Optimizing separate phase light hydrocarbon recovery from contaminated unconfined aquifers

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A modeling approach is presented that optimizes separate phase recovery of light non-aqueous phase liquids (LNAPL) for a single dual-extraction well in a homogeneous, isotropic unconfined aquifer. A simulation/regression/optimization (S/R/O) model is developed to predict, analyze, and optimize the oil recovery process. The approach combines detailed simulation, nonlinear regression, and optimization. The S/R/O model utilizes nonlinear regression equations describing system response to time-varying water pumping and oil skimming. Regression equations are developed for residual oil volume and free oil volume. The S/R/O model determines optimized time-varying (stepwise) pumping rates which minimize residual oil volume and maximize free oil recovery while causing free oil volume to decrease a specified amount. This S/R/O modeling approach implicitly immobilizes the free product plume by reversing the water table gradient while achieving containment. Application to a simple representative problem illustrates the S/R/O model utility for problem analysis and remediation design. When compared with the best steady pumping strategies, the optimal stepwise pumping strategy improves free oil recovery by 11.5% and reduces the amount of residual oil left in the system due to pumping by 15%. The S/R/O model approach offers promise for enhancing the design of free phase LNAPL recovery systems and to help in making cost-effective operation and management decisions for hydrogeologists, engineers, and regulators. © 1998 Elsevier Science Limited. All rights reserved.

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1 INTRODUCTION

Hydrocarbon contamination of soil and water by petroleum products (primarily fuels and lubricants) has created widespread environmental problems in the United States. These hydrocarbons, having a density less than water, are referred to as light non-aqueous phase liquids (LNAPL). Remediation of petroleum contaminated sites usually requires several steps: containment and recovery of mobile, free product LNAPL, that exists as a separate phase above the water table; 25 pumping and treatment of dissolved phase contamination; and final removal of residual contamination by soil vapor extraction, 33 enhanced bioremediation, or natural attenuation. The first task, free product LNAPL recovery, is the remediation step that is optimized in the present work.

In describing the problem of LNAPL recovery some preliminary concepts should be discussed. Nonaqueous oil contamination in the aquifer is categorized into two forms, free oil and residual oil. Free oil is mobile and can be detected in monitoring wells. Its movement is related to forces from gravity, fluid saturations, and fluid-table gradients. Residual oil is immobile and is typically considered to be hydraulically discontinuous in both unsaturated and saturated zones. Because residual oil is difficult to remove and extract by conventional pumping alone and remains as a continuing source of contamination, it becomes a primary remediation concern. 9

One of the most serious impediments to the rapid reduction of contaminant concentrations to very low levels is the presence of residual contamination sources that replace the solutes removed by pumping. Potential residual sources include contaminants adsorbed on the soil grains, vapor phase contamination in the vadose zone, and mobile and immobile LNAPL. At sites with extensive LNAPL pools, it is
recognized that significant reductions in solute concentrations will not occur until the residual (or free oil) sources have been removed. Therefore, the remediations at these sites are focusing initially on plume stabilization and removal of LNAPL.

Residual oil is entrapped in the soil matrix as a result of flow mechanisms and inherent aquifer properties. The flow mechanisms consist of multiphase flow due to forces of gravity, natural groundwater flow gradients, fluctuations in the water table, and man-made induced effects from pumping. Significant aquifer properties are related to the soil matrix, hydraulic conductivity, and the residual saturation values. The events of spreading, entrapment, movement, and recovery of the free oil plume are governed by these flow mechanisms and porous media properties.36

Recovery of light hydrocarbons is usually accomplished via a dual-extraction well that: (1) pumps water to cause water table drawdown and hydrocarbon phase flow towards the well; (2) the simultaneous pumping of hydrocarbon from the same well using a separate oil extraction pump. This pumping system is recommended because field experience has shown that free product recovery can be significantly enhanced by controlled depression of the water table through groundwater pumping.9 When designing such an operation, a number of factors must be considered to assure efficient free oil recovery. These may include the rate of pumping at the well, steady versus time-varying pumping rates, length of time for remediation, location of pumping wells, and other design issues related to system operation.

The purpose of this paper is to present a methodology for determining optimal gradually increasing pumping rates that control drawdown to maintain an adequate gradient toward a recovery well. This approach causes minimal residual oil while causing free oil to shrink to a prespecified volume within a specific planning period. This is equivalent to maximizing recovery of free oil (since the less trapped/residual oil, the more available for recovery). The method utilizes nonlinear optimization coupled with nonlinear regression curve fitting. We demonstrate how the proposed monotonically increasing stepwise pumping strategy is an improvement over the best steady water pumping strategy that can be developed by simulation models alone.

2 LITERATURE REVIEW

2.1 Optimizing aquifer remediation

Many optimization techniques have been developed for groundwater management and contamination remediation. These have been limited mostly to aqueous phase or miscible contaminant transport. Such models coupling simulation expressions and optimization algorithms are termed management or simulation/optimization (S/O) models. They have addressed plume containment, pump-and-treat remediation, and related contamination problems. S/O models addressing groundwater quality management have utilized linear programming,2,8,21,34 quadratic programming,3,16,17,19,20,41,49,50 nonlinear programming,5,7,19,24,31 dynamic programming,18,45 genetic algorithms,44 and simulated annealing.10

Although aqueous phase contamination has been addressed with S/O modeling, the LNAPL multiphase flow problem has not been addressed previously. The governing equations of multiphase flow of hydrocarbon and water are highly nonlinear and coupled. The fact that previous literature contains no S/O modeling addressing this nonlinear problem attests to the problem’s computational difficulty.

An innovative simulation/regression (S/R) modeling technique using statistical regression equations describing system response to unit stimuli was developed by Alley4 and applied by Lefkoff and Gorelick.32 Alley optimized steady pumping to intercept and remove migrating contaminants by a pump-and-treat system. Lefkoff and Gorelick addressed the transient hydrologic processes for irrigated agriculture in a saline stream-aquifer system.

A modified regression approach is applied here in a simulation/regression/optimization (S/R/O) model. Because of system hysteresis and numerous flow paths, the effect of pumping on the movement of LNAPL in soils and groundwater is dependent upon previous fluid distribution history. To represent that history here, we use a simulation model (external to the optimization model) that can predict the movement and interaction between air, water, and LNAPL. Thus, the functional relationships of permeabilities $k$, saturations $S$, and pressures $P$ must be known.39

The modified regression approach requires that we develop system responses to multiple pumping sequences, rather than responses to individual unit stimuli. In other words, responses to single steady pumping events cannot be used to represent time-varying pumping. As described below this requires a multiple step approach in developing the nonlinear predictive functions (regression equations).

First, one systematically determines system response to a wide range of simple pumping rate sequences. Through regression analysis, predictive functions are developed that can replicate these system responses. These linear or nonlinear predictive functions are used as objectives and constraints within a S/R/O model to predict system response to pumping. Initial inaccuracy or error in system response prediction are eliminated by cycling through the regression steps. This method can save computational time and improve efficiency in optimizing LNAPL management, because the simulation model is utilized in developing model response functions before the S/R/O model optimization begins. This avoids calling upon the simulation model during optimization. It reduces the total number of required simulations and associated computer run time. This approach should compare favorably to simulated annealing or genetic algorithms which may require more than 1000 simulations10 (neither of those two approaches have been used to address NAPL management). Our methodology is the first reported S/R/O model addressing
free product recovery of LNAPL from contaminated, unconfined aquifers.

2.2 Multiphase flow simulators

Initially, finite difference models came into use for simulating single phase saturated flow.43,48 Then models representing the unsaturated flow regime were developed.15,46 These early models did not include consideration of non-aqueous phase liquids. Later, several researchers developed computer simulation models to predict and analyze multiphase flow of water, air, and nonaqueous phase liquids in the subsurface. Abriola and Pinder,1 Faust,14 Falta and Javandel,12 Faust et al.,13 Kia,29 developed finite difference models for multiphase flow through vertical cross-section media in the unsaturated and saturated zones. Huyakorn and Pinder,22 Osborne and Sykes,35 Kuppusamy et al.,40 Kaluarachchi and Parker,23,28 developed finite element models for multiphase flow. Such models were subsequently applied to analyze remediation techniques. Notwithstanding, many of these models had limited applicability for analyzing LNAPL problems, because of complex geometry and boundary conditions encountered by designers.38

To provide enhanced modeling capabilities, Kaluarachchi et al.25 assumed vertical flow equilibrium in developing a new method for modeling multiphase flow of LNAPL and oil recovery. Their finite element model, ARMOS Version 3.0,11 is a 2-D areal flow simulator. Although we could possibly have used a different model to perform pre-optimization simulations, ARMOS was utilized because: we are familiar with it, it is available to others, and it is widely used for analysis of field LNAPL problems1 and for design of remediation systems. ARMOS simulation abilities have been presented previously.11,25,37,40 Cooper et al.5 summarizes the model’s assumptions and development.

3 THEORY AND MODEL DESCRIPTION

3.1 Multiphase flow analysis

The flow domain is a two fluid-phase porous media system—water and a separate LNAPL in an unconfined aquifer. The numerical model employs the simplifying assumptions of near-equilibrium vertical conditions and negligible gas pressure gradients to reduce the dimensionality of the problem from 3-D to 2-D areal multiphase flow.35 The vertical equilibrium assumption relies on vertical fluids redistributing quickly enough such that vertical pressure distributions constantly approximate hydrostatic conditions, i.e. \( \partial p / \partial z = 0 \) and \( \partial \rho / \partial z = 0 \). In such circumstances, the vertical pressure distributions can be characterized for all phases in terms of various fluid ‘table’ elevations.38

As a result, the oil lens is described by an air–oil table elevation, \( z_{oa} \), at which point the gauge oil pressure is zero, and an oil–water table elevation, \( z_{ow} \), at which water and oil pressures are equal. A hypothetical air–water table elevation, \( z_{aw} \), is also defined within the oil lens at which location gauge water pressure is zero. This (locally) hydrostatic system is depicted in Fig. 1. It shows a hypothetical screened well and the respective fluid ‘table’ interfaces for the three phase of air (\( z_{oa} \)), oil (\( z_{ow} \)), and water (\( z_{aw} \)). The various fluid ‘table’ elevations are defined38 as:

\[
\begin{align*}
  z_{aw} &= z_{ow} + \rho_w H_o \\
  z_{ow} &= (z_{aw} - \rho_o z_{oa})/(1 - \rho_o) \\
  H_o &= z_{oa} - z_{ow}
\end{align*}
\]

where \( \psi_w = z_{aw} \); \( \psi_o = \rho_o z_{oa} [\text{L}] \); \( z \) is elevation above an arbitrary datum [\text{L}]; \( \rho_o \) is the oil specific gravity [\text{L}^{-1}]; and \( H_o \) is the apparent oil thickness [\text{L}].

The vertically integrated governing flow equations for the two phase system can be defined in an areal 2-D domain as:

\[
\begin{align*}
  \frac{\partial V_w}{\partial t} &= \frac{\partial}{\partial x} \left( T_w \frac{\partial z_{aw}}{\partial x} \right) + \frac{\partial}{\partial y} \left( T_w \frac{\partial z_{aw}}{\partial y} \right) + J_w \\
  \frac{\partial V_o}{\partial t} &= \frac{\partial}{\partial x} \left( T_o \frac{\partial z_{oa}}{\partial x} \right) + \frac{\partial}{\partial y} \left( T_o \frac{\partial z_{oa}}{\partial y} \right) + J_o
\end{align*}
\]

where \( V_w \) and \( V_o \) are the water and oil volumes per horizontal area \([\text{L}^2 \cdot \text{T}^{-1}]\), respectively, at a location in the \( x-y \) plane; \( T_w \) and \( T_o \) are water and oil transmissivities \([\text{L}^2 \cdot \text{T}^{-1}]\); \( J_w \) and \( J_o \) are vertically integrated source–sink terms for water and oil \([\text{L}^3 \cdot \text{T}^{-1}]\); \( x \) and \( y \) are Cartesian horizontal–spatial coordinates [\text{L}]; and \( t \) is time [\text{T}].

The saturation–capillary pressure model used in the analysis is an extension of the van Genuchten (VG) model.
The three-phase van Genuchten model is defined as:

\[ S_w = (1 - S_m) \left[ 1 + (\alpha \beta_{so} h_{ow})^{n} \right]^{-m} + S_m \] (3a)

\[ S_i = (1 - S_m) \left[ 1 + (\alpha \beta_{so} h_{oi})^{n} \right]^{-m} + S_m \] (3b)

where \( S_w \) is water saturation; \( S_i \) is total liquid saturation which includes water and oil; \( S_m \) is the irreducible water saturation at which capillary heads appear to extrapolate to infinity; \( h_{ow} = (1 - \rho) (z - z_{ow}) \) is the oil–water capillary head [L]; \( h_{oi} = \rho \alpha (z - z_{oi}) \) is the air–oil capillary head [L]; \( \alpha \) [L\(^{-1}\)] and \( n \) [L\(^{0}\)] are VG model parameters specific to the soil media with \( m = 1 - 1/n \); \( \beta_{so} \) is a scaling parameter that is approximated by the ratio of water surface tension to oil surface tension; and \( \beta_{oi} \) is another scaling parameter approximated by the ratio of water surface tension to oil–water interfacial tension.

Residual oil in the saturated and unsaturated zones is defined to permit predicting the effects of drawdown and water table fluctuation upon the free oil recovery process. Total oil specific volume is accounted for in the system as:

\[ V_r = V_{or} + V_{ocr} + V_{og} \] (4a)

where \( V_r \) is the total oil specific volume per unit area [L\(^3\)-L\(^{-3}\)]; \( V_{or} \) is the free oil specific volume [L\(^3\)-L\(^{-3}\)]; \( V_{ocr} \) is the residual oil specific volume in the saturated zone caused by oil entrapment during water imbibition (i.e., rising water table) [L\(^3\)-L\(^{-3}\)]; and \( V_{og} \) is the residual oil specific volume in the unsaturated zone due to retention after gravity drainage [L\(^3\)-L\(^{-3}\)]. Total residual oil volume is the sum of \( V_{or} \) and \( V_{og} \).

Fluid entrapment occurs with fluctuations of \( z_{on} \) and \( z_{om} \). The rising and lowering of the water table and associated fluid ‘table’ interfaces affect the values of \( V_{or} \) and \( V_{og} \). Also, the initial infiltration and redistribution events at an oil spill site are important in how they occur and their effects on residual oils. \(^{26}\) The respective oil quantities are determined from the fluid entrapment model of Parker et al. \(^{37}\) by numerical integration and are evaluated via the following empirical functions:

\[ V_{or} = \phi S_{or} F(z_{on} - z_{on}^{\min}) \] (4b)

\[ V_{og} = \phi S_{og} (z_{og}^{\max} - z_{og}) \] (4c)

where \( \phi \) is the porosity [L\(^3\)-L\(^{-3}\)]; \( S_{or} \) is the maximum entrapped oil saturation in the saturated zone; \( F \) is a factor that provides a measure of total oil specific volume prior to water imbibition and varies between 0 and 1, \( F = 0 \) (small oil volume) to \( F = 1 \) (large oil volume) [L\(^0\)]; \( z_{on}^{\min} \) is the historical minimum oil–water table elevation since oil has reached a given areal location; \( S_{og} \) is the residual oil saturation in the unsaturated zone; \( z_{og}^{\max} \) is the historical maximum air–oil table elevation since oil has reached a given area location; and \( z_{on} \) and \( z_{om} \) are the current oil–water and air–oil table elevations at a given location, respectively. Typical values for \( S_{or} \) are in the range of 0.2 to 0.4 and values for \( S_{og} \) are 0.04 to 0.08. \(^{37}\)

The factor \( F \) is related to \( H_{ow}^{\max} \) (the maximum historical apparent oil thickness), that has occurred at the specific areal location prior to water imbibition. This is used to compute values for the function \( F(H_{ow}^{\max}) \) once for each soil type and for various imposed histories of \( z_{on} \) and \( z_{om} \). \(^{37}\) Similar relationships are defined and utilized in ARMOS to calculate other equation variables.

### 3.2 Optimization methodology

The proposed S/R/O model computes the optimized pumping rates required to minimize residual oil subject to a constraint on final free oil volume. This combination of objective and constraint actually maximizes free oil recovery while minimizing residual oil. This can be explained by first defining total oil in the system as the sum of three components:

\[ V_{tot} = V_{rs} + V_{ro} + V_{fo} \] (5a)

where \( V_{tot} \) (same as \( V_r \)) is total oil volume [L\(^3\)]; \( V_{rs} \) is total residual oil volume \( (V_r + V_{og}) \) [L\(^3\)]; \( V_{ro} \) is total recovered oil from the well [L\(^3\)]; and \( V_{fo} \) is total remaining free oil volume [L\(^3\)]. Hereafter, total residual oil volume will be referred to as ‘residual oil volume’. Objectives are to recover as much free oil as possible from the system, to minimize residual oil left behind, and to reduce total free oil volume in the system. If a pumping strategy can be determined so that the maximum amount of oil is recovered while minimizing residual oil and forcing the free oil volume to a known quantity or preselected value (for example, less than or equal to some specified percentage of the initial free oil volume), then subtracting \( V_{fo} \) from both sides of eqn (5a) yields a known on the left hand side and two unknowns (extracted and residual oil volumes) on the right. In that case, minimizing residual oil is the same as maximizing oil recovery:

\[ V_{tot} - V_{fo} = V_{rs} + V_{ro} \] (5b)

\[ \therefore \text{Minimizing } V_{rs} = \text{Maximizing } V_{ro} \] (5c)

The problem formulation is developed for a single well pumping water at varying rates for multiple pumping stress periods (later termed pumping periods). The well consists of a dual-pumping system that extracts water and oil simultaneously. The water pump and screen are located at an elevation below the oil/water interface and only extract water. Oil is extracted via separate skimmer pump and screen.

The model formulation for optimizing free oil recovery by pumping water and oil for a specific planning period is represented mathematically as:

\[ \text{Minimize } Z = V_{rs} \] (6)

Subject to the constraints:

\[ V_{fo} \leq V_{U} \] (7a)
\[ P_1 \leq P_2 \leq P_3 \]  
(7b)

\[ V_{n0} = F_1 \{ P_1, P_2, P_3 \} \]  
(7c)

\[ V_{f0} = F_2 \{ P_1, P_2, P_3 \} \]  
(7d)

where \( Z \) is the objective function of minimum residual oil volume \( (V_{n0}) \); \( V_{f0} \) is the free oil volume; \( V_{f0}^u \) is the upper bound on free oil volume; \( P_t \) is water pumping rate during pumping periods \( (t = 1, 2, \text{ and } 3) \); \( F_1 \{ P_t \} \) is a response function describing residual oil volume \( (V_{n0}) \) remaining after pumping at varying rates in pumping periods \( (t = 1, 2, \text{ and } 3) \); \( F_2 \{ P_t \} \) is a response function describing free oil volume \( (V_{f0}) \) remaining after pumping at varying rates in pumping periods \( (t = 1, 2, \text{ and } 3) \). Eqn (7a) describes the constraint that final free oil volume must not exceed a prescribed value (upper bound). Eqn (7a) will always be a tight constraint or binding, because without any pumping, the final free oil volume would exceed this upper bound. Therefore, the final free oil volume is selected and known before optimization.

Eqn (7b) describes the constraint of requiring monotonic, increasing water pumping rates at the well. Parker et al.\textsuperscript{37} stated that oil entrapment could probably be reduced by implementing a stepped (gradually increasing) pumping strategy for oil recovery, but did not prove that by simulation. This idea was incorporated into our optimization model formulation by adding a stepwise pumping requirement (eqn (7b)) to ensure that pumping cannot decrease with respect to time.

The decision variables in the above formulation are the water pumping rate for each pumping period. Oil extraction is a result of oil flow due to pumping and water table drawdown around the well. The assumed boundary condition for oil recovery is zero oil thickness in the well. The oil pumping rate is sufficient that all product entering the well is removed, leaving no accumulated oil (well oil thickness is negligible compared to the thickness of the floating plume). The effect of water pumping on oil recovery is described through the state variables of residual oil volume and free oil volume, eqns (7c) and (7d), respectively.

The model formulation includes response functions (eqns (7c) and (7d)) relating nonlinear system response to transient, variable pumping stimuli for a specified planning period. Response functions for residual oil and free oil area are developed using a set of ARNOS simulations followed by regression analysis. Specific response functions developed in Section 4.3 for an illustrative example use a power law relationship for regression. These functions describe the relationships between state variables and pumping and are determined by optimizing the regression analysis using MINOS.\textsuperscript{33} Optimal stepwise pumping strategies are also computed utilizing MINOS. MINOS is an optimization algorithm available for solving linear or nonlinear problems. It solves nonlinear problems using projected Lagrangian and augmented reduced-gradient algorithms.\textsuperscript{33}

### 3.3 Minimizing residual oil

Our remediation objective (eqn (6)) is to minimize residual oil subject to a free oil volume constraint (eqn (7a)). The computed stepwise pumping strategy contains the floating oil plume and provides for adequate time-varying drawdown to cause oil flow towards the recovery well. Containment is desired to prevent expansion and migration of free oil away from the recovery well. Drawdown is necessary to provide for efficient oil recovery by maintaining an adequate gradient toward the recovery well.

To realize why a stepped pumping strategy is desirable, consider how low and high steady (constant) pumping rates affect free product lens surrounding the pumping well. At very low pumping rates, the plume continues to spread laterally, free oil moves away from the well, and residual oil increases. On the other hand, a much greater pumping rate might capture the entire free oil lens, but the greater pumping causes increased drawdown, a larger cone of depressing, and more residual oil in the depressed region.

Increasing drawdown increases oil entrapment. A tradeoff exists between extracting free oil and causing its entrapment. The tradeoff changes with time as the free product lens shrinks and the water gradient needed to maintain oil flow toward the well changes.

Pumping that increases in steps (stepwise pumping) can help maintain the proper gradient towards the well. A balance between preventing oil plume spreading and causing a large drawdown is needed. To address this, the S/R/O model constrains final free oil volume to compute an optimal stepwise pumping strategy that minimizes residual oil while achieving plume containment. This is discussed further in the following section by contrasting steady versus stepwise pumping strategies and examining the effects on recovered oil, residual oil, and free oil volumes.

### 4 APPLICATION AND RESULTS

#### 4.1 Problem description

A hypothetical LNAPL problem was developed consisting of a plume of gasoline lying in a single layer, unconfined aquifer. A single pumping well is located at the center of the plume. The assigned finite element mesh has 361 nodes, and is symmetrical about the well. The finest mesh spacing is 3 meters near the well (Fig. 2). The initial water table gradient is approximately 0.312% (0.50/160 m). Initially the oil plume is floating on the water table. The size of the study area is large enough that the oil plume never reaches the boundaries. Dirichlet boundary conditions are used on all sides of the study area. Soil and fluid properties are assumed to be homogeneous and isotropic (Table 1) and appropriate for a gasoline spill in a medium sand aquifer.
The gasoline spill volume in the problem is approximately 164 m$^3$. Initial conditions for the floating plume (Fig. 3) were simulated using ARMOS and are based on oil depths measured in field monitoring wells at the site. The contours of total oil specific volume in Fig. 3 represent the sum of both free and residual oil volumes. Initial simulation results also indicated that negligible residual oil exists in the system. The study area has not experienced fluctuations in the water table. The initial total LNAPL spill area predicted by ARMOS at time = 0.0 is 4475 m$^2$.

4.2 Predicting the results of the unmanaged scenario

The unmanaged scenario or 'do nothing strategy' is discussed here. If the oil plume is left alone and no attempt is made to remediate it, simulation indicate that after 360 days residual oil volume and total spill area will be about 28 m$^3$ and 7200 m$^2$, respectively. The change in total spill area represents a 60% increase from initial conditions. Figure 4 shows a contour plot of the total oil specific volume distribution after 360 days. It is a true indicator of total oil contamination (residual and free oil) remaining at the site. Figure 4 also shows how the oil plume has spread and expanded since initial conditions (Fig. 3). ARMOS estimates that after 2 years (720 days) with no pumping, residual oil volume will be 46.2 m$^3$, free oil area equal to 7402 m$^2$, and total LNAPL spill area will equal 8190 m$^2$ (83% increase in total spill area).

4.3 Developing regression equations

A time lag exists between water pumping and significant oil lens response. This lag differs with each site—depending upon soil and fluid properties, water table gradient, and

![Fig. 3. Initial conditions for LNAPL plume: contours of total oil specific volume in meters.](image-url)

![Fig. 4. Unmanaged scenario (no pumping) for LNAPL plume after 360 days: contours of total oil specific volume in meters.](image-url)
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Table 2. Regression equations for residual oil and free oil volume response to pumping from one well

<table>
<thead>
<tr>
<th>Variable type</th>
<th>Pumping period</th>
<th>Coefficient values ($\beta_i$)</th>
<th>Exponent values ($E_i$)</th>
<th>Pumping range for equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Residual oil vol.</td>
<td>1</td>
<td>0.000807</td>
<td>1.907144</td>
<td>50–200 m$^3$/day</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0.808685</td>
<td>0.571138</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>4.753794</td>
<td>0.460634</td>
<td></td>
</tr>
<tr>
<td>Free oil volume</td>
<td>1</td>
<td>22,958.69</td>
<td>-1.989796</td>
<td>50–200 m$^3$/day</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>331,461.16</td>
<td>-2.303800</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1,542,692.60</td>
<td>-2.300906</td>
<td></td>
</tr>
</tbody>
</table>

Note: Planning period is 360 days with three 120 day pumping periods. Pumping rates can vary and increase with each pumping period.

floating plume characteristics (i.e. oil thickness, plume size, shape of the plume). Too small a pumping rate will not significantly affect the lens within a reasonable time period.

The S/R/O model requires response functions describing the response of residual oil volume and free oil volume to pumping. Preliminary simulations of system response to steady water pumping helped guide design of the response functions—selection of: (a) minimum and maximum potential pumping rates, (b) number of pumping periods and (c) reasonable total planning period for oil recovery. Early selection of these three parameters helps reduce the total number of computer simulation runs required to develop the response functions and to define a more manageable solution space prior to the optimizing step. Therefore, it is imperative that preliminary simulations be performed to establish a range for each parameter.

It should be noted that the range of values for pumping rates, the length and/or number of pumping periods, and the total pumping time will be highly dependent upon site specific conditions. It is only reasonable to say that the number of simulations, including time constraints on computing time and resources, will dictate the level of effort expended to achieve optimality within the solution space. This is a restrictive element upon which a final optimal pumping strategy can be determined by the S/R/O model.

A total of 13 preliminary simulations were run for steady pumping rates ranging from 15 to 240 m$^3$/day over a time period of 420 days (run time was 4.5 h on a SUN SPARC/IXP work station). Results of the preliminary steady pumping simulations showed that the lowest pumping rate which prevented the oil lens from further expansion was approximately 70–80 m$^3$/day. The highest pumping rate at which oil recovery did not improve significantly was 200 m$^3$/day. Also, oil recovery reached a maximum threshold after about 360 days using the highest pumping rate. Lag time was observed to be about 90–100 days for the lower pumping rates (time required before the oil plume decreased in size and thereafter did not increase). Thus, a pumping range of 50–200 m$^3$/day and a 360 day planning period consisting of three 120 day pumping periods were selected for developing the response functions. The one year planning horizon and 120 day pumping periods were considered reasonable and practical for implementation in the field.

The following process was used to actually create the response functions. A matrix of 30 incrementally increasing stepwise pumping strategies was devised to cover the specified range of pumping values. These three-period pumping strategies were simulated by ARMOS in approximately 9.5 h on a SUN SPARC/IXP work station. The results were summarized and analyzed by attempting to fit several regression equation types (i.e. linear, quadratic, and polynomial) to the data.

A power law relationship provided the best predictive accuracy. This is reasonable since the governing equations of multiphase flow are nonlinear. Furthermore, it was clear from the simulation results that the residual oil and free oil relationships must be increasing and decreasing functions, respectively. This was used to establish the sign of the respective exponents in each relationship. The regression analysis performed by minimizing the sum of squared residuals between observed and predicted values yielded nonlinear regression relationships of the following general form:

$$Y_n = \sum_{t=1}^{3} \beta_{nt} P_t^E$$

where $Y_n$ is the dependent variable for residual and free oil volume, respectively, $(n = 1, 2)$; $P_t$ is the independent variable for water pumping rates during pumping periods $(t = 1, 2, \text{and } 3)$; $\beta_{nt}$ and $E_{nt}$ are the coefficient and exponent for each dependent variable respectively, for pumping periods $(t = 1, 2, \text{and } 3)$. Coefficient and exponent values for the regression equations are given in Table 2. Coefficients of determination equal 0.9984 and 0.9898 for the residual oil and free oil volume equations, respectively.

4.4 Computing optimal stepwise pumping strategies and post-optimization results

The model consisting of eqns (6)–(7d) illustrate application of the E constraint method of solving a multi-objective optimization problem. The primary objective is displayed as minimizing residual oil remaining after pumping (eqn (6)). The secondary objective is to remove free oil (this is accomplished via eqn (7a) which limits the amount of free oil remaining after pumping).

Applying the E constraint method requires performing several optimizations, each employing a different bound on the secondary objective. Here, ten values of free oil volume ($V_r$) were preselected and used as the upper bound on $V_n$ (i.e. used as $V_{r0}$) for ten optimization scenarios
Table 3. Optimal stepwise pumping strategies computed by S/R/O model for one well

<table>
<thead>
<tr>
<th>Strategy number</th>
<th>Free oil vol. U.B. (m³)</th>
<th>Pumping rate period (1) (m³/day)</th>
<th>Pumping rate period (2) (m³/day)</th>
<th>Pumping rate period (3) (m³/day)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>25.5</td>
<td>72.61</td>
<td>121.98</td>
<td>147.52</td>
</tr>
<tr>
<td>2</td>
<td>23.5</td>
<td>74.61</td>
<td>126.57</td>
<td>153.31</td>
</tr>
<tr>
<td>3</td>
<td>21.5</td>
<td>76.87</td>
<td>131.79</td>
<td>159.89</td>
</tr>
<tr>
<td>4</td>
<td>19.5</td>
<td>79.43</td>
<td>137.77</td>
<td>167.45</td>
</tr>
<tr>
<td>5</td>
<td>17.5</td>
<td>82.37</td>
<td>144.74</td>
<td>176.28</td>
</tr>
<tr>
<td>6</td>
<td>15.5</td>
<td>85.82</td>
<td>153.00</td>
<td>186.77</td>
</tr>
<tr>
<td>7</td>
<td>13.5</td>
<td>89.93</td>
<td>163.03</td>
<td>199.52</td>
</tr>
<tr>
<td>8</td>
<td>13.0</td>
<td>93.00</td>
<td>170.63</td>
<td>200.00</td>
</tr>
<tr>
<td>9</td>
<td>12.5</td>
<td>96.86</td>
<td>180.28</td>
<td>200.00</td>
</tr>
<tr>
<td>10</td>
<td>12.25</td>
<td>99.02</td>
<td>185.75</td>
<td>200.00</td>
</tr>
</tbody>
</table>

Note: U.B. is \( V_{fo} \) (upper bound value) in constraint eqn (7).

(Table 3). The \( V_{fo} \) varied between 7.5 and 15% of the initial free oil volume (164 m³). The S/R/O model was run separately for each different \( V_{fo} \) value. Mathematically optimal stepwise pumping strategies were calculated by the S/R/O model for each scenario (Table 3). The upper bound on \( V_{fo} \) was binding (the value of \( V_{fo} \) precisely equaled \( V_{fo}^{ub} \)) for all scenarios (i.e. minimizing residual oil was equivalent to minimizing free oil recovery for the \( V_{fo} \) remaining).

The upper curve in Fig. 5 illustrates the tradeoff between the objectives of minimizing residual oil and maximizing free oil removal. The strategy having the smallest total pumping is at the left end of the curve. The best optimal strategy is at the top of the curve (all are optimal pumping strategies). Increasing pumping beyond that of the best strategy reduces free oil removal while increasing residual oil.

Normally, one performs post-optimization simulations to demonstrate that the accuracy of the employed simulation expressions (the regression expressions here) were acceptable (i.e. that the S/R/O model suitably considered system response to pumping while optimizing). Thus, in these verification simulations, computed optimal pumping rates were used as ARMOS inputs. Error (difference in \( V_{n} \) and \( V_{fo} \) computed by S/R/O model versus that computed later by simulation model) was greatest for strategies 1 and 10 (Table 4) because these had pumping rates at the limits of the range of data used to develop the regression equations. Error was insignificant for strategies in the center of the range and varied between 1 and 2% for residual oil volume values and 1–13% for the free oil volume values.

### 4.5 Comparing stepwise vs steady pumping strategies

It is illustrative to contrast the computed stepwise pumping strategies with the best steady pumping strategies one could possibly develop. This comparison was made because employing steady pumping is standard practice. The best steady pumping rate for a single well system could be determined by simulation only without applying formal mathematical optimization. This was accomplished by making many different ARMOS simulations, each differing only in the steady water pumping rate that was used. Employed steady pumping rates ranged from 74 to 210 m³/day.

Figure 5 illustrates oil recovery performance of the steady pumping strategies. Again notice that increasing pumping beyond a certain point is counterproductive. The best (empirically optimal) steady pumping rate is

![Graph](image)

Fig. 5. Plot of (%) recovered oil versus (%) residual oil (360 days) for comparison of optimal stepwise pumping vs steady pumping strategies.

Table 4. Residual and free oil volumes: predicted by S/R/O model versus simulated ARMOS for optimal stepwise pumping strategies for one well

<table>
<thead>
<tr>
<th>Strategy</th>
<th>Residual oil (m³)</th>
<th>Free oil (m³)</th>
<th>Residual oil (m³)</th>
<th>Free oil (m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>62.86</td>
<td>25.5</td>
<td>64.09</td>
<td>27.39</td>
</tr>
<tr>
<td>2</td>
<td>64.13</td>
<td>23.5</td>
<td>65.47</td>
<td>25.39</td>
</tr>
<tr>
<td>3</td>
<td>65.55</td>
<td>21.5</td>
<td>66.56</td>
<td>23.35</td>
</tr>
<tr>
<td>4</td>
<td>67.15</td>
<td>19.5</td>
<td>67.54</td>
<td>20.91</td>
</tr>
<tr>
<td>5</td>
<td>68.98</td>
<td>17.5</td>
<td>68.25</td>
<td>18.51</td>
</tr>
<tr>
<td>6</td>
<td>71.12</td>
<td>15.5</td>
<td>69.74</td>
<td>15.32</td>
</tr>
<tr>
<td>7</td>
<td>73.64</td>
<td>13.5</td>
<td>72.56</td>
<td>11.04</td>
</tr>
<tr>
<td>8</td>
<td>74.38</td>
<td>13.0</td>
<td>74.64</td>
<td>9.61</td>
</tr>
<tr>
<td>9</td>
<td>75.24</td>
<td>12.5</td>
<td>76.45</td>
<td>8.40</td>
</tr>
<tr>
<td>10</td>
<td>75.72</td>
<td>12.2</td>
<td>79.46</td>
<td>7.20</td>
</tr>
</tbody>
</table>

Note: Optimal stepwise pumping strategies determined by the S/R/O model (Table 3) and post-optimization simulations performed by ARMOS.
168.4 m$^3$/day. The best (mathematically optimal) stepwise pumping strategy has rates of 89.93, 163.03, and 199.52 m$^3$/day.

Note that the stepwise strategy recovers more oil and leaves less residual oil behind. Even the poorest optimal stepwise strategy recovers about as much oil as the best steady strategy, and causes less residual while requiring less total pumping.

Table 5 summarizes simulated response to the best pumping strategies. The best optimal stepwise strategy recovers 11.5% more oil and causes 15.0% less residual oil than the best steady pumping strategy. The best optimal stepwise pumping strategy requires less total pumped water in 360 days (44200 m$^3$) than the best steady pumping strategy (49400 m$^3$).

Figure 6 further contrasts steady and stepwise strategies. It shows final oil volumes for three steady and three stepwise strategies taken from Fig. 5. These are the strategies having the least, best and greatest pumping for the steady and stepwise approaches respectively. The stepwise pumping strategies provide more oil recovery and cause less residual oil than the steady pumping strategies.

Examining free oil area changes with time helps explain why time-varying stepwise pumping improves oil recovery. Figure 7 compares free oil area ($FO_a$) versus time for the unmanaged scenario and three pumping strategies. Free oil is not contained and continues to expand for the unmanaged scenario. The low steady pumping rate of 74 m$^3$/day achieves containment (final $FO_a = 4664$ m$^3$) with some lateral spreading, but oil recovery is low compared to other pumping strategies (Fig. 6). In this case, insufficient gradient is produced to draw much free oil into the recovery well. At the higher best optimal steady pumping rate of 168 m$^3$/day, oil recovery is improved and free oil area decreases significantly to 712 m$^3$, but residual oil dramatically increases (Fig. 6).

The plot of $FO_a$ for the best optimal stepwise pumping strategy lies between those of the two steady pumping strategies (final $FO_a = 982$ m$^3$). Figure 7 shows that there is no immediate increase or decrease in $FO_a$ for the time-varying, stepwise pumping. Instead, $FO_a$ increases only slightly up to about 180 days of pumping. After 180 days $FO_a$ decreases as oil is removed and pumping increases to maintain sufficient drawdown and oil flow towards the recovery well.

Figures 8 and 9 show how the three oil volumes change with time for the best optimal steady and optimal stepwise pumping strategies, respectively. For steady pumping, recovered and residual oil volumes initially increase at approximately the same rate, but residual oil exceeds recovered oil after 180 days of pumping (Fig. 8). However, the results from stepwise pumping show that recovered oil volume is always greater than residual oil for the entire pumping period of 360 days (Fig. 9). Over the long term, stepwise pumping creates less residual oil than steady pumping, permitting more free oil recovery.

Final total oil specific volume contours (representing the

### Table 5. Pumping rates and simulation results for best single-well pumping strategies

<table>
<thead>
<tr>
<th>Best scenario</th>
<th>Pumping rate (m$^3$/day)</th>
<th>Recovered oil volume (m$^3$)</th>
<th>Residual oil volume (m$^3$)</th>
<th>Free oil volume (m$^3$)</th>
<th>Free oil area (m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steady</td>
<td>168.40</td>
<td>72.45</td>
<td>85.38</td>
<td>6.57</td>
<td>712</td>
</tr>
<tr>
<td>Optimal stepwise</td>
<td>89;163;199</td>
<td>80.80</td>
<td>72.56</td>
<td>11.04</td>
<td>982</td>
</tr>
</tbody>
</table>

Note: Values shown are results after simulating for 360 days at given pumping rates. Initial free oil area = 4475 m$^3$. Total oil volume = 164.4 m$^3$. 

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**Fig. 6.** Total oil volumes after oil recovery (360 days) for selected steady and stepwise pumping strategies.

**Fig. 7.** Plot of free oil area versus time (360 days) for selected pumping strategies.
sum of residual and free oil volumes) resulting from the best optimal stepwise pumping strategy (Table 3, No.7) are shown in Fig. 10. The oil plume is contained and total oil specific volume has decreased significantly. Final total spill area equals 5194 m² compared to 4475 m² initially. The best optimal stepwise strategy removed approximately 49% (80.80 m³) of the free oil volume after 360 days. By comparison, the unmanaged scenario yields no oil removal, a residual oil volume of 17% (28.09 m³) and a total spill area equal to 7200 m² after one year. After two years residual oil is 28% (46 m³) and total spill area equals 8190 m² for the unmanaged scenario.

5 SUMMARY AND CONCLUSIONS

The presented modeling approach optimizes free phase LNAPL recovery for a single dual-extraction well in a homogeneous, isotropic unconfined aquifer. Optimal free oil recovery is achieved by minimizing residual oil subject to a free oil volume constraint. By minimizing residual oil, more free oil is available for recovery and recovered oil is maximized. The best-optimal solution is at least locally optimal—global optimality cannot be mathematically proven for such a nonlinear problem.

The developed S/R/O model computes optimal time-varying, increasing stepwise pumping strategies at a single recovery well for a selected final free oil volume. In this case stepwise pumping improves free oil recovery by reducing residual oil. Optimized stepwise pumping strategies recover more free oil and cause less residual oil for a specified planning period than the best steady pumping strategy.

The stepwise strategies better manage drawdown and water table gradients for oil recovery. Stepwise pumping improves free oil recovery and manages the free oil plume better than steady pumping because: (1) the free-product is more gradually captured and drawn into the recovery well; (2) the optimal water table gradient is maintained better (compensating for decreasing free oil volume and a rising water table); (3) the stepped drawdown does not create excessive residual oil due to a deep cone of depression. All this is accomplished with less water pumping than the best steady pumping strategy.

The complexity of heterogenous conditions and well interference between multiple wells were not considered. Notwithstanding, regression analysis can be performed and response functions developed for a variety of problem applications. The proposed S/R/O methodology should be applicable to other free oil recovery problems. Post-optimization simulations should be used to verify the performance and robustness of computed remediation strategies. The S/R/O model approach offers promise for enhancing the design and operation of free phase LNAPL recovery systems.
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REFERENCES


