extraction wells fails to contain the LNAPL plume during the given pumping period; free product escapes and moves towards the shoreline. Consequently, future work will focus on identifying optimal locations for drilling new wells that can satisfactory contain and remove the LNAPL contamination in the area. In addition, the number and length of pumping periods to ensure successful remediation can be included as a design parameter when constructing the optimization problem.

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