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S/O MODELING TECHNIQUE FOR OPTIMAL CONTAINMENT OF LIGHT HYDROCARBONS IN CONTAMINATED UNCONFINED AQUIFERS

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ABSTRACT

An innovative approach is presented to minimize pumping for immobilizing a floating plume of a light non-aqueous phase liquid (LNAPL). The best pumping strategy is determined to contain the free oil product and provide for gradient control of the water table. This approach combined detailed simulation, statistical analysis, and optimization.

This modeling technique uses regression equations that describe system response to variable pumping stimuli. The regression equations were developed from analysis of systematically performed simulations of multiphase flow in an areal region of an unconfined aquifer. Simulations were performed using **ARMOS**, a finite element model. **ARMOS** can be used simulate a spill, leakage from subsurface storage facilities and recovery of hydrocarbons from trenches or pumping wells to design remediation schemes.

Two gradient control points were located inside the area of the symmetric floating plume. Air-oil interface drawdowns with respect to water pumping rates were taken from **ARMOS** simulations at the two locations. These drawdowns were used to calculate elevation changes in air-oil table elevations (Z_{ao}) between the control points. These elevation changes of Z_{ao} between Points #1 and #2 versus pumping were plotted and fitted by statistical regression analysis for a pumping range of 150 m^3/day to 240 m^3/day. The resulting regression equation

was used to represent system response to pumping in the simulation/optimization (S/O) model called Utah State Model for Optimizing Management of Stream/Aquifer Systems Using the Response Matrix Method (**US/REMAX**). The containment problem was then optimized by **US/REMAX** to determine the minimum pumping rate required to reverse the water table gradient and immobilize the floating plume.

Once regression equations are developed the optimal pumping state for alternative containment goals and scenarios can be quickly determined. A range of gradient control values can be easily evaluated to determine minimized pumping rates. Then, their impacts can be compared between alternatives for minimum pumping versus time to containment, residual or trapped oil volumes, and free oil area at containment time.

INTRODUCTION

Over the last 40 years, groundwater aquifers have been contaminated by a wide range of inorganic and organic chemicals. Regulatory agencies, contractors, and clients responsible for cleanup need feasible and cost-effective strategies for remediating contamination sites.

Contamination sites associated with light non-aqueous phase liquids (LNAPL) are numerous and represent difficult cleanup problems (Gangadharan, 1988). Sources of LNAPL contamination include long-term leakage from underground storage tanks, pipeline leaks, transportation accidents involving vehicles carrying hazardous chemical, and uncontrolled or unauthorized discharge of industrial hydrocarbon contaminants. These contamination sites have created numerous environmental problems that will be with us for years to come. In many circumstances, the contamination is not detected immediately after the discharge and groundwater aquifers across the United States have been exposed to continously increasing contamination problems.

Once groundwater contamination is detected, remediation actions are usually implemented based on a plan of environmental and management goals. Environmental goals establish soil and water quality standards necessary for cleanup. Management goals include two components. First, applicable remediation methods are identified and selected to accomplish site cleanup. Second, a management plan is developed to outline the sequence of remediation steps necessary so desired environmental goals can be achieved.

In most situations natural biodegradation or attenuation of contaminants is inadequate. Thus, some remediation is required. Typically, groundwater contamination remediation includes three tasks: plume containment, extraction, and in-situ remediation. Containment involves containing, immobilizing, or preventing the spread of contamination in the aquifer. Extraction involves extracting LNAPL product and/or treating contaminated water using pumping wells. In-situ remediation includes remediating the residual/trapped contaminants found in the aquifer by soil venting, enhanced bioremediation, etc.

In particular, this paper focused on the task of containment of a floating LNAPL plume. Containment is part of the remediation actions taken to capture the free oil product that is not considered part of the residual oil, but is free to move through the soil media. The immobilization of the free oil plume helps to prevent further spreading of contaminants down-gradient from the source.

THEORY

Remediation methods for cleanup of LNAPL contaminant plumes have evolved with the development of various technologies for pump-and-treat, soil venting, etc. (Johnson et al., 1990). Many researchers have evaluated the effectiveness of remediation techniques, as well as attempted to improve their efficiency. Their efforts have included the development of computer simulation models to predict and analyze the flow of water, air, and nonaqueous phase liquids in the subsurface soil media. The numerical models were developed for multiphase flow in the unsaturated and saturated zones using finite difference methods (Abriola and Pinder, 1985; Faust, 1985) and finite element methods (Huyakorn and Pinder, 1978; Kuppusamy, et al., 1987).

Kaluarachchi and Parker (1989) developed a new numerical modeling method for multiphase flow of LNAPL's and oil recovery. The finite element method was devised using upstream weighting techniques and influence coefficient methods for evaluating element matrices. These techniques greatly improved the efficiency and accuracy of finite element methods for simulating multiphase flow. A finite element model called Areal Multiphase Organic Simulator, **ARMOS** (ES&T, 1991), was developed to incorporate these improved modeling techniques (Parker and Kaluarachchi, 1989; Kaluarachchi et al., 1990;). The same model was enhanced and updated to account for residual oils in the vadose zone and trapped oils in the saturated zone (ES&T, 1991). The application and use of **ARMOS** has been illustrated and compared to other multiphase models. It appears to be an accurate and efficient model for simulating LNAPL spill and recovery operations (Kaluarachchi et al., 1990; Kaluarachchi and Parker, 1990).

Deterministic Multiphase Flow Model

The numerical model **ARMOS** uses 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 (Parker and Lenhard, 1989). The use of vertically integrated flow equations also reduces the severe nonlinearity associated with three-phase constitutive relationships.

It is assumed in **ARMOS** that the time factor for vertical redistribution of fluids is sufficiently short that vertical pressure distributions are locally approximated by hydrostatic conditions. In such circumstances, the vertical pressure distributions can be characterized for all phases in terms of various fluid "table" elevations (Parker and Kaluarachchi, 1989). Thus, the oil lens is described by an air-oil table elevation, z_{ao}, 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. An air-water table elevation, z_{aw}, is also defined at which location gauge water pressure is zero. Based on hydrostatics conditions ($\partial\psi_w/\partial z=0$ and $\partial\psi_o/\partial z=0$), the following equations can be written:

$$\psi_w = h_w + z \tag{1a}$$

$$\psi_o = h_o + \rho_{ro} z \tag{1b}$$

$$\psi_w = z_{aw} \tag{1c}$$

$$\psi_o = \rho_{ro} z_{ao} \tag{1d}$$

The hydrostatic vertical pressure distributions for air-water and oil-water table elevations is described as:

$$z_{aw} = z_{ow} + \rho_{ro} H_o \tag{2a}$$

$$z_{ow} = (z_{aw} - \rho_{ro} z_{ao})/(1 - \rho_{ro}) \tag{2b}$$

$$H_o = z_{ao} - z_{ow} \tag{2c}$$

where ψ_w and ψ_o are water and oil piezometric heads, respectively; z is elevation above an arbitrary datum; h_w and h_o are water height-equivalent pressure heads in water and oil; ρ_{ro} is the ratio of oil to water density; and H_o is the apparent oil thickness.

The vertically integrated governing flow equations are written as follows:

$$\frac{\partial V_w}{\partial t} = \frac{\partial}{\partial x}\left(T_w \frac{\partial z_{aw}}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_w \frac{\partial z_{aw}}{\partial y}\right) + \overline{J_w} \tag{3a}$$

$$\frac{\partial V_o}{\partial t} = \frac{\partial}{\partial x}\left(T_o \frac{\partial z_{ao}}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_o \frac{\partial z_{ao}}{\partial y}\right) + \overline{J_o} \tag{3b}$$

where V_w and V_o are the water and oil volumes per horizontal area, respectively, at a location in the x-y plane; T_w and T_o are water and oil transmissivities; $\overline{J_w}$ and $\overline{J_o}$ are vertically integrated source-sink terms for water and oil; x and y are Cartesian horizontal-spatial coordinates; and t is time.

The saturation-capillary pressure model used in **ARMOS** is an extension of the van Genuchten model which does not include fluid entrapment (Parker and Lenhard, 1989). The impact of residual oil in the saturated and unsaturated zones are further defined to allow for the effects of drawdown and water table fluctuation upon the free oil recovery process. See Parker et al. (1990) for definitions of residual/trapped oil relationships. The three-phase van Genuchten (VG) model is defined as:

$$S_w = (1 - S_m)\ (1 + (\alpha\ \beta_{ow}\ h_{ow})^n)^{-m} + S_m \tag{4a}$$

$$S_t = (1 - S_m)\ (1 + (\alpha\ \beta_{ao}\ h_{ao})^n)^{-m} + S_m \tag{4b}$$

where S_w is water saturation; S_t is total liquid saturation which includes water and oil; S_m is the "irreducible" water saturation; α and n are VG model parameters specific to the soil media with $m = 1\text{-}1/n$; β_{ao} is a scaling parameter that is approximated by the ratio of water surface tension to oil surface tension; and β_{ow} is another scaling parameter approximated by the ratio of water surface tension to oil-water interfacial tension.

S/O Model Formulation

The objective of the simulation/optimization (S/O) model was to optimize the required pumping for immobilization of the LNAPL plume in a contaminated, unconfined aquifer. The task of containment was accomplished by completing the following items:

1. Develop an approach using the deterministic multiphase flow model, **ARMOS**, to determine system response to pumping (i.e., ΔZ_{ao}), then use elevation changes in Z_{ao} to develop appropriate regression equations that are used in the S/O model.

2. Develop an optimization model to minimize water pumping necessary to capture the free oil product or floating plume and prevent further spreading of the plume due to a water table gradient.

3. Analyze one hypothetical example problem to evaluate the applicability of the S/O model to remediation designs and work encountered by engineers.

The S/O model uses an regression approach proposed by Alley (1986) and Lefkoff and Gorelick (1990) to optimize the pumping for aqueous plume containment. The S/O model was restricted to a single well pumping water at a constant rate. The water pump was located at an elevation below the oil/water interface and only pumped water. The *model formulation* for optimizing plume immobilization by pumping water is:

$$\text{Minimize } Z_1 = P_{ew} \tag{5}$$

Subject to the constraints:

$$[Z_{aw}]_{i,t} < [Z_{aw}]_{j,t} \tag{6a}$$

$$\Delta Z_{ao} \leq [Z_{ao}]_{i,t} - [Z_{ao}]_{j,t} \tag{6b}$$

$$[Z_{aw}]_{i,t} = [Z_{aw}]_{i,0} - [d_{aw}]_{i,t} - P_{ew}\{f_1(P_{ew})_{i,t}\} \tag{6c}$$

$$[Z_{ao}]_{i,t} = [Z_{ao}]_{i,0} - [d_{ao}]_{i,t} - P_{ew}\{f_2(P_{ew})_{i,t}\} \tag{6d}$$

where Z_1 is the objective function of total water pumping for P_{ew} (extraction); Z_{aw} is the air-water table elevation; Z_{ao} is the air-oil table elevation; d_{aw} and d_{ao} are initial air-water and air-oil fluid-table drawdowns, respectively, under unmanaged conditions; $f_1(P_{ew})_{i,t}$ and $f_2(P_{ew})_{i,t}$ are response functions describing fluid-table drawdown per unit pumping rate for Z_{aw} and Z_{ao}, respectively; ΔZ_{ao} is the elevation difference between control points, i and j; t is a given time period; and i (Point #1) and j (Point #2, see Figure 1) represent paired gradient control points. Equation [6a] describes the constraint of requiring a water gradient towards the pumping well. Equation [6b] describes the constraint for gradient control across the down-gradient side of the floating plume towards the pumping well. Equations [6c] and [6d] describe the relationship between changes in fluid-table elevations and pumping rates at the well for Z_{aw} and Z_{ao}, respectively.

EXAMPLE PROBLEM

The following hypothetical contamination problem illustrates the simulation/optimization approach. The study area is 160 meters by 160 meters with a single pumping well located at the center. The initial water table gradient lies left to right across the study area. The water table gradient is approximately 0.312% (0.50/160 m). The domain of the problem lies in a single layer, unconfined aquifer. The study area is shown in Figure 1 and shows the contours of the initial oil lens, direction of the water table gradient, locations of gradient control points, and location of the well.

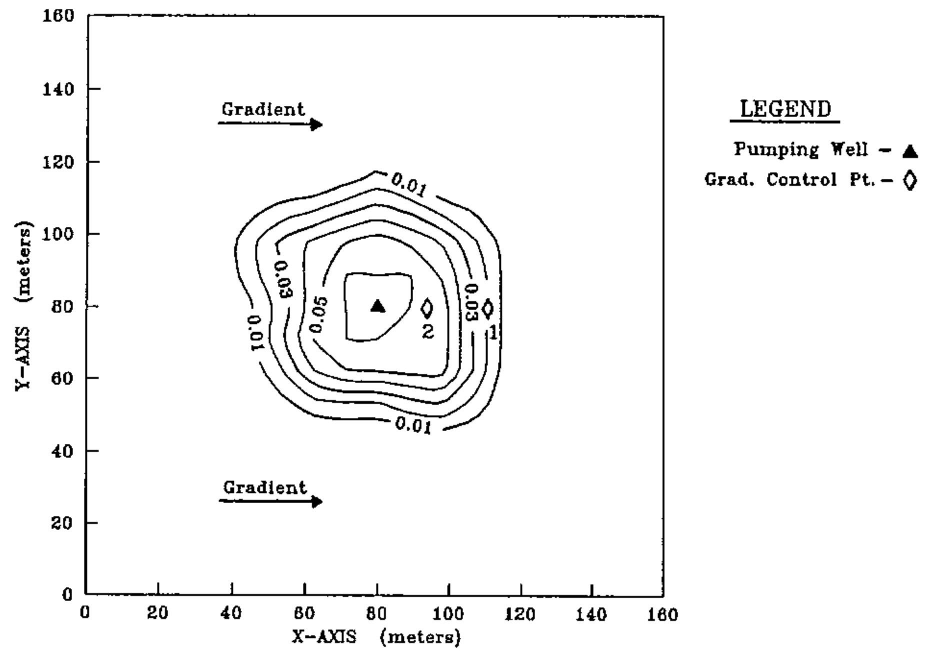

Figure 1 – Contours of LNAPL plume at initial conditions in meters.

Initial conditions consist of an oil plume floating on the water table. The assumption is made that the oil plume never reaches the boundaries. In all modeling simulations, the boundary conditions for the water table are maintained at initial elevations (constant head) on the domain perimeter. The soil and fluid properties for the study area, summarized in Table 1, represent a gasoline spill in a medium sand aquifer.

TABLE 1 - SOIL AND FLUID PROPERTIES

Fluid Properties	Soil Properties
$\rho_{ow} = 0.80$	$K_{sw} = 10$ m/day
$\eta_{ow} = 2.00$	$\phi = 0.41$
$\beta_{ao} = 3.20$	$\alpha = 6.00$
$\beta_{ow} = 1.45$	$n = 2.70$
	$S_m = 0.20$
	$S_{og} = 0.08$
	$S_{or} = 0.21$

Note: ρ_{ow} - ratio of oil to water density; η_{ow} - ratio of oil to water absolute viscosity; β_{ao} - ratio of water surface tension to oil surface tension; β_{ow} - ratio of water surface tension to oil-water interfacial tension; K_{sw} - saturated hydraulic conductivity; ϕ - porosity; α - van Genuchten model curve parameter; n - van Genuchten model exponent; S_m - irreducible water saturation; S_{og} - unsaturated zone residual oil saturation; S_{or} - saturated zone residual oil saturation.

The gasoline spill volume in the problem is approximately 164 m^3. Initial conditions for the floating plume (Figure 1) represent infiltration and redistribution events simulated by **ARMOS**. The study area has not experienced any fluctuations in the water table. Therefore, no residual oil exists in the system initially. The initial total spill area predicted by **ARMOS** (2-D areal multiphase flow model) at time = 0.0 is estimated to be 4475 m^2.

The hypothetical problem was analyzed using a modified version of Utah State Model for Optimizing Management of Stream/Aquifer Systems Using the Response Matrix Method (**US/REMAX**), a linear or nonlinear S/O model. **US/REMAX** (Peralta and Aly, 1993) can be used to analyze and optimize a variety of groundwater management problems. The modified version incorporated a new nonlinear constraint option. It used regression equations to describe system responses to pumping. These equations were generated externally using **ARMOS** and a statistical package. The results of the S/O model are presented below.

RESULTS AND DISCUSSION

The purpose of the analysis is to determine the best pumping strategy to capture or contain the floating plume. The optimization problem objective is to minimize pumping subject to constraints at selected gradient control points. Containment was approached using different variations of the gradient control constraint in the model formulation for three scenarios (Table 2).

TABLE 2 - GRADIENT CONTROL CONSTRAINTS

Scenario	Gradient Control Constraints	System Resp. Type & S/O Model Used
1	$0.02 \leq [Z_{aw}]_{1,t} - [Z_{aw}]_{2,t}$	Z_{aw}: US/REMAX
2	$0.00 \leq [Z_{ao}]_{1,t} - [Z_{ao}]_{2,t}$	Z_{ao}: US/REMAX with ARMOS
3	$0.02 \leq [Z_{ao}]_{1,t} - [Z_{ao}]_{2,t}$	Z_{ao}: US/REMAX with ARMOS

The third column of Table 2 indicates the type of system response function (i.e., air-water or air-oil) used in the S/O model to describe system response to pumping. It also indicates which simulation model was utilized with **US/REMAX** to compute the system response functions, $f_1(P_{ew})$ and $f_2(P_{ew})$.

Air-water table drawdowns for Scenario 1 were calculated directly within **US/REMAX** for the gradient control points without considering the effects of oil. **US/REMAX** utilized **MODFLOW** (McDonald and Harbaugh, 1988) to automatically generate the system response function, $f_1(P_{ew})$. **MODFLOW** does not simulating multiphase flow. The two gradient control points are located east of the well (down-gradient), but lie within the oil plume (Figure 1). For Scenarios 2 and 3, the air-oil table drawdowns were calculated in **ARMOS** from simulation runs for a pumping range of 15 to 240 m^3/day. The simulation runs in **ARMOS** were also done for time periods of 60 to 180 days. Drawdown data for Z_{ao} was then used to calculate the system response function, $f_2(P_{ew})$. Z_{ao} elevation changes between gradient control points (Points #1 and #2) versus pumping rates were plotted and fitted statistically. Based on preliminary simulations, it was estimated that optimal pumping would lie between 150 to 240 m^3/day. Regression equations were fitted to drawdown data for this range of pumping. A plot of ΔZ_{ao} versus pumping is given in Figure 2 for a time simulation of 180 days.

Linear and quadratic regression equations were determined for ΔZ_{ao} versus pumping using different time simulations (length of stress period). The R^2 values for the expressions describing ΔZ_{ao} response to pumping are given in Table 3. To perform the optimization, computed regression equations were substituted into **US/REMAX** as system response functions which represent Equation (6d) for Scenarios 2 and 3. Optimal pumping rates were computed for each scenario using the modified **US/REMAX**. This was done using regression equations for different time simulations (Table 3).

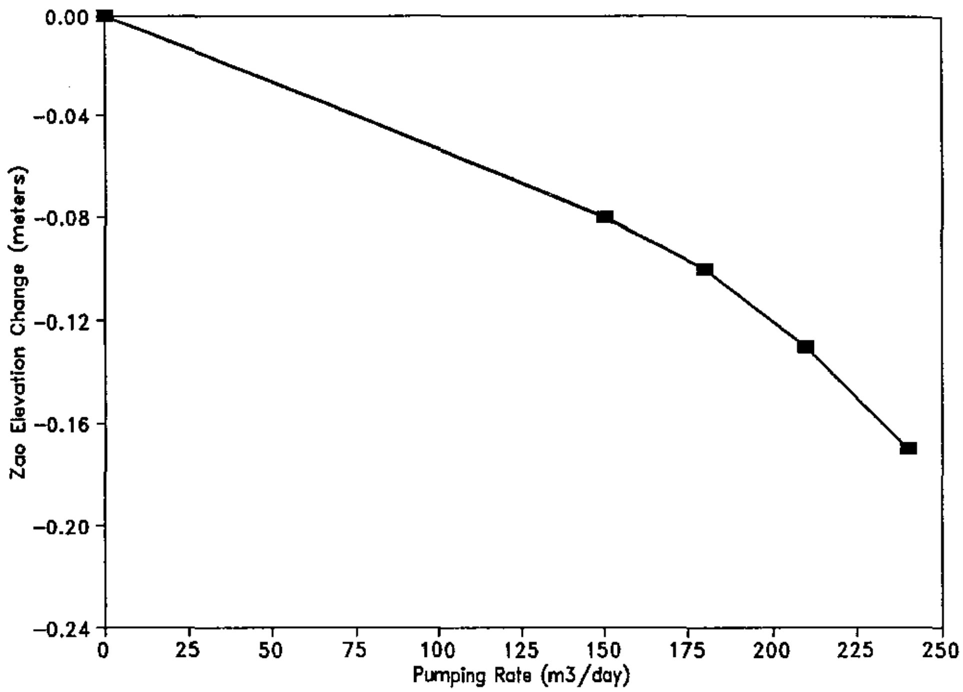

Figure 2 - ΔZ_{ao} between gradient control points #1 and #2 versus water pumping rate at time = 180 days.

A comparison of optimal pumping in Table 3 shows a variation in pumping rates. The optimal pumping rates determined using linear regression equations for different time simulations vary by 25 to 32 m^3/day, depending on which gradient control constraint is examined. The variation in optimal pumping rates derived using quadratic equations is between 5 to 6.5 m^3/day (a 3% variation) for all time simulations and scenarios.

The next step was to verify whether containment of the LNAPL plume was achieved. Tested were the optimal pumping rate for Scenario 1 (115.7 m^3/day) and the optimal pumping rates of 164.5 and 189.9 m^3/day from Table 3 (based on quadratic regression equations and a containment time of 90 days). Post-optimization simulations were performed using **ARMOS.**

Results of simulating the Unmanaged Scenario (no pumping) and the optimal pumping strategies are shown in Table 4. Figures 3 thru 6 show longitudinal cross-sections of the floating plume after 90 days for the Unmanaged Scenario and Scenarios 1-3, respectively. One sees that the oil will continue to spread in the Unmanaged Scenario and in Scenario 1. Clearly, controlling the air-water surface is not enough to immobilize the floating contaminant for Scenario 1. The LNAPL plume is immobilized in Scenarios 2 and 3. Less pumping is required in Scenario 2 than in Scenario 3. Pumping in Scenario 2 leaves substantially more residual oil in the aquifer compared to the Unmanaged Scenario. But, if

TABLE 3 - SUMMARY OF OPTIMAL PUMPING RATES USING DIFFERENT SIMULATION TIMES

Simulation Time (days)	Regression Equation	R^2 - Coeff. of Determination	Grad. Control Constraint (meters)	Optimal Pumping (m^3/day)
60	Linear	0.9995	0.00	180.50
60	**Quadratic**	0.9997	0.00	**168.35**
60	Linear	0.9995	0.02	204.57
60	**Quadratic**	0.9997	0.02	**190.80**
90	Linear	0.9998	0.00	163.52
90	**Quadratic**	0.9998	0.00	**164.56**
90	Linear	0.9998	0.02	188.68
90	**Quadratic**	0.9998	0.02	**189.87**
120	Linear	0.9962	0.00	160.21
120	**Quadratic**	0.9975	0.00	**163.58**
120	Linear	0.9962	0.02	186.91
120	**Quadratic**	0.9975	0.02	**185.34**
180	Linear	0.9916	0.00	148.54
180	**Quadratic**	1.0000	0.00	**163.55**
180	Linear	0.9916	0.02	179.17
180	**Quadratic**	1.0000	0.02	**184.34**

Note: Pumping range used to develop $f_2(P_{ew})$ via regression analysis is 150 to 240 m^3/day.

the floating plume were allowed to spread unchecked, then residual oil in the Unmanaged Scenario would eventually far exceed that created in Scenario 2. In summary, Scenario 2 would be recommended for immobilizing the plume within 90 days. The total spill area for Scenario 2 is approximately the same size as Scenario 3 and produces less residual oil in the aquifer compared to Scenario 3 (Table 4).

Lastly, the results of this S/O modeling exercise can be evaluated by considering residual oil volume. Figure 7 shows a plot of residual oil volume versus water pumping rate for two different time periods, one being containment time and the other at 360 days. Figure 7 shows that residual oil volume existing at time of containment does not increase substantially with increases in pumping. Thus, water pumping could be used as a short-term strategy without causing significant trapped oils.

TABLE 4 - FINAL SIMULATION RESULTS FROM ARMOS

Scenario	Pumping Rate (m^3/d)	Total Spill Area (m^2)	Free Oil Area (m^2)	Containment Achieved (days)	Residual Oil (m^3)
Unmanaged	0.0	5,832	5,832	N/A	9.4
1	115.7	4,725	4,632	N/A	28.1
2	164.5	4,538	4,238	83	41.2
3	189.9	4,475	4,063	47	48.4

Note: Total spill area, free oil area, and residual oil volume are results after simulating for 90 days at the given pumping rates. N/A indicates that containment was not achieved.

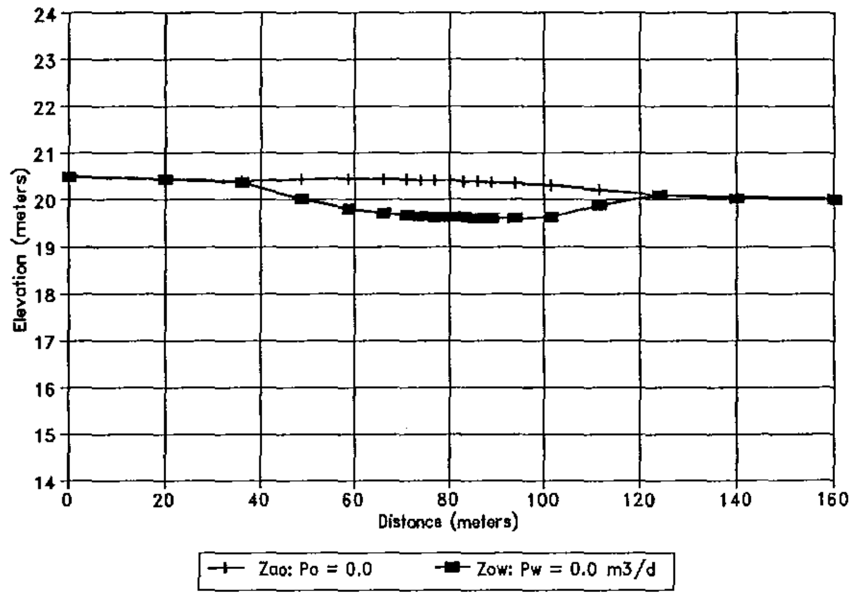

Figure 3 - Unmanaged Scenario: plot of air-oil and oil-water elevations across centerline of study area after 90 days.

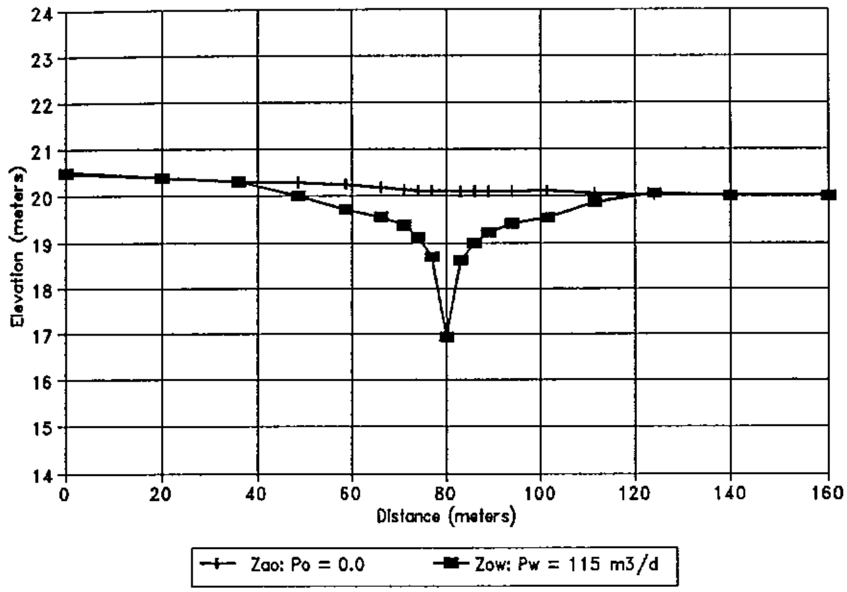

Figure 4 - Scenario 1: plot of air-oil and oil-water elevations across centerline of study area after 90 days.

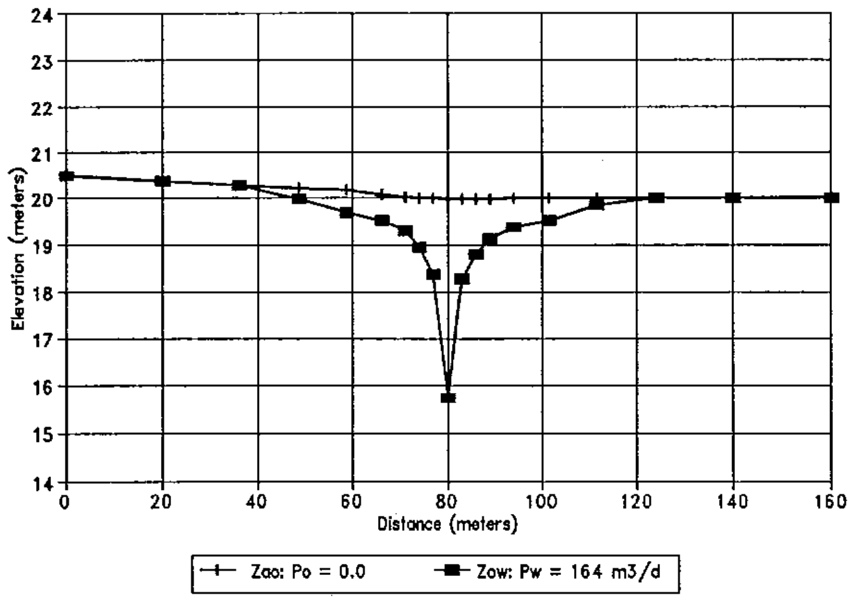

Figure 5 - Scenario 2: plot of air-oil and oil-water elevations across centerline of study area after 90 days.

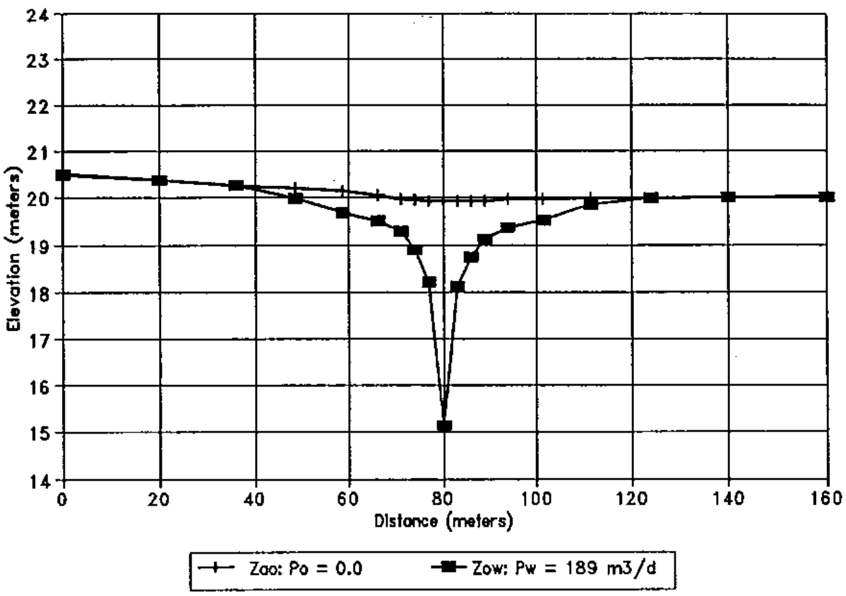

Figure 6 - Scenario 3: plot of air-oil and oil-water elevations across centerline of study area after 90 days.

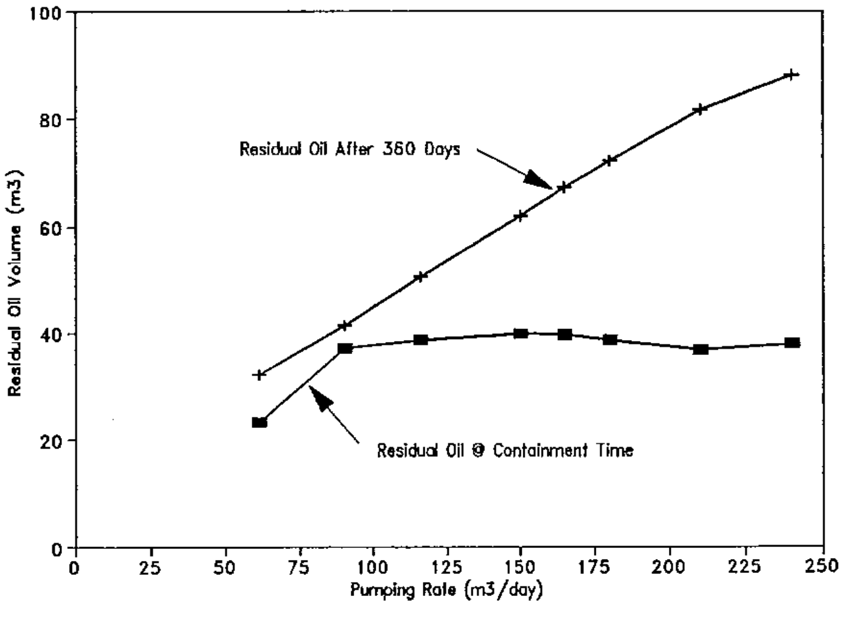

Figure 7 - Effect of water pumping rate on residual oil volume at containment time and after 360 days of steady pumping.

SUMMARY AND CONCLUSIONS

This hypothetical containment problem highlights the need for detailed simulation and optimization using **ARMOS** and the nonlinear feature of **US/REMAX**. The problem also illustrates how containing a floating plume is aided by an S/O model. It would be a tedious process to determine the pumping rate of Scenario 2 using **ARMOS** alone and then compare alternatives. This S/O model allows the engineer to make management decisions with regards to different containment strategies. A range of gradient control values can be easily evaluated to determine minimized pumping rates.

The general application of the proposed methodology can be applied to other containment problems. This approach should be valid using simulation data having time simulations greater than or equal to the desired time to containment. Also, the pumping range analyzed should be defined so that the optimal pumping rate lies within that range. This can be accomplished by looking at the statistical analysis of ΔZ_{ao} data and the best fit obtained for the regression equations. A comparison of pumping rates using data for different time simulations should not vary more than 5% for the optimal pumping rate. And finally, post-optimization simulations should be used to verify the achievement of containment for gradient control and the desired time requirements.

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