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Optimizing ethanol enhanced NAPL remediation using evolutionary algorithms

Zoi Dokou[a,*], George P. Karatzas[a], Derya Aydin Sarikurt[b], Nadim K. Copty[b]

[a]*School of Environmental Engineering, Technical University of Crete, University Campus, Chania, 73100, Greece*
[b] *Institute of Environmental Sciences, Bogazici University, Hisar Campus, Bebek, Istanbul, 34342, Turkey*

Abstract

In the past decades, subsurface non-aqueous phase liquid (NAPL) contamination has been recognized as one of the most widespread and challenging environmental problems. Thus, researchers have focused their efforts on developing and testing the efficiency of remediation methodologies, able to address the unique nature of these contaminants. Recently, in-situ flooding techniques for the accelerated removal of NAPLs trapped in the subsurface have been proposed, where additives are injected together with water upgradient of the NAPL-contaminated area in order to alter the physio-chemical properties of the contaminants, such as interfacial tension, and enhance their solubilities. In this work, the efficiency of ethanol enhanced NAPL remediation is addressed. To this end, a non-linear, multi-objective optimization strategy is developed by combining a multiphase flow simulation model with evolutionary algorithms. Two conflicting optimization objectives are considered: minimizing operation cost and maximizing remediation efficiency, while preventing uncontrolled NAPL mobilization. More specifically, the first objective involves the operation cost of the procedure, which is directly proportional to the pumping rate, duration and ethanol volume used. The second represents the environmental considerations of the problem that, in this work, are described by the maximization of free product removal and the prevention of DNAPL vertical spreading.

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Keywords: NAPLs; cosolvent flushing; groundwater remediation; evolutionary algorithms; particle swarm optimization

* Corresponding author. Tel.: +30-28210-37793; fax: +30-28210-37847.
E-mail address: zoi.dokou@enveng.tuc.gr

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1. Introduction

The accidental release of organic contaminants in the form of non-aqueous phase liquids (NAPLs) is a widespread and challenging environmental problem that poses a serious threat to groundwater reserves worldwide and compromising future opportunities for economic development of local communities.

Since the late 1980's considerable efforts have been directed towards developing new technologies for the remediation of NAPL-contaminated groundwater. Among the more promising technologies that have been emerged is in-situ cosolvent flushing which involves the injection of chemical to enhance the solubility of the NAPL and possibly instigate its mobility as a separate phase by reducing the interfacial tension [1].

Successful remediation of the contaminated sites is of paramount importance to ensure the protection of groundwater resources and human health but it 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 [2]. Such tools include algorithms that couple groundwater contaminant transport simulation models with optimization techniques. While many models focused on optimizing pump and treat designs, very few attempted to optimize surfactant flushing [3,4], and none to the best of our knowledge has attempted to optimize cosolvent flushing, which is the focus of this work.

In this work, a non-linear, multi-objective optimization strategy is proposed that seeks the optimal pumping rates and pumping pattern of cosolvent flushing experiments conducted in a 2D experimental porous media tank. Two conflicting objectives were combined: the first is associated with the economical aspect of the problem, in this case the pumping wells installation and operation cost as well as the flushing chemical (ethanol) cost, and the second involves the environmental considerations represented by the maximization of NAPL recovery and the minimization of the required cleanup time. More specifically, the first objective involves the operation cost of the procedure, which is directly proportional to the pumping rate, duration and ethanol volume used. The second objective is described by the maximization of free product removal and the prevention of DNAPL vertical spreading, which was formulated in the form of a penalty in the objective function. The above problem was solved using an evolutionary computation algorithm, namely Particle Swarm Optimization (PSO).

2. Methodology

2.1. Multiphase modeling

For the purpose of modeling the ethanol enhanced flushing process, a three-dimensional, multiphase, finite-difference numerical model (UTCHEM) was used. UTCHEM was originally developed by Pope and Nelson [5] to simulate the enhanced recovery of oil using surfactant and polymer processes and is one a very few models are capable of modeling cosolvent flushing. The UTCHEM code was modified by Roeder and Falta [6], to model unstable conditions which may occur during cosolvent flushing of NAPLs. A modified version of the multiphase flow simulator UTCHEM-9.0 was used in this modeling study, equipped with the interfacial tension calculation method developed by Li and Fu [7] and implemented by Liang and Falta [8]. This method enables UTCHEM to accurately simulate the process of ethanol concentration-dependent interfacial tension lowering.

UTCHEM accounts for effects of surfactants/cosolvents on interfacial tension, phase behavior, capillary trapping, and surfactant/cosolvent adsorption. Capillary pressures, relative permeabilities, dispersion and molecular diffusion as well as the partitioning of NAPL to the aqueous phase (under equilibrium and non-equilibrium assumptions) are some of the important components of the simulator that were utilized in this work. More details can be found in a previous study [9] that involved the model development and calibration of the ethanol flushing experiments, which is linked here to the multi-objective optimizer. A schematic representation of the 2D experimental tank used for the experiments is provided in Fig. 1.

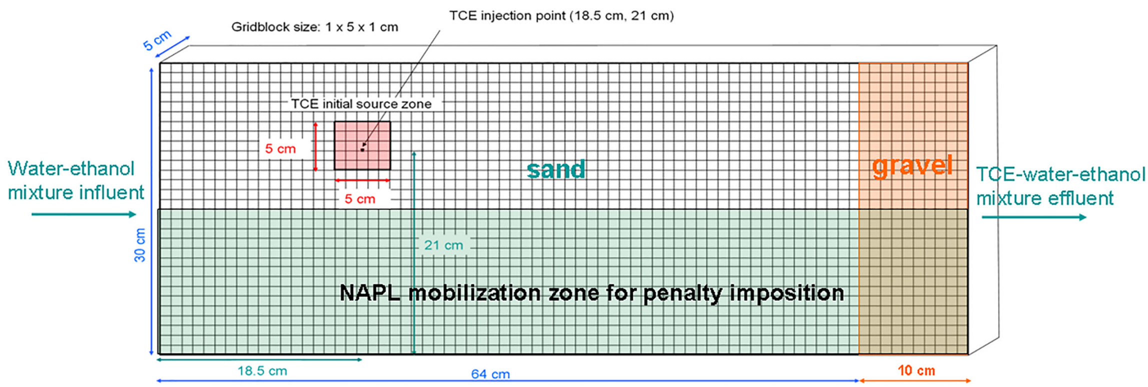

Fig. 1. Model and 2D tank setup and TCE mobilization zone for penalty imposition

2.2. Optimization problem formulation

The objective of the proposed optimization algorithm is twofold: maximizing the remediation efficiency (NAPL product removal) while minimizing operation cost. The decision variables of the problem are the NAPL pumping rates, the amount of chemical (ethanol) needed for the remediation process and the remediation time. The first objective of the optimization problem is associated with the economical aspect of the NAPL recovery and flushing process. More specifically, the first objective involves the minimization of the installation and operation cost (that is directly proportional to the pumping rate, duration and ethanol volume). The second objective involves the environmental considerations of the problem that in this work are represented by the maximization of the volume of TCE recovered.

In single objective optimization problems, the main focus is on the decision variable space while in a multi-objective concept the interest switches on the objective space. Due to the contradiction of the objective functions it is not possible to find a single optimal solution for all of them simultaneously. The most common approach to overcome this problem is to combine the objectives into a single objective function assigning weights to each of them according to their relative importance (weighted aggregation). Based on the above, the optimization problem formulation has the following form:

$$\min \; w_1\left[c_{fixed} + c_1\sum_{j=1}^{m} Q_j + c_2\, t\sum_{j=1}^{m} D_j Q_j + c_3\, t\right] - w_2\sum_{j=1}^{m} V_i + w_3 \tag{1}$$

Where: c_{fixed} cost related to well installation, c_1 is the unit cost of well operation, t is the remediation period duration, Q_j the pumping rate of each well and m is the number of pumping wells, c_2 is the unit cost per volume of ethanol, D_j the percentage of ethanol introduced into the aquifer at each well and V_i is the NAPL free phase volume recovered during the remediation period.

The parameters w_1 and w_2 are weights that define the relative importance of the two terms of the objective function and w_3 is a penalty term imposed whenever the current algorithm solution results in DNAPL vertical spreading below a certain depth. The penalty is imposed when the total NAPL mass below the line of 15 cm height (represented by the light blue rectangle in Fig. 1) exceeds 1% of the initial TCE mass injected, indicating TCE vertical spreading. The mass that was injected in the system was 14600 mg.

As can been seen on Equation 1 the two objectives have different units of measurement. To compensate for differences in magnitude (e.g. cost in thousands of euros, volume in m^3) between the two objectives, they were transformed to a common distance scale [4,10]. From the initial, randomly selected population in the PSO algorithm, the transformation functions were deducted. Both objective functions were first normalized and then transformed in order to have the same distance from the origin to the optimum of the initial sample. The transformation function is given by:

$$g_i(F_i) = \frac{F_i}{\sigma_i} + \varepsilon_i, \quad i = 1,2 \tag{2}$$

$$\varepsilon_i = \max\left\{\min\left\{\frac{F_j}{\sigma_j}\right\}, j = 1,2 - \min\left\{\frac{F_i}{\sigma_i}\right\}\right\} \tag{3}$$

Where: Fi is the objective function, σi the standard deviation calculated by the initial PSO population. In this case the objective function transform to:

$$F_{final} = w\left(\frac{F_1}{\sigma_1} + \varepsilon_1\right) + (1-w)\left(\frac{F_2}{\sigma_2} + \varepsilon_2\right) \tag{4}$$

Where w is a weight between 0-1. In the case of w=0.5 the two objective are considered to have equal importance, as was the case selected here.

A population of 25 particles was used and a maximum number of 200 iterations were defined as the stopping criteria, corresponding to 12500 calls to the simulation model. The initial population was created randomly in all cases. Table 1 summarizes the basic parameters used in this optimization problem (costs, upper and lower bounds etc.). The fixed and ethanol costs were taken as market values for the experiments while the pumping and treatment and remediation time costs were taken from the literature [4]. It is assumed that only one recovery well (m=1) is present, located at the end of the tank.

Table 1. Optimization parameters.

Parameter	Value
Number of particles	25
Number of iterations	200
Lower and upper bounds for pumping: Q_{min}, Q_{max}	0 m^3/d , 0.017 m^3/d
Lower and upper bounds for ethanol content (%)	0-100
Lower and upper bounds for remediation time (t)	0 – 4 d
Objective function weight: w	0.5
Fixed cost (κ_{fixed})	5000 €
Pumping and treatment cost (κ_1)	0.25 €/m^3
Ethanol cost (κ_2)	18000 €/m^3
Remediation time cost (κ_3)	240 €/d

2.3. Particle Swarm Optimization algorithm

The PSO algorithm was inspired by the behaviour of swarms of animals. In this method, each individual is considered as a particle in multidimensional space with a specific position and velocity. A record of each particle's best position that has been achieved so far is kept [11]. The collection of particles is called a swarm, a term analogous to the population term in genetic algorithms and differential evolution algorithms. At each iteration, a particle moves to a new position in space by adding a velocity to its current position. The velocity term is a random combination of three components: i) the inertia component, causing the particle to continue moving in the direction it was moving in the previous iteration, ii) the cognitive component, causing the particle to move towards the best position it has ever been in and iii) the social component, steering the particle towards the best position of any particle of the entire swarm or in its neighborhood [12]. The above process is summarized by the following equations:

$$\boldsymbol{v}_i(t) = \boldsymbol{v}_i(t-1) + \phi_1 rand_1\left(\boldsymbol{p}_i - \boldsymbol{x}_i(t-1)\right) + \phi_2 rand_2\left(\boldsymbol{p}_g - \boldsymbol{x}_i(t-1)\right) \tag{5}$$

$$\boldsymbol{x}_i = \boldsymbol{x}_i(t-1) + \boldsymbol{v}_i(t) \tag{6}$$

Where: $\boldsymbol{v}_i$ is the velocity of the particle, ϕ_1, ϕ_2 are two positive numbers (weights) that represent the particle's own experience (ϕ_1) and the experiences of the other particles of the swarm (ϕ_2), $rand_1$, $rand_2$ are two uniformly distributed random numbers in the range of [0,1], $\boldsymbol{p}_i$ and $\boldsymbol{p}_g$ is the best previously recorded positions of the i^{th} particle and of the entire swarm, respectively.

During the implementation of the particle swarm optimization there are certain parameters that need to be taken into account in order to avoid the "explosion" of the swarm and to speed convergence. In the literature there are different methods to ensure this: i) the maximum velocity multiplier, ii) the constriction factor or iii) the inertia constant. In this work, the maximum velocity method in combination with the constriction factor are used. The maximum velocity is limited by a multiplier between 0 and 1:

$$v_{max} = kx_{max} \tag{7}$$

Where: k is the multiplier and x_{max} is the variable's upper bound. The constriction factor method [13] updates Equation 5 as follows:

$$\boldsymbol{v}_i(t) = \chi \cdot \left\{\boldsymbol{v}_i(t-1) + \phi_1 rand_1\left(\boldsymbol{p}_i - \boldsymbol{x}_i(t-1)\right) + \phi_2 rand_2\left(\boldsymbol{p}_g - \boldsymbol{x}_i(t-1)\right)\right\} \tag{8}$$

$$\chi = \frac{2}{\left|2 - \phi - \sqrt{\phi^2 - 4\phi}\right|}, \quad \phi = \phi_1 + \phi_2 > 4 \tag{9}$$

In order to select the parameter values that would produce the best results for the multiplier for the maximum velocity (k), tests were made with different values and the one with the best results (k=0.4) was finally selected. The parameters ϕ_1 and ϕ_2 were assumed both equal to 2.05 (corresponding to a constriction factor of χ =0.729) as suggested by Clerk [13].

3. Results

The optimization algorithm gave the following values to the decision variables of the problem: Pumping rate: Q = 0.017 m3/d (equal to the upper bound), % ethanol: D=82 % and remediation time: t = 0.6865 days or 16.5 hours. It was observed that the optimal ethanol content found by the algorithm is high (82%), a value that can cause the IFT to become zero and thus TCE to completely dissolve and mobilize. It is worth mentioning though that in the experimental setting the recovery well fully penetrates the tank, thus all mobilized TCE mass is finally recovered by the well. Thus, no penalty is imposed for high ethanol contents, providing the remediation time is adequate. It is observed that the algorithm tends to discard solutions with high remediation times that could have good recovery results, if combined with low pumping rates, because this will not be as cost effective as the current optimal solution. Finally, additional increase in ethanol content does not improve the solution as TCE is fully mobile and dissolved in lower than 100% ethanol contents, such as the optimal value produced by the optimization algorithm.

The PSO algorithm converged very fast, as seen in Fig. 2 that shows convergence for the first 100 iterations. In iteration 62, the algorithm converges to the optimal solution. Due to the low objective function values the differences between the values are not very clear in Fig. 2. The final objective function value is -6.06655 (normalized) that has a cost of 5335€ (5000€ fixed cost plus 335€ for ethanol and time costs) and recovers almost all TCE mass injected (14431 mg out of 1460 mg that was injected, corresponding to 98.8% recovery).

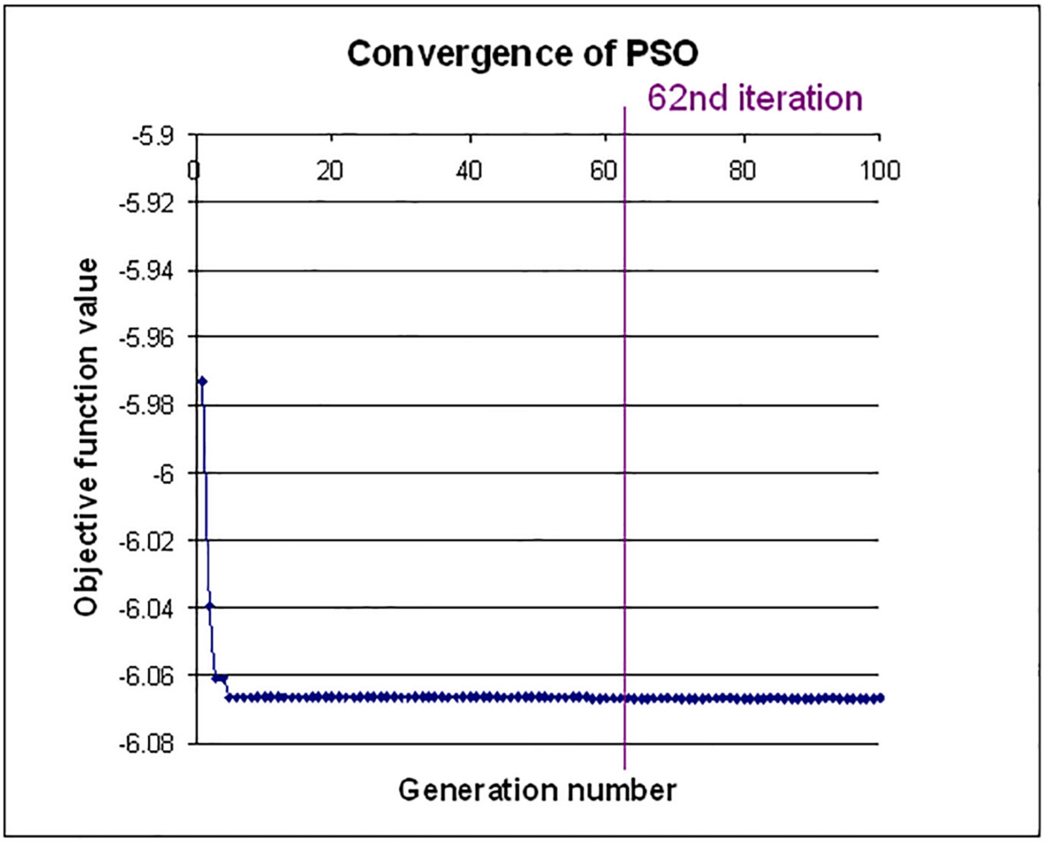

Fig. 2. PSO convergence

4. Conclusions

In this work, the efficiency of ethanol enhanced NAPL remediation is addressed by developing a non-linear, multi-objective optimization strategy that combines a multiphase flow simulation model with particle swarm optimization algorithm. Two conflicting optimization objectives are considered: minimizing operation cost and maximizing remediation efficiency (NAPL product removal), while preventing uncontrolled NAPL mobilization. More specifically, the first objective involves the operation cost of the procedure, which is directly proportional to the pumping rate, duration and ethanol volume used. The second represents the environmental considerations of the problem that, in this work, are described by the maximization of free product removal and the prevention of DNAPL vertical spreading.

The results show that the optimal ethanol content found by the algorithm is high (82%), a value that can cause the IFT to become zero and the TCE to completely dissolve and mobilize. It is worth mentioning though that, contrary to what one might expect in field conditions, in the experimental setting the recovery well fully penetrates the tank, thus all mobilized TCE mass is finally recovered. Thus, no penalty is imposed for high ethanol contents, if the remediation time is adequate. It is also observed that the algorithm tends to discard solutions with high remediation times that could have good recovery results if combined with low pumping rates because this will not be as cost effective as the current optimal solution. Finally, additional increase in ethanol content does not improve the solution as TCE is fully mobile and dissolved in lower than 100% ethanol contents, such as the optimal solution found by the optimization algorithm.

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