Using Simulation-Optimization Techniques to Improve Multiphase Aquifer Remediation

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Abstract

The T2VOC computer model for simulating the transport of organic chemical contaminants in non-isothermal multiphase systems has been coupled to the ITOUGH2 code which solves parameter optimization problems. This allows one to use linear programming and simulated annealing techniques to solve groundwater management problems, i.e. the optimization of operations for multiphase aquifer remediation. A cost function has to be defined, containing the actual and hypothetical expenses of a cleanup operation which depend - directly or indirectly - on the state variables calculated by T2VOC. Subsequently, the code iteratively determines a remediation strategy (e.g. pumping schedule) which minimizes, for instance, pumping and energy costs, the time for cleanup, and residual contamination. We discuss an illustrative sample problem to discuss potential applications of the code. The study shows that the techniques developed for estimating model parameters can be successfully applied to the solution of remediation management problems. The resulting optimum pumping scheme depends, however, on the formulation of the remediation goals and the relative weighting between individual terms of the cost function.

Introduction

The design of a cleanup operation for a contaminated aquifer comprises problems of a hydrological, technical, environmental, and economic nature. The main task is to select an effective and efficient remediation technology. The suitability of a proposed method depends on the chemical properties of the contaminant, the characteristics of the aquifer, and the overall remediation goals. Once a technology has been chosen, the operational scheme (e.g. pumping schedule) can be further optimized to reduce remediation costs.

Standard groundwater remediation operations include some form of pumping through extraction wells and subsequent treatment of the contaminated groundwater. Hazardous volatile nonaqueous phase liquids may be efficiently removed from contaminated soils and aquifers by injecting steam, thus vaporizing and displacing the contaminant toward the extraction wells. The use of numerical models to study different remediation designs requires simulating the transport of organic chemical contaminants in non-isothermal multiphase flow systems. In this study, we use the T2VOC code [*Falta et al.*, 1994], which is an adaptation of the STMVOC numerical simulator developed at Lawrence Berkeley Laboratory by R. Falta and K. Pruess [*Falta and Pruess*, 1991], for modeling contaminant transport.

The management of groundwater remediation by means of optimization techniques usually aims at maximizing contaminant removal by a minimum of capital, operating, and maintenance costs. Furthermore, technical constraints and regulatory cleanup standards have to be observed. The purpose of this paper is to demonstrate how standard parameter estimation methods can be used to optimize remediation strategies. The ITOUGH2 code [*Finsterle*, 1993; *Finsterle and Pruess*, 1993, 1995] was originally developed for the estimation of hydrogeologic model parameters for the TOUGH2 code [*Pruess*, 1991] and some of its descendants, such as T2VOC. ITOUGH2 solves the inverse problem by automatic model calibration using non-linear optimization techniques. In principle, the same methodology can be applied to optimize remediation strategies by minimizing an appropriately defined objective (or cost) function. The example discussed in the paper examines the remediation of a large contaminant plume by an array of extraction wells. The pumping rate in each well is optimized to reduce cleanup costs.

Optimizing Pumping Schedule For Aquifer Cleanup Operation

Consider a confined aquifer of uniform thickness (10 m), contaminated by a spill of xylene. It is assumed that 3 years after release, the pollution is discovered, stopped, and the spatial distribution of the plume is determined. Subsequently, an array of wells is installed to extract the contaminated groundwater. The aquifer is assumed heterogeneous in hydraulic conductivity with a mean permeability of 10^{-11} m^2, a standard deviation of one order of magnitude, a correlation length of 100 m along the main west-east flow direction, and a correlation length of 20 m in the perpendicular direction. Effective porosity is 0.3. A natural hydraulic gradient of 0.01 is imposed across the model domain of 200 m length. There is no flow across the northern and southern boundaries. We realize that the unsaturated zone as well as density effects (concentration of low-density xylene near the top of the aquifer) are important aspects of plume migration which are not accounted for due to the two-dimensional nature of our schematic model.

The permeability field, the location of the contaminant source (square), and the pumping wells (circles) are shown in Figure 1. Superimposed are the contours of the contaminant plume after 3 years of continuous release.

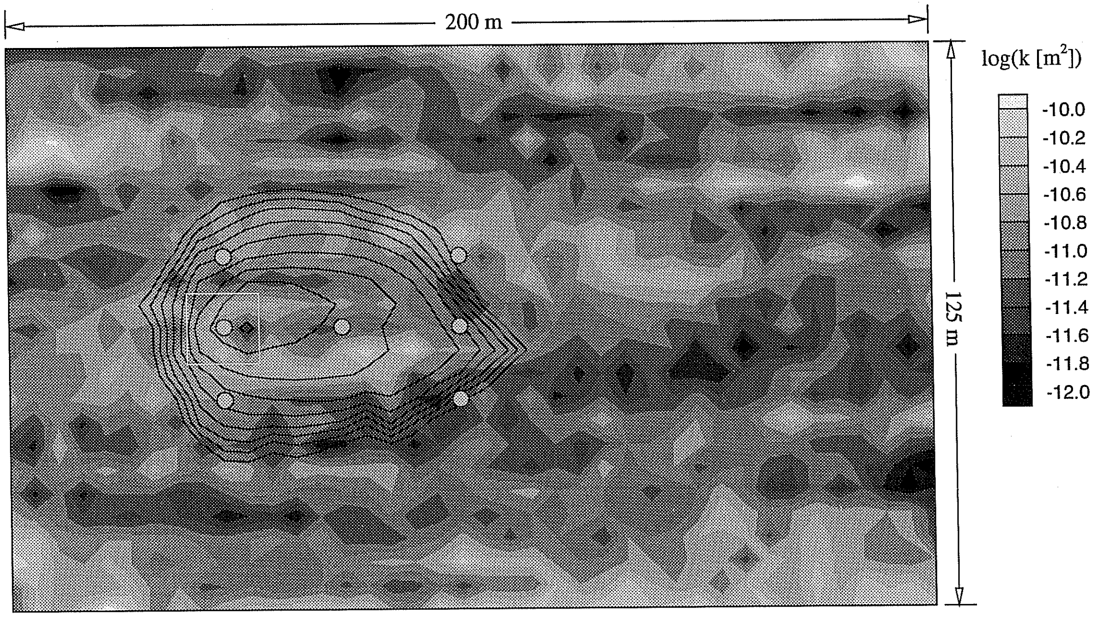

Figure 1: Log-permeability field of hypothetical contaminant site and NAPL saturation prior to remediation

The T2VOC code has been slightly modified so that the simulation automatically stops when the total amount of hydrocarbon in the system is lower than a certain predefined value (e.g. 70 % of the initial inventory). The actual cleanup time is then calculated by linear interpolation between the two last time steps. The cost function to be minimized is simply the total amount of fluid that needs to be pumped and treated, i.e. the product of pumping rate and cleanup time, totaled for all wells. Furthermore, each pump is assumed to have a maximum capacity of 4 kg/s which is the upper bound not to be exceeded during the optimization process.

The problem can now be formulated as follows: A set of pumping rates has to be determined that minimizes the total amount of contaminated groundwater extracted from the system. In inverse modeling terminology, the individual pumping rates are the unknown T2VOC input parameters to be determined, and the data point to be matched is a dummy measurement of zero, representing the desired cleanup costs.

We decided to determine three optimum pumping schedules for three phases of the cleanup operation. Since the location of the plume as well as its spreading changes with time, it is expected that the pumping rates have to be changed with time to achieve maximum aquifer remediation within a reasonable time frame. In this study we change the pumping schedule after 30 and 60 % of the contaminant has been removed.

The pumping schedule, cleanup time, and mean NAPL concentration of the extracted two-phase NAPL-groundwater mixture, as well as the total amount pumped are summarized in Table 1. The values for an alternative design which assumes pumping at a constant rate of 2 kg/s in each well is also included for comparison.

The location of the plume, i.e. the NAPL saturation, is shown in Figures 2, 3, and 4 after 30, 60, and 90 % of the original amount of contaminant is removed, respectively. Note that a relatively small percentage of the total contaminant inventory is dissolved in the water phase, flowing downstream at a higher velocity than the NAPL plume. Initially, most of the xylene is present as a free and mobile NAPL phase. The time required to remove the first 30 % of the total initial contaminant mass is calculated to be 20 days, whereas it takes more than 8 years to remove an additional 60 %. This is mainly due to the strongly reduced effective permeability at low NAPL saturations, i.e. the contaminant is removed basically by pumping groundwater, in which the chemical is dissolved.

Table 1: Optimum pumping schedule

	Pumping rate [kg/s]			
	optimized			not optim.
Contaminant removed	30 %	60 %	90 %	90 %
Well NW	1.9	0.1	0.0	2.0
Well NE	0.0	0.0	0.0	2.0
Well CW	4.0	0.9	0.6	2.0
Well CC	4.0	3.1	3.2	2.0
Well CE	4.0	3.9	3.0	2.0
Well SW	2.1	0.1	0.5	2.0
Well SE	0.2	0.6	0.0	2.0
Total pumping rate [kg/s]	16.3	8.7	7.3	14.0
Total cleanup time [day]	20	180	3110	3060
NAPL/water ratio at wells [gr/kg]	16.7	6.3	0.6	0.4
Total mass pumped [10^6 kg]	28	148	2270	3700

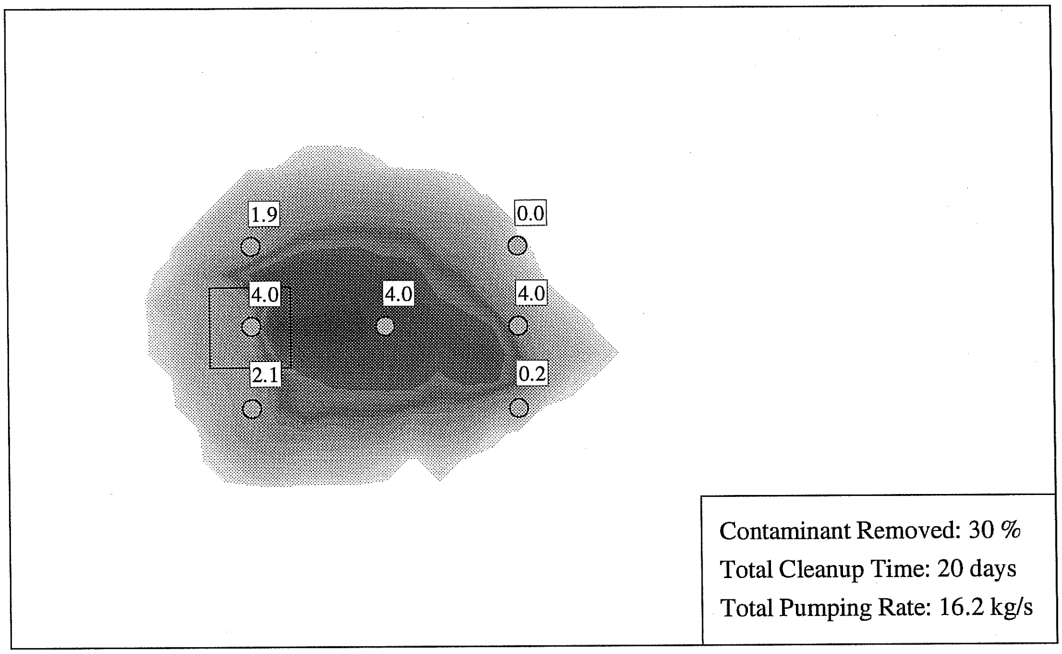

Figure 2: NAPL saturation after 30 % of the contaminant has been removed. Individual pumping rates are shown in boxes at wells.

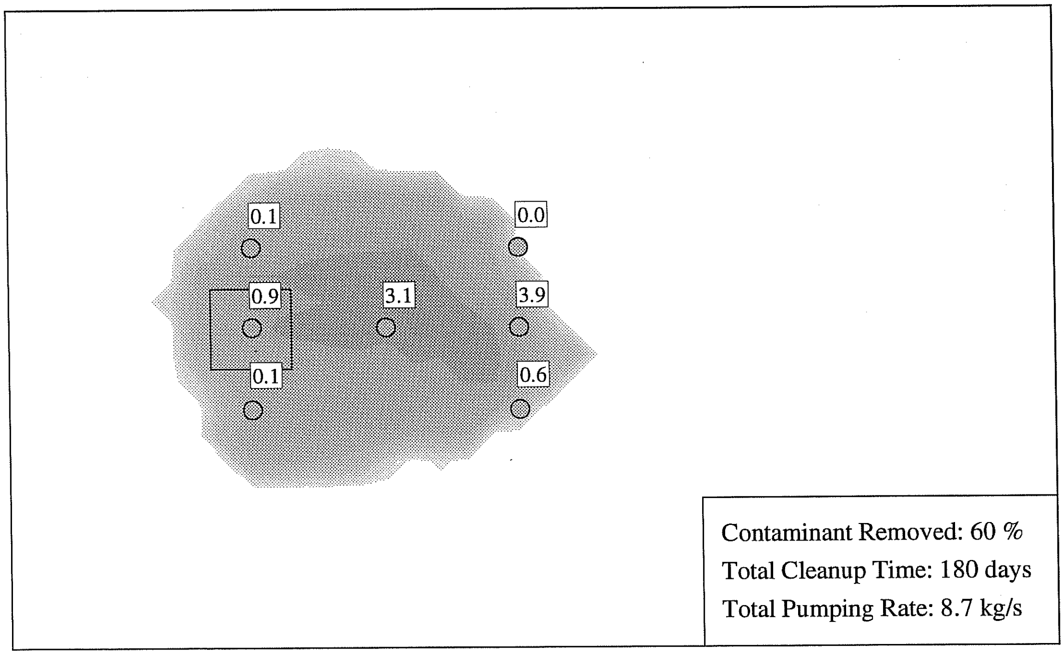

Figure 3: NAPL saturation after 60 % of the contaminant has been removed. Individual pumping rates are shown in boxes at wells.

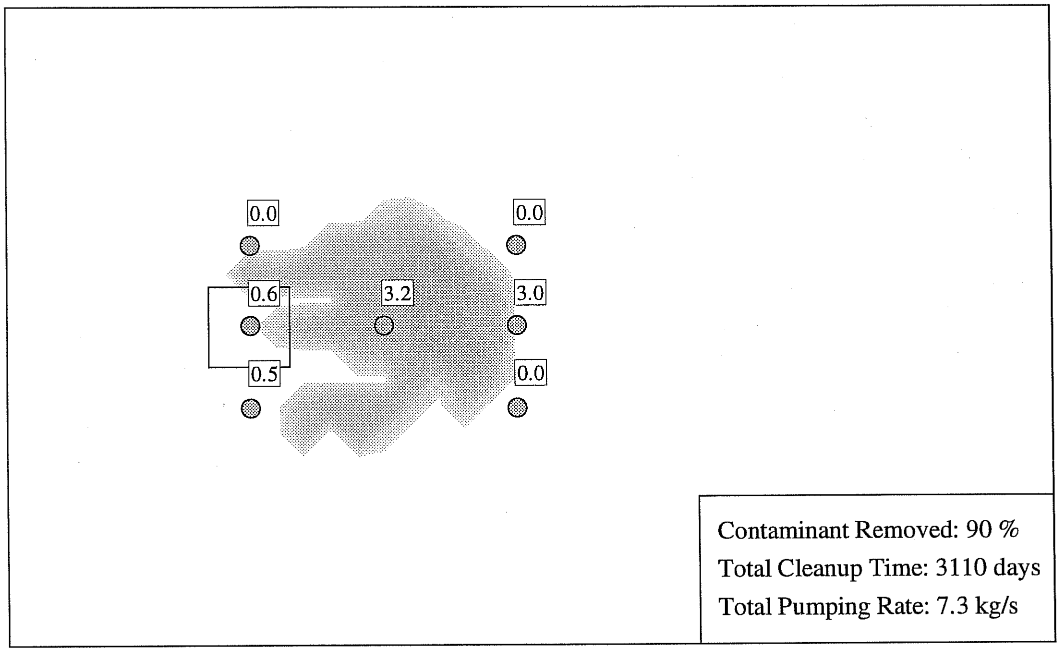

Figure 4: NAPL saturation after 90 % of the contaminant has been removed. Individual pumping rates are shown in boxes at wells.

For the initial period of the cleanup operation, the result of the optimization procedure suggests pumping the center wells at full capacity, and extracting contaminated groundwater also from the two wells on the west side of the field. The two wells to the east are almost shut down, because the water has low NAPL concentrations in that region.

During the second cleanup period, where the total contaminant content will be reduced from 70 to 40 % of the initial amount, the pumping rates in the western wells are lowered to avoid the formation of a stagnation zone. Part of the plume has moved east following the regional gradient, favoring extraction from wells center-east (CE) and south-east (SE) which are further downstream. Extracting an additional 30 % of the initial contaminant content requires pumping for a long period at a relatively low rate. Notice that the total duration of the cleanup operation is slightly longer than for the alternative design, but the total volume of removed groundwater is reduced by more than 50 %, leading to a higher contaminant concentration in the extracted fluid.

One might argue that the solution of the optimization is non-unique and strongly depends on the pumping rate initially assigned to each well. There is a hydrological reason for this unstable behavior. If a certain well starts out with a higher pumping rate than an adjacent well, the flow field and therefore the contaminant plume moves preferentially toward this well. This makes the neighboring well even less efficient because water of lower contaminant concentration is extracted. In addition, local heterogeneities may induce preferential flow of contaminant, thus influencing the selection of certain extraction wells for most effective remediation. Depending on the flow distances and the size and shape of the plume, it is often preferable to shut down peripheral wells, thus concentrating the remediation effort to a few wells in the center of the plume. It should be pointed out that a detailed site characterization study is required, and that the location of the plume has to be accurately determined, so that the effects discussed above are correctly accounted for.

Despite the problem of non-uniqueness, each proposed solution of similar efficiency is a valuable alternative which can help conceive of an improved remediation design. Given the optimum pumping schedule presented above, one might want to revise the number and location of the wells, thus reducing installation costs. The new well configuration can then be optimized in the same manner. Moreover, the long pumping period required to remove the contaminant suggests that another remediation technique may be more appropriate. For example, one might consider using air or steam injection to enhance the recovery of contaminant since the low mobility of the contaminant near residual saturation is the main reason for the inefficiency of the pump and treat method.

Concluding Remarks

The T2VOC numerical simulator has been linked to the ITOUGH2 code to optimize multiphase aquifer remediation operations. One simplified sample problem is discussed in this paper to demonstrate the methodology. More details can be found in *Finsterle and Pruess* [1994]. These studies show that the techniques developed for estimating model parameters can be successfully applied to solve remediation problems. A cost function has to be defined, representing the part of the management objective that is influenced by the hydrological properties of the aquifer. This means that optimization reduces the costs that depend - directly or indirectly - on state variables calculated by T2VOC. ITOUGH2 is flexible enough to handle complicated, discontinuous cost functions that may include pumping rates, energy costs, duration of total cleanup operation, capital costs for well installation, operational costs for the treatment of contaminated groundwater, etc. It is important to realize that the resulting optimum pumping scheme strongly depends on the formulation of the remediation goals, and the relative weighting between individual terms of the cost function. Nevertheless, the solution of the optimization process points towards alternative remediation schemes which have the potential to increase effectiveness with decreasing costs.

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