Optimization of Hydrocarbon Recovery

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STEP
Strategies for Today's
Environmental Partnership

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Optimization of Hydrocarbon Recovery

Manufacturing, Distribution and Marketing Department

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Optimization of Hydrocarbon Recovery

SECTION 1—INTRODUCTION

The concept of recovery optimization is, in its broadest sense, to achieve an environmentally sound site closure in the appropriate time frame for the least cost (That is, to maximize efficiency of the selected system). Optimization can be applied at various levels and is a function of the goals and the evaluation criteria against which a system's effectiveness is measured. For example, optimization could be applied to a recovery system using the concept of maximizing light non-aqueous phase liquid (LNAPL) recovery as the goal. At the lowest level, optimization could be applied to the design and operation of a single well. At the highest level, optimization would be applied to the design and operation of an entire remediation system. There is essentially a continuum of remedial choices ranging from containment to implementation of the most complex recovery systems, all of which can be optimized to enhance efficiency and lower costs. In general, remediation optimization should consider this continuum of technologies required to achieve appropriate cleanup target levels for the site. Typical technologies may consist of pump and treat for plume control and hydrocarbon recovery, followed by soil venting for removal of residual hydrocarbons in the vadose zone. The advantages and disadvantages of various remedial systems have been discussed in detail in API Publication 1628 Section 7.0 [1]. This document will focus on site-wide recovery system optimization, as system designs and operation and maintenance (O&M) are covered in separate documents.

SECTION 2—LNAPL MIGRATION

Understanding the migration of LNAPL in the subsurface is important to all of the remedial technologies and their subsequent optimization. Thus, a brief review of the mechanics of this migration will be presented. When a release of a petroleum product that is less dense than water, LNAPL, occurs in the subsurface, it can be distributed in the subsurface in several phases. Some of the LNAPL will adhere to the soil particles and become trapped in the small pore spaces, becoming immobile; this is called *residual LNAPL* or *residual hydrocarbon*. (Note: In this document, the terms *LNAPL* and *oil* are used interchangeably.) The LNAPL will also volatilize and form a vapor phase, assuming that the hydrocarbon mixture has a volatile component. If a water table is present, as the LNAPL migrates vertically in the pore spaces of the formation, it will encounter pores filled with water. Due to the differences in density and capillary pressures, it will begin to accumulate and a two-phase flow system, consisting of water (the wetting phase) and LNAPL (the non-wetting phase), will develop.

Figure 1 presents a conceptual illustration of the distribution of water, LNAPL, and air in a porous medium, as presented in API Publication 1628, [1]. The continuous pore volume is occupied by water, LNAPL, and/or air and the spaces between represent the porous medium. Several zones are present in the porous medium:

a. A three-phase zone containing water, LNAPL, and air, where the relative saturations of the three fluids will determine the mobility of each. This section is considered part of the vadose or unsaturated zone.
b. A two-phase zone, or capillary zone, containing water and LNAPL, where the relative saturation of these fluids will determine their mobility.
c. A two-phase zone below the water table, but within the limits of water-table fluctuations, where residual hydrocarbons are present.
d. A one-phase zone containing only water at some distance below the water table and outside the zone of water-table fluctuations, where only dissolved hydrocarbons are present.

The primary zone of lateral movement of LNAPL near the water table is the two-phase zone (water and LNAPL), where LNAPL saturation can reach a high enough level to become mobile. Figure 2 shows the relative saturation curves for water and LNAPL in this zone and the relationship to LNAPL accumulation in a monitoring well. In general, there is an over-accumulation of LNAPL in the well relative to the formation; this accumulation can be calculated through the saturation-capillary pressure relationships (Chiang and Kemblowski, [2]; Farr, et al., [3]).

This concept of a two-phase system where both water and LNAPL occupy the pore spaces is extremely important in the evaluation of remedial systems and the recovery of LNAPL. The ability of the porous medium to transmit fluids (its permeability) is a function of the relative saturation of the two fluids and is referred to as relative permeability. Relative permeability involves the flow behavior of two immiscible fluids existing in the same porous medium. It means that as the saturation of one fluid decreases relative to the second fluid, its flow capacity will also decrease. Thus, as the saturation of LNAPL decreases relative to water, the

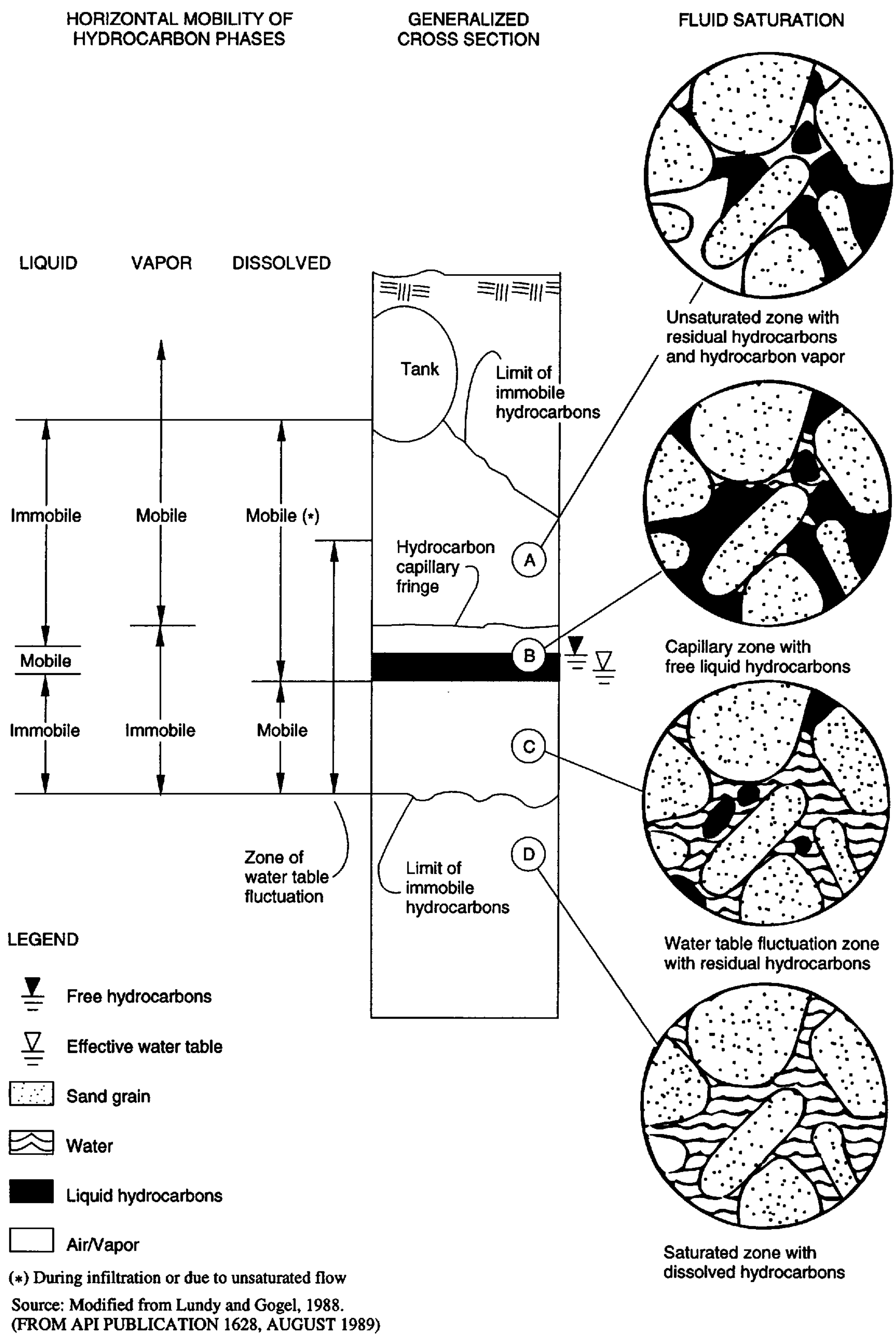


Figure 1—Vertical Distribution and Degrees of Mobility of Hydrocarbon Phases in Earth Materials

ability of the LNAPL to flow will also decrease (as shown in Figure 3). The relative saturation of the LNAPL (the non-wetting phase) must reach a certain level for it to become mobile; then its mobility and relative permeability increases rapidly with increased saturation. The increase in relative permeability of the wetting phase (water) is more gradual and proportional to the incremental increase in saturation. The relative permeability effect, coupled with the entrapment of LNAPL below the water table and residual losses in the unsaturated zone, result in the relatively low recoverability of LNAPL.

Residual LNAPL losses are very important to overall remediation at a site. In addition to residual losses that occur above the water table in the unsaturated zone, fluctuations of the water table will also result in entrapment of LNAPL below the water table. Fine-grained sands tend to retain more of the liquids in a residual state than coarse-grained sands. The type of hydrocarbon also impacts LNAPL residuals, and residual LNAPL tend to increase with more viscous products. These residual LNAPL are immobile and remain as a source of dissolved and vapor phase concentrations.

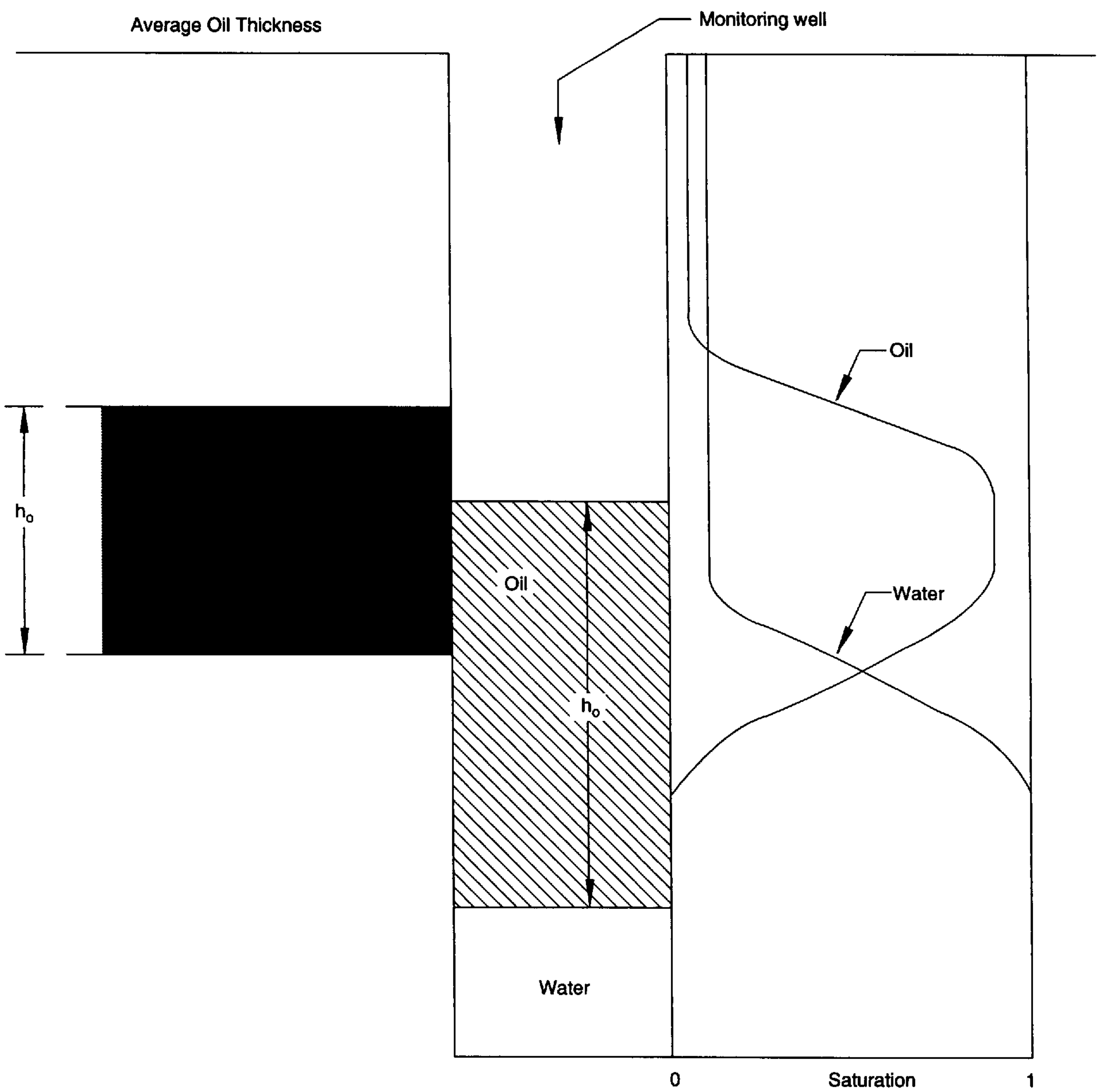


Figure 2—Hydrocarbon Distribution in Formation and Monitoring Well

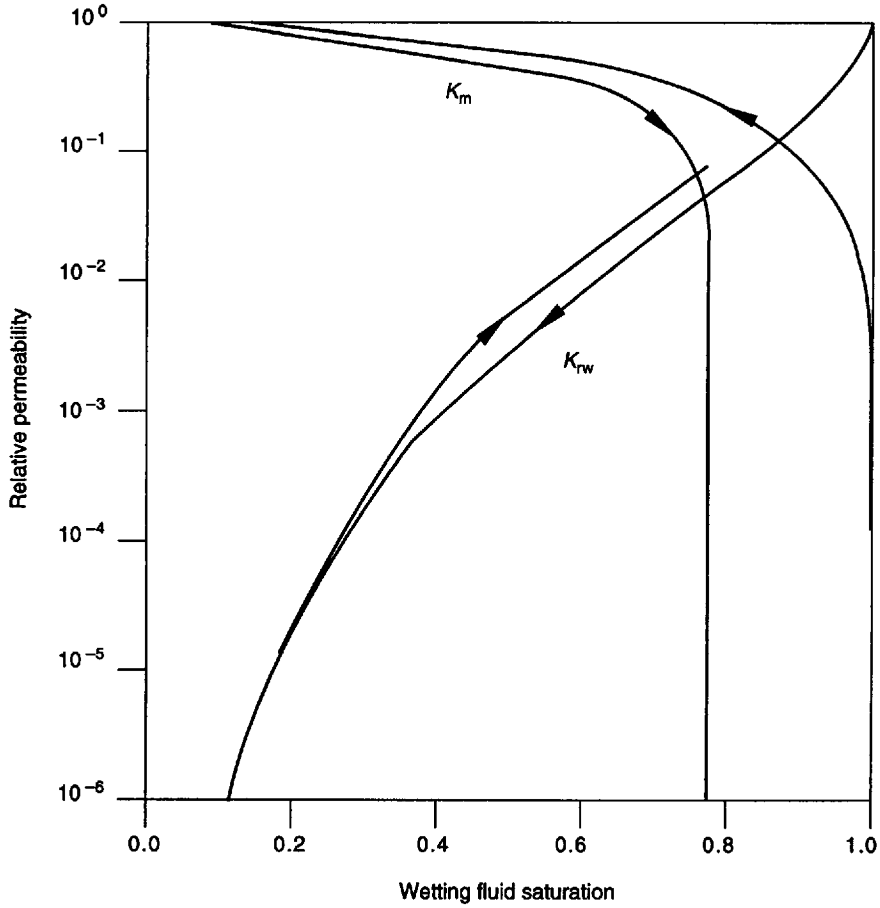


Figure 3—Relationship Between Wetting Fluid Saturation and Relative Permeability

SECTION 3—GOAL DEFINITION AND THE EFFECT ON OPTIMIZATION

3.1 General

Establishing the goals or cleanup target levels for the remediation of a site is of primary importance since the goals determine the selection of the remedial technology. An example would be a one-acre site, located in an arid environment, with a 200-foot depth to groundwater, with 1.0 part per million (ppm) of benzene in the soil, that originated from a gasoline release. If the goal at this site is to achieve cleanup target levels that provide an acceptable level of risk to human health and the environment, the optimal solution based on a risk assessment may be no further action or monitoring only. On the other hand, if the goal is to achieve regulatory-driven benzene levels of 5 parts per billion (ppb) in the soil in one year, venting may be selected as the remedial technology, and optimization would take the form of maximizing the efficiency of the venting system.

3.2 Factors Affecting Remedial Goals

The goals define the selection of the remedial technology that is to be optimized. Selection of the goals at a particular remedial site can be based on numerous factors, including the following:

a. Composition and distribution of the chemical(s) of concern.
b. Exposures to human and environmental receptors.
c. Effectiveness and limitations of available technologies.
d. Costs.
e. Business management requirements.
f. Regulatory requirements.

It should be noted that every remediation technology has a range of effectiveness depending upon the following:

a. Chemical(s) of concern.
b. Distribution of chemical(s) of concern within the subsurface.
c. Subsurface hydrogeology (e.g. soil types, depth to groundwater). In many cases where remediation is required, several types of systems may be needed to achieve

cleanup target levels. In other instances, it may not be possible to practically remediate to required cleanup target levels. In these instances, institutional controls or containment measures should be considered.

3.3 Remedial System Evaluation Criteria

The evaluation criteria against which a system is being measured define whether it is effective and whether it is operating at an optimal level. The primary evaluation criteria against which remedial systems are typically measured include the following:

a. Performance (i.e., comparison of design assumptions to field results).
b. Reliability.
c. Cost.
d. Safety.
e. Institutional controls.
f. Constructability.
g. Environmental impacts.
h. Progress towards achieving cleanup target levels.

3.4 Factors Affecting Optimization Complexity

Each remedial approach can be optimized at different levels of complexity. In general, the simplest approach to optimization is also the least costly, requires the least amount of data, and requires the least rigorous analysis. The key is to ask a series of questions and evaluate the factors that will determine the level of complexity required for a particular site.

The following questions should be considered prior to deciding on the optimization approach and its associated complexity:

a. Scale of problem?	Small__ Large__
b. Risk associated with an error?	Low__ High__
c. Level of effort ($)?	Low__ High__
d. Knowledge of hydrogeology?	Low__ High__
e. Complexity of hydrogeology?	Low__ High__
f. Knowledge of distribution of chemical(s) of concern (available data)?	Low__ High__
g. Knowledge of hydrogeologic parameters (physical and chemical)?	Low__ High__
h. Confidence in field data?	Low__ High__

A small site with a limited problem, a homogeneous formation, and limited risk would require a less complex optimization. However, a large complex site with complex hydrogeology and high risk would require a more complex optimization, as well as a more aggressive data collection program to support that optimization.

SECTION 4—APPROACHES TO REMEDIATION AND OPTIMIZATION

4.1 General

Based on the range of remedial alternatives, there is also a large number of alternative approaches to optimization. Three basic remedial approaches will be discussed here: (a) containment and withdrawal of dissolved hydrocarbons, (b) LNAPL recovery, (c) Residuals remediation and venting. The general approaches to optimization and the methods available will be presented.

4.2 Containment and Withdrawal of Dissolved Hydrocarbons

In general, the design of containment and withdrawal systems is based on the concept of capturing the dissolved hydrocarbon plume with as few extraction points as possible and at the lowest possible flow rate. Again, the goals of the remediation, such as limiting drawdown to maximize LNAPL recovery, may impact this basic scenario. This issue will be discussed in subsequent sections.

4.2.1 BASICS OF CONTAINMENT AND RECOVERY

A *capture zone* is the area within which LNAPL, groundwater or hydrocarbon vapors will flow to an extraction point. In more technical terms, the capture zone is the zone of hydraulic influence within which liquids will flow to a recovery well. As depicted in Figure 4, the capture zone is developed by establishing and maintaining a cone of depression (created by pumping) in the water table.

When a groundwater extraction system is being designed, the extraction well locations and the pumping rates should create a capture zone that will encompass and prevent migration of the dissolved plume. In a system where the established goal is simply containment of a dissolved plume, the design optimization of the system may involve the adjustment of the well locations and pumping rates to achieve capture at the lowest possible flow rate with the least number of wells. On a more complex level, the time frame to achieve capture and the degree of containment could also be considered. The optimization process can take several forms, from simply calculating the capture zone of a single well and then assuring that the wells have overlapping cones, to the use of complex groundwater flow and associated linear optimization models. The complexity of the design optimization process selected will depend on the desired accuracy and on the costs associated with the potential inaccuracies in the result, as discussed in Section 3.4. These approaches deal with the optimization of the design prior to installation. "Optimizing" the performance of the

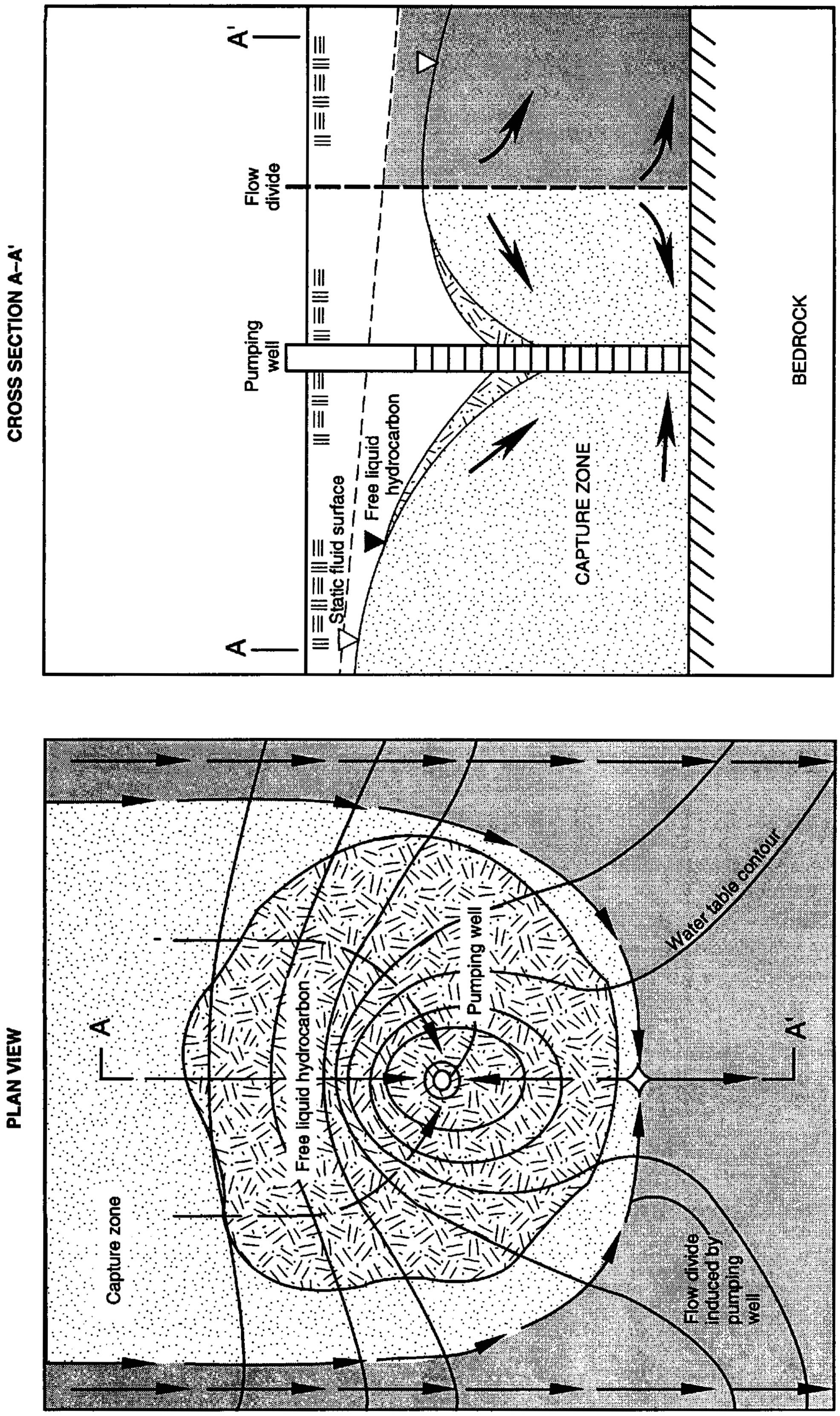


Figure 4—Recovery System Capture Zone

system can only be accomplished after the system is installed and operating. Once in operation, the actual performance of the system can be compared to the predicted design. If performance is observed to be outside of the design parameters, then modifications can be made to optimize system performance relative to design.

If residual hydrocarbons are present, pump and treat containment systems will not be sufficient to remediate a site due to the continued dissolution of chemical(s) of concern into the groundwater. Pump and treat systems must be coupled with other remedial techniques to address the residual concentrations of chemical(s) of concern and achieve the desired remedial goals. Thus, pump and treat systems have three common uses:

a. Containment of dissolved plumes.
b. Enhancing LNAPL recovery through gradient control.
c. Dewatering to enhance the use of venting systems for volatization of residuals.

Containment implies that the area within the capture zone may not be remediated in a reasonable time frame. Residual hydrocarbons may always remain in the soil pore spaces following recovery of the mobile LNAPL. The amount of residual LNAPL is a function of (a) hydrocarbon type and properties,(b) soil type, and (c) distribution of LNAPL before pumping.

As noted above, the methods for optimizing the design of a containment system and selecting the number, location, and pumping rates of extraction systems vary with the level of effort expended and the complexity of the site. The approaches to design can be divided into three categories: (a) those that use radius of influence calculations, (b) basic or screening models, or (c) detailed models. These methods and their data requirements are summarized below.

4.2.2 RADIUS OF INFLUENCE/CAPTURE ZONE METHOD

Radius of influence calculations using analytical solutions to determine well spacing for optimizing the containment of a groundwater plume are a very common approach. This method is normally accomplished using analytical techniques based on aquifer hydraulic properties collected during pumping or slug tests of the aquifer at the site. At a minimum, slug tests, sieve analyses, and core samples should be taken to estimate the aquifer parameters required to use the radius of influence methods. The amount of field data that is collected and the effort used to develop these values (slug test versus multiple long-term aquifer tests) will be a function of the factors affecting site complexity, as discussed in Section 3.4. Some of the equations available for estimating these properties are presented in Table 1.

In this approach to design optimization, analytical equations are applied to the hydraulic properties calculated for the site to obtain an estimated radius of influence. The groundwater containment system is then designed based on this radius, with the wells placed to assure that the capture zones overlap and encompass the plume. It is important to note that the stagnation point is the point directly downgradient of the pumping well where the forces on the groundwater are balanced. The forces are that of the natural gradient away from the well and the gradient created by the pumping towards the well. Any groundwater or LNAPL beyond the stagnation point will not be pulled back to the pumping well. This calculated distance is important in designing recovery well networks to capture plumes. Limiting assumptions must be made when considering the analytical solution to be used. The questions that must be answered or assumptions made concerning the hydrogeology include the following:

a. Confined or unconfined?
b. Leaky or non-leaky?
c. Artesian or non-artesian?
d. Equilibrium or non-equilibrium?
e. Homogeneous or heterogeneous?
f. Isotropic or anisotropic?
g. Recharge effects?
h. Boundary effects?
i. Partially penetrating wells?
j. Seasonal effects/tidal effect?

Thus, the analytical solutions may be simple to use, but a good understanding of the hydrogeology is required for them to be applied correctly. Table 1 lists a few of the analytical solutions available; the details on these methods can be obtained from Groundwater Hydrology Bower [4], Driscoll [5]; and Kruseman and deRidder [6].

Analytical approaches should be modified to include the additional consideration of the natural gradients at the site. The natural gradient will skew the capture zone for an individual well in the upgradient direction, making the capture zone elliptical in shape rather than circular. The effect of the site groundwater gradient on the capture zone and the resultant stagnation point is depicted on Figure 4. These modified analytical solutions give a much more realistic evaluation of the expected capture zone of an individual well, given the existing site conditions.

One option to incorporating the effect of gradients is to do a flow net analysis and superimpose the calculated cones of depression from the analytical solutions onto a plot of the site gradients. This is a simple matter of addition and subtraction of the calculated drawdowns from the analytical solutions to the site gradient map.

Another approach is to use an analytical solution developed by Keely and Tsang [7] to evaluate the effectiveness of a containment system that incorporates the natural gradient. The first step is to calculate the distance from the recovery well to the downgradient stagnation point using the following equation:

Table 1—Examples of Analytical Solutions

Description	Equation	Terms	Reference
		Solutions for Determining Hydraulic Parameters	
Unconfined Equilibrium Equations	$K = \frac{1055\ Q \text{ Log } r_2 / r_1}{(h_2^2 - h_1^2)}$	*Where:* r_1 = distance to the nearest observation well, in ft r_2 = distance to the farthest observation well, in ft h_2 = saturated thickness, in ft, at the farthest observation well h_1 = saturated thickness, in ft, at the nearest observation well Q = pumping rate in gpm	Driscoll [5]
Slug Test Solution Bower and Rice	$K = \frac{r_c^2 \ln (R_e / r_w)}{2 L_e} \frac{1}{t} \ln \frac{Y_o}{Y_t}$	*Where:* R_e = effective radial distance over which the head difference y is dissipated r_w = radial distance between well center and undisturbed aquifer (rc plus thickness of gravel envelope or developed zone outside casing) L_e = height of perforated, screened, uncased, or otherwise open section of well through which groundwater enters y_o = y at time zero y_t = y at time t t = time since y_o	Driscoll [4]
		Solutions for Determining Radius of Influence	
Unconfined Equilibrium Equations	$Q = \frac{K(H^2 - h^2)}{1055 \text{ Log } R/r}$	*Where:* Q = well yield or pumping rate, in gpm K = hydraulic conductivity of the water-bearing formation, in gpd/ft^2 H = static head measured from bottom of aquifer, in ft h = depth of water in the well while pluming, in ft R = radius of the cone of depression, in ft r = radius of the well, in ft	Driscoll [5]
Modified Nonequilibrium Cooper and Jacob	$S = 264 \frac{Q}{T} \text{ Log } \frac{.3Tt}{r^2 S}$	*Where:* s = drawdown, in ft, at any point in the vicinity of a well discharging at a constant rate Q = pumping rate, in gpm T = coefficient of transmissivity, in gpd/ft t = time since pumping started, in days S = coefficient of storage (dimensionless)	Driscoll [5]
Capture Zone Analysis	$r_{stag} = \frac{Q}{2\pi hKI}$	*Where:* r_{stag} = distance from well to stagnation point, (ft) Q = pumping rate from the well, (ft 3/day) h = Saturated thickness of the aquifer, (ft) I = hydraulic gradient, and (ft/ft) K = hydraulic conductivity (ft/day)	Keely and Tsang [7]

$$r_{stag} = \frac{Q}{2\pi hKI}$$

Where:

r_{stag} = distance from well to stagnation point.
Q = pumping rate from the well.
h = saturated thickness of the aquifer.
I = hydraulic gradient.
K = hydraulic conductivity.

Note that the units must be consistent in this equation. That is, all length units must be the same (e.g., feet) and all time units must be the same (e.g., days). For example, the following could be used in the above equation:

Q = ft^3/day.
h = ft.
K = ft/day.
r_{stag} = ft.
I = ft/ft or dimensionless.

After computing r_{stag}, the capture zone is constructed based upon the following relationships (see Figure 5):

The maximum width of the upgradient inflow to the well, or the maximum capture zone width, is equal to 2π times the stagnation distance:

$$r_{max} = 2\pi r_{stag}$$

The width of the capture zone (CZ) at the well is equal to half the maximum capture zone width ($\frac{1}{2} r_{max}$).

$$\text{CZ @ Well} = \frac{1}{2} r_{max}$$

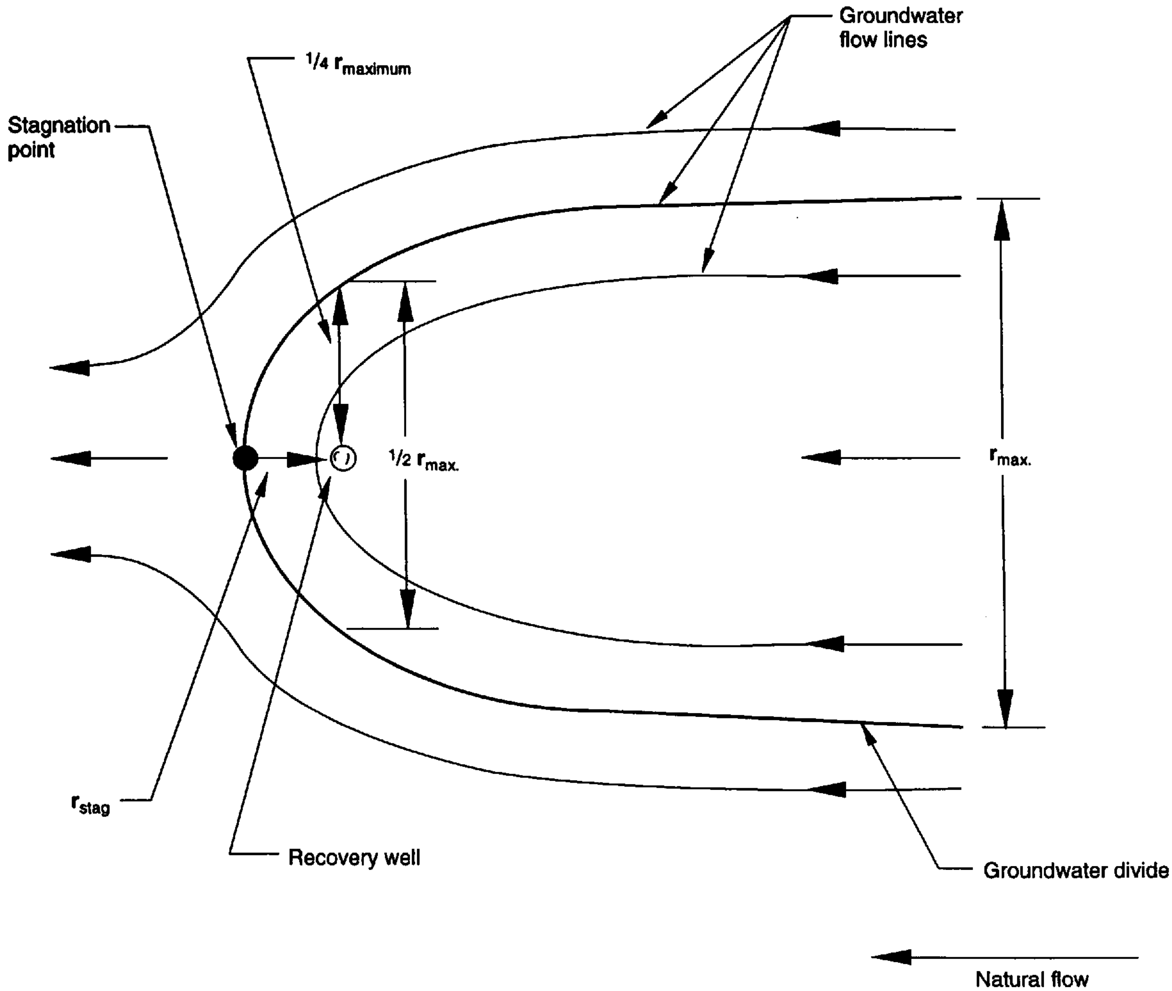


Figure 5—Estimation of the Width of the Capture Zone at the Recovery Well

As shown on Figure 5, the width of the capture zone at the well is configured perpendicular to the natural hydraulic gradient.

Data requirements for these analytical approaches include hydraulic conductivity, transmissivity, storage coefficient, effective porosity, saturated thickness, and the existing hydraulic gradient across the plume. These requirements are summarized in Table 1. These analytical approaches are simple and efficient methods of evaluating capture zones, but do not address the interference effects or the optimization of pumping rates for the entire system. All can result in an under- or over-designed system that is either inefficient or costs more to operate than desirable.

4.2.3 BASIC FLOW MODELS OR SCREENING MODELS

Screening models can be used to resolve one of the remaining optimization issues (well interference effects) and aid in the optimization of well location and pumping rates. The optimization of well location and pumping rates with these screening models is accomplished using iterations inside the model. Most screening models can be run with a minimum of effort, can provide a quick and effective way of evaluating various pumping scenarios at a particular site, and can significantly increase the confidence level of the proposed system. All models should be calibrated with actual site data.

Computer models are becoming more widely applied to groundwater remediation. Rumbaugh and Ruskauff {8} conducted a survey of groundwater modelers in the United States and identified about 200 different models. Very few are commonly used. Table 2 presents examples of models that can be used to simulate groundwater flow, dissolved phase transport, multiphase (separate-phase) flow, air flow or venting, and linear optimization. Table 3 summarizes model type, developer, availability, applications, and output obtained from each. Examples of simple screening models include QuickFlow (Rumbaugh, [9]), an analytical flow model, and FLOWPATH (Franz and Guiguer, [10]), which combines a numerical two-dimensional flow model with a particle-tracking model.

Table 2—Common Computer Models Used in Recovery Optimization

Model Types	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Groundwater Flow Models																				
Analytical																•		•		
Numerical		•				•		•	•			•	•		•				•	
Dissolved Transport Models																				
Analytical					•															
Numerical						•			•		•		•	•			•		•	
Multiphase Flow Models			•										•							
Venting (Air Flow) Models	•			•			•			•										•
Linear Optimization	•	•																		

Model Types:

1. AIRFLOW	6. BIOPLUME II	11. MOC	16. *QUICKFLOW
2. AQMAN	7. CSUGAS	12. MODFLOW	17. Random Walk
3. ARMOS	8. *FLOWPATH	13. MOTRANS	18. RESSQ
4. AIRTEST	9. HST3D	14. MT3D	19. SWIF II
5. *AT123D	10. *HYPERVENTILATE	15. PLASM	20. *Venting

*Basic (Screening) Models
Note: See Tables 3, 4, and 5 for a description and reference for each of these models.

Each model type has its own data requirements. The amount of data increases with the complexity of the model. All require a thorough understanding of the groundwater flow system, the model assumptions, and the chemicals of concern. Data requirements by model type are presented in Table 4.

4.2.4 DETAILED FLOW MODELS

Detailed flow models are generally used on large sites with complex hydrogeology, where the risk of under- or over-designing the containment system outweighs the cost of the modeling effort. The questions in Section 3.4 will help to determine the proper level of complexity necessary for a particular site. These models can incorporate a linear optimization routine that will locate wells and adjust pumping rates automatically. This feature resolves the last optimization problem of balancing the number and location of wells with the goal of minimizing the water production and still achieving containment. However, it is very important that the user verify and understand the parameters going into the model, as all models are simplifications of reality and may not accurately reflect site conditions.

An example of a detailed numerical model is MODFLOW (McDonald and Harbaugh, [11]), the most commonly used numerical model in the U.S. (Rumbaugh and Ruskauff, [8]). Particle tracking can be performed using MODPATH (Pollock, [12]), which interfaces with MODFLOW to define the capture zone around the pumping system. Tables 2 and 3 provide a summary of these models, their uses, and output. For more information on the application of groundwater flow and particle-tracking models to the design of recovery systems, see Anderson and Woessner ([13]).

As discussed above, the amount of data required increases with model complexity. Most detailed flow models require detailed information on containment and hydrogeologic parameters and also require information on the horizontal and vertical variations of these parameters. Knowledge and confidence in the field data and hydrogeologic parameters are essential to the use of detailed models. If the data are limited or of questionable accuracy, then the use of a detailed model is not justified, as the level of effort would increase but the model accuracy may not. The model results are only as good as the data entered. Data requirements for these detailed models are presented in Table 4.

4.3 LNAPL Recovery

4.3.1 GENERAL

Optimization of LNAPL recovery at a site is very problematic, due to the complexity of evaluating the flow of LNAPLs in a water-table aquifer. This is essentially a three-phase (water/LNAPL/air) flow problem for which it is difficult to develop simple analytical solutions that will predict the recoverability of the LNAPL, as discussed in Section 2. Thus, the options for optimizing LNAPL recovery are limited to the simple and the complex.

In general, the same techniques presented in the previous section concerning optimization of withdrawal systems are also applied to the optimization of LNAPL recovery sys-

Table 3—Summary Matrix of Groundwater Models

Model Name	Model Type	Developer	Availability	Applications	Output
AQMAN	Complex; 2-D; Finite - difference	Lekoff & Groehick [22], USGS	USGS; $40	Optimization for pump and treat systems	Optimum well locations/rates No graphics
ARMOS	Complex; 2-D; Finite - element	Environmental Systems & Technology, Inc., (ES & T) [16]	ES & T	Prediction of separate phase hydrocarbon cleanup time/volume/product thickness	Listing of head at each node Product thickness at each node Product recovery rates No graphics
AT123D	Basic; 3-D; semi-analytical	Yeh, [23], Oak Ridge National Lab	Internatinal Ground Water Modeling Center	Simple analyses of dissolved contaminant migration under uniform gradient	Listing of concentration at each node No graphics
Bioplume II	Complex; 2-D; method of characteristics	Rifai et al. [24] Rice University	Rice University	Dissolved contaminant migration with biodegradation	Listing of head at each node Listing of concentration at each node Dissolved contaminant recovery rates No graphics.
DREAM	Basic; 2-D; Analytical	Bonn & Rounds [25]	Lewis Publishers	Capture zone of pump and treat in 2D	Listing of head at each node Plots of streamlines
Flowpath	Basic; 2-D; finite - difference	Waterloo Hydrologic Software		Analysis of recovery system capture zones in 2D	Listing of head at each node Contour plots Plots of streamlines/particle paths
HST3D	Complex; 3-D; finite - difference	Kipp [26] USGS	USGS	Dissolved contaminant migration in 3D	Listing of head at each node Listing of concentration at each node Dissolved contaminant recovery rates No graphics
MOC	Complex; 2-D; method of characteristics	Konikow & Bredehoeft [27], USGS	USGS	Dissolved contaminant migration in 2D	Listing of head at each node Listing of concentration at each node Dissolved contaminant recovery rates No graphics
MODFLOW	Complex; 3-D; finite - difference	McDonald and Harboaugh [12], USGS	USGS	Capture zone of pump and treat systems in 3D	Listing of head at each node No graphics
MOTRANS	Complex; 2-D; finite - element	Env. Systems & Technologies [17]	ES & T	Separate phase remediation/volatization	Listing of head at each node Listing of concentration at each node Product recovery rates Dissolved contaminant recovery rates No graphics
MT3D	Complex; 3-D; method of characteristics	Zheng [28], USEPA	Papadopulos & Assoc.	Dissolved contaminant migration (fate and transport) in 3D	Listing of concentration at each node Dissolved contaminant recovery rates No graphics
PLASM	Complex; 3-D; finite - difference	Prickett and , Lonquist [29], Illinois State Water Survey	T. Prickett	Capture zone of pump and treat in 2D	Listing of head at each node No graphics
QuickFlow	Basic; 2-D; analytical	Geraghty & Miller, Inc., [30]	Geraghty & Miller, Inc.	Capture zone of pump and treat in 2D	Listing of head at each node Contour plots Plots of streamlines/particle paths
Random Walk	Complex; 3-D; random walk	Prickett et al. [31], Illinois State Water Survey	T. Prickett	Dissolved contaminant migration in 2D	Listing of concentration at each node Dissolved contaminant recovery rates No graphics
RESSQ	Basic; 2-D; semi-analytical	Javandel et al. [32]	Internatinal Ground Water Modeling Center	Capture zone in 2D	Plots of streamlines/particle paths
SWIFT II	Complex; 3-D; finite - difference	Reeves et al. [33]	NTIS	Dissolved contaminant migration	Listing of head at each node Listing of concentration at each node Dissolved contaminant recovery rates No graphics

Table 4—Data Requirements for Models Used in Recovery Optimization

Model Types	Data Requirements 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Groundwater Flow Models																			
Analytical	•	•	•		•	•	•	•											
Numerical	•	•	•	•	•	•	•	•											
Dissolved Transport Models																			
Analytical	•	•	•		•	•	•	•	•	•	•								
Numerical	•	•	•	•	•	•	•	•	•	•	•								
Multiphase Flow Models	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•			
Venting (Air Flow) Models			•			•	•					•				•	•	•	•
Linear Optimization	•	•	•	•	•		•	•											

Model Types:

1. hydraulic conductivity	6. porosity	11. half-life or decay coefficient	16. intrinsic permeability
2. hydraulic gradient	7. extent of product	12. product density/vapor pressure	17. residuals distribution
3. aquifer thickness	8. extent of dissolved plume	13. product viscosity	18. subsurface pressure distribution
4. recharge rate	9. dispersivity coefficient	14. product saturation	19. effluent vapor concentrations
5. storage coefficient	10. retardation factor or K_d	15. relative permeability curves	

Note: There is little difference in the categories of data required for the basic or screening models and the detailed models. The difference is in the level of detail. The detailed models usually require the spatial distribution of the hydrogeologic parameters and a heterogeneous site. The screening models usually assume constant or homogeneous site-wide hydrogeologic parameters.

tems. The same concepts apply in terms of developing capture zones and overlapping cones that will encompass the LNAPL plume. However, once the evaluation has been performed to develop a system that will capture and contain the LNAPL, optimization of the liquid (both groundwater and LNAPL) recovery process still remains to be accomplished. Again, the established goals of the cleanup will determine the approach to this optimization process; in most instances, the objective is to maximize the LNAPL recovery while minimizing both the production of water and residuals in the formation. Minimizing residuals is extremely important as a significant percent of the LNAPL can be left in the formation. For this reason, it is also important to limit drawdown and reduce smearing of the LNAPL in the formation. As discussed in Section 2, the effect of hydrocarbon entrapment, residuals loss, and relative permeability combine to severely limit the recoverability of LNAPLs. The approaches to system design optimization can be divided into 3 categories: (a) graphical solutions, (b) modified flow models, and (c) three-phase flow models.

4.3.2 GRAPHICAL SOLUTION METHODS—SINGLE WELL

Movement of LNAPL is a very difficult process to model. Consequently, few analytical or simple calculations are available to perform design optimization of recovery of the LNAPL. Chiang and Charbeneau [14] have developed a set of nomographs that can be used as a tool to estimate the amount of LNAPL that can be recovered by a single pumping well. They used a two-layer oil and water model to simulate LNAPL recovery over a range of hydraulic parameters, oil thicknesses, and hydrocarbon properties. The rate and/or volume of hydrocarbon removal can be estimated based upon the following data:

a. Hydraulic conductivity.
b. Hydrocarbon viscosity and density (degree API).
c. Hydrocarbon thickness.

Examples of these nomographs are shown on Figures 6 and 7, for K = 0.01 centimeters per second (cm/s), K = 0.001 cm/s, and K = 0.0001 cm/s, respectively.

These nomagraphs should be interpreted as approximations or general guidelines to be used to aid in evaluating what might be expected at a particular site. The variability between sites and other hydrogeologic complexities make these "rule of thumb" approximations only.

4.3.3 FLOW MODELS—MODIFIED

Another approach to design optimization for LNAPL recovery systems from a site-wide perspective is to use flow models to predict groundwater flow and containment. Tables 2, 3, and 4 list flow models that could be used for this groundwater modeling and their associated data requirements. Particle tracking is then applied to the model to obtain information on groundwater travel times to the extraction wells. These travel times for the groundwater particle tracks can then be modified for LNAPL migration based on a calculated retardation factor (accounting for viscosity and relative permeability) for the migration of the LNAPL in accordance with the following approach:

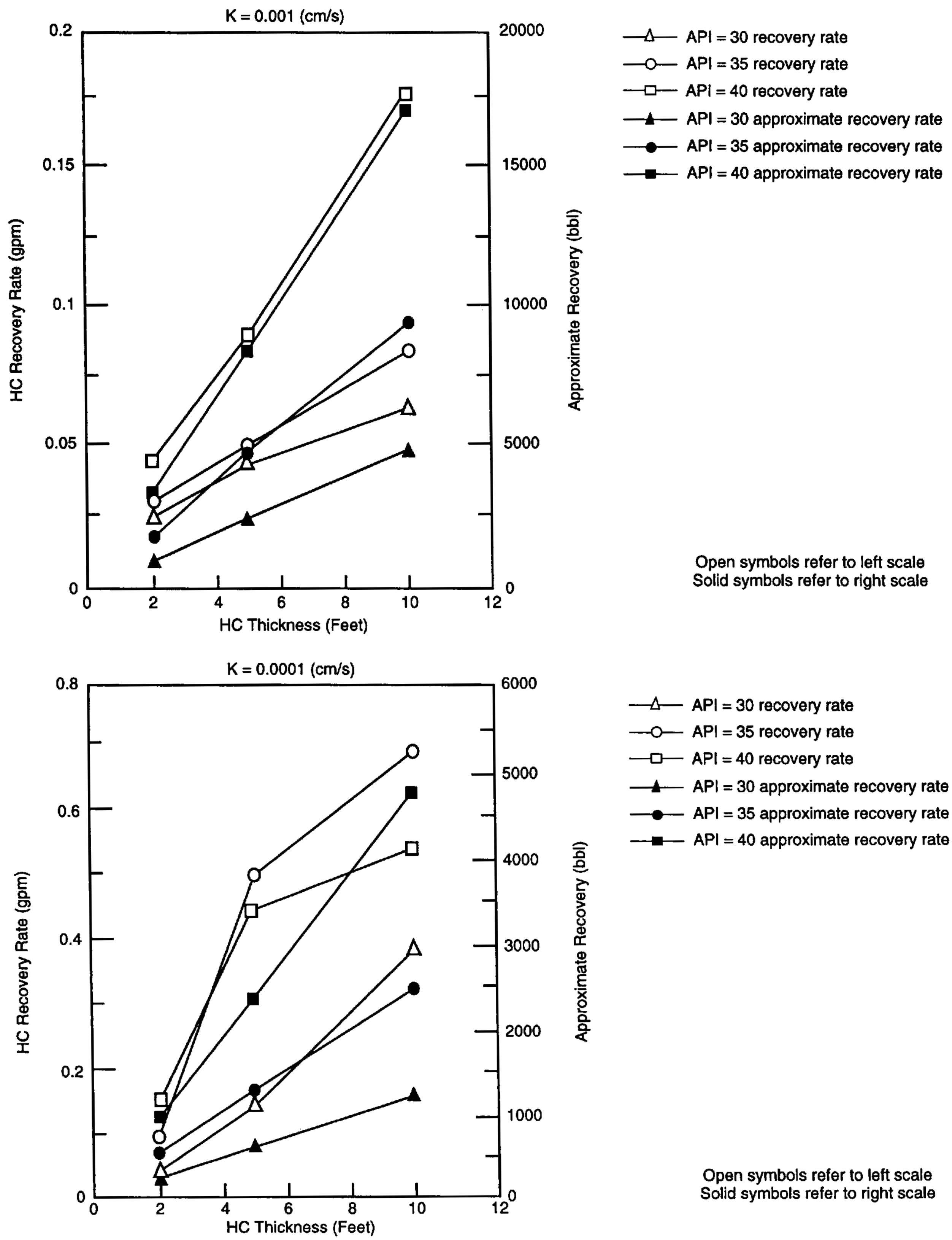
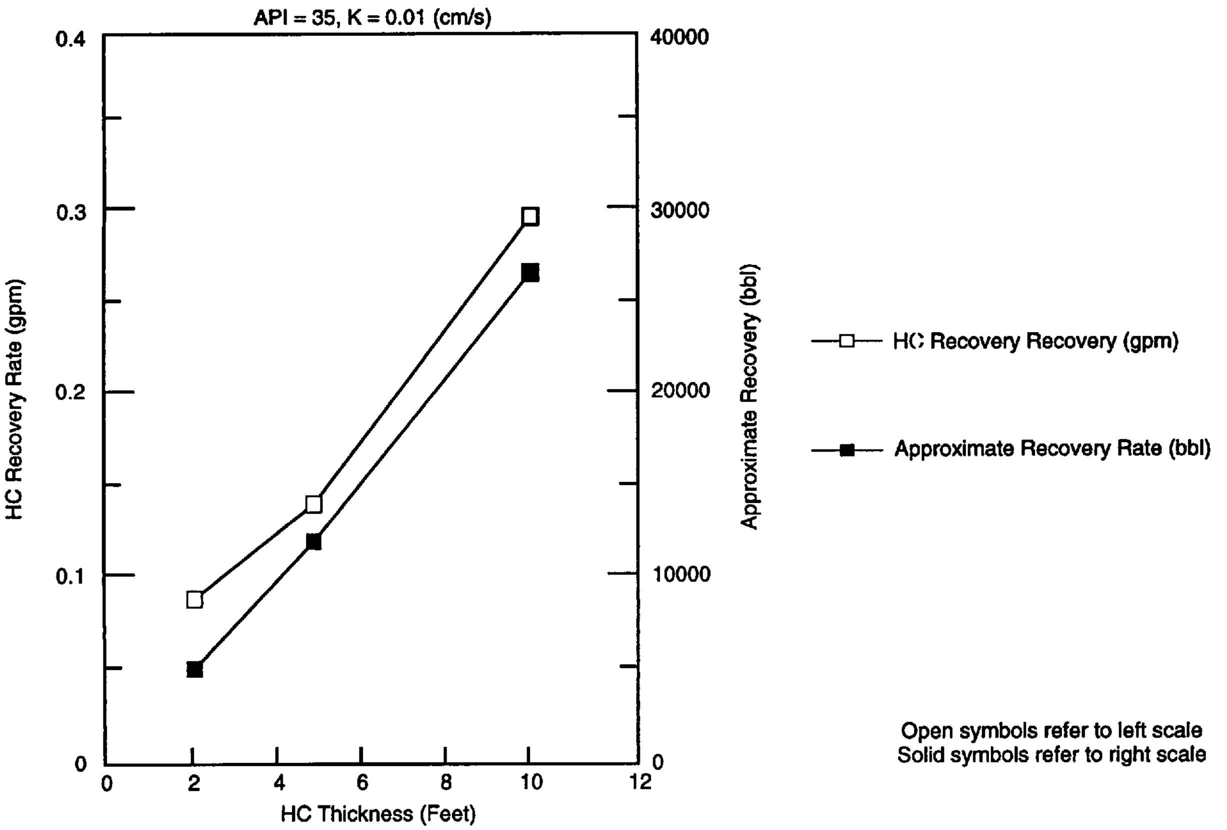


Figure 6—Optimal LNAPL Recovery Rates and Total Recovery from a Single Pumping Well for an API 30, 35, and 40 Oil at a K-value of 0.001 cm/s and 0.0001 cm/s



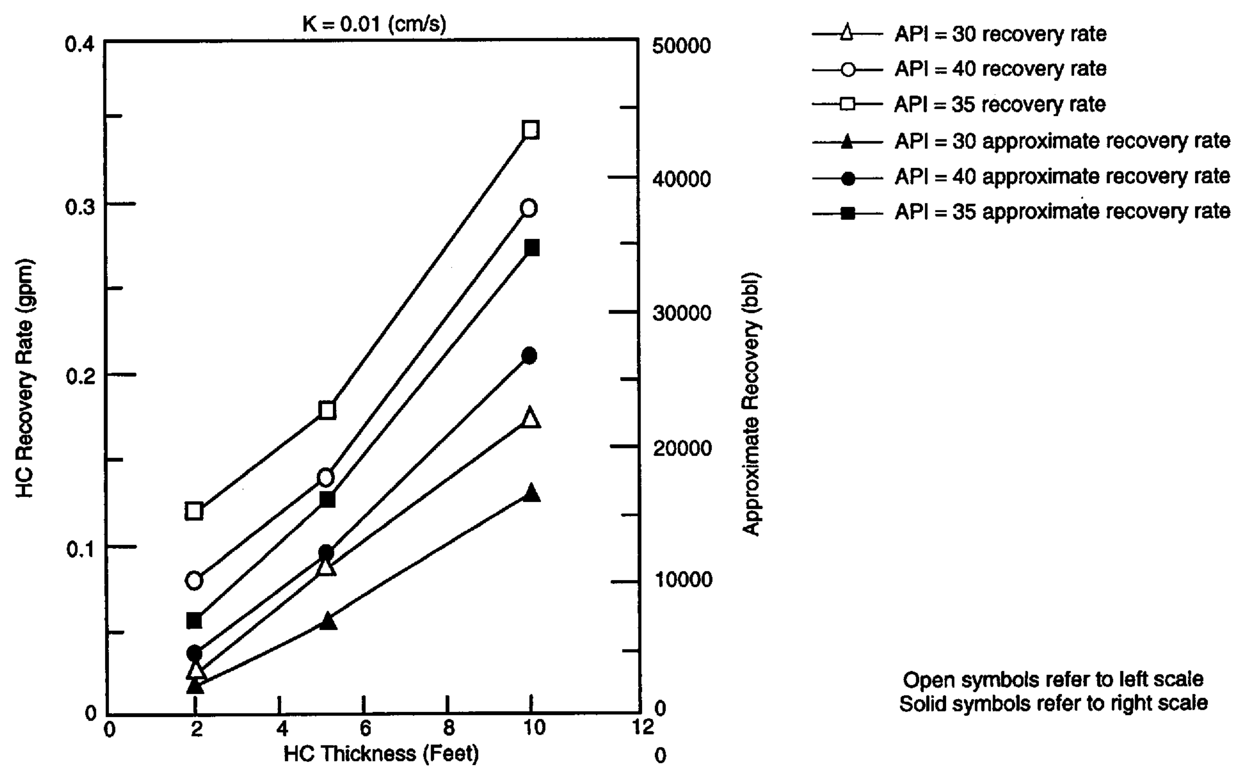


Figure 7—Optimal LNAPL Recovery Rates and Total Recovery from a Single Pumping Well for an API 30, 35, and 40 Oil at a K-value of 0.01 cm/s and 0.001 cm/s

The relative permeability of the formation to oil (i.e., LNAPL) can be calculated from the following (Charbeneau et al., [15]:)

$$K_o = K[(\rho_o/\rho_w)(\mu_w/\mu_o)\, k_{ro}]$$

Where:

- K_o = hydraulic conductivity to oil.
- K = saturated water conductivity.
- ρ_o = density of oil.
- ρ_w = density of water.
- μ_w = dynamic viscosity of water.
- μ_o = dynamic viscosity of oil.
- k_{ro} = relative permeability to oil.

The value of $[(\rho_o/\rho_w)(\mu_w/\mu_o)\, k_{ro}]$ will give the ratio or factor that can be used to adjust the water conductivity to that for oil. This same factor can then be applied to the migration times calculated for the water, since there is a direct relationship between the K and the rate of migration, (i.e., if K_o is two times smaller than K, travel times for the oil will decrease by the same factor of two).

Estimation of k_{ro} requires the evaluation of the relative saturation of the two fluids and determination of several characteristic constants that must be obtained experimentally or estimated from the literature (Charbeneau et al., [15]. This factor can be applied to the water travel times to obtain travel times for the LNAPL to the wells. The well locations can then be adjusted in the model until travel times for the LNAPL, which meet the remedial goals for the site, are reached. It is very important to remember that the analysis of relative permeability is a function of the oil saturation relative to that of water. As the LNAPL accumulations in the formation decline, so will the relative saturation of oil in the formation. Once the relative oil saturation drops to a critical value (See Figure 3), the LNAPL will be immobile.

4.3.4 THREE-PHASE FLOW MODELS

At the most complex sites, the use of three-phase flow models may be justified. These models can be used to simulate the migration of the water/LNAPL/air continuum, evaluate the LNAPL recovery effectiveness of various pumping scenarios, and optimize the flow system. However, these are very complex models and only skilled modeling practitioners should use these codes. These models also require a significant amount of experimental or field data, or these data must be estimated from the literature. Without adequate field data to support these complex models, the results of the modeling will be questionable.

ARMOS is a two-dimensional finite-element model developed by Environmental Systems & Technologies, Inc. [16] to model the movement of groundwater and LNAPL. MOTRANS, also by Environmental Systems & Technologies, [17] is a more complex model that can simulate the movement of air, water, and LNAPL, including the partitioning of the LNAPL in the dissolved and vapor phases. Both models require a significant degree of experience on the part of the modeler and also require significantly more site data (see Tables 2, 3, and 4). Refer to the questions in Section 3.4 to aid in determining the level of complexity that is justified at a given site before these approaches are used for design optimization.

4.4 Residuals Remediation and Venting

4.4.1 GENERAL

The concepts of optimization and capture zones discussed previously for groundwater extraction systems, are equally applicable to soil vapor extraction (SVE). The primary difference is that capture zones for SVE systems are generated by extraction of air in the vadose zone rather than water from the saturated zone.

The approaches to optimization of SVE presented herein are from the work of Johnson and Peargin in the soils remediation workshop conducted by the U.S. Environmental Protective Agency (USEPA [18]. They present several basic methods for design and optimization of SVE, which can be put into three basic categories: (a) those that use radius of influence calculations, (b) screening models, and (c) detailed modeling. Two other methods (empirical and system matching), which have been used in the past, are also presented. However, they are not endorsed by USEPA [18] and are not recommended for use as they may result in inadequate system design.

4.4.2 RADIUS OF INFLUENCE

While the radius of influence approach to SVE design is commonly used, but has one basic flaw: it defines an area of capture, but not an area of remediation. Based on the evaluation of the extent of the concentrations of chemical(s) of concern, an SVE is designed so that it will have sufficient influence to encompass the area of concentrations that are above site target levels. A pilot test is usually run to obtain an estimate of the area of influence from the monitoring of vacuum at vapor monitoring points. The radius of influence is interpreted as the distance at which the vadose zone vacuum can no longer be measured. The SVE system is designed based on this radius of influence using enough wells to encompass the area of concentrations of chemical(s) of concern that are above site target levels. This is the same approach used in the radius of influence calculations for containment using groundwater systems discussed previously.

The problem with this approach is that the radius of influence defines a zone of capture or containment, but not a region of remediation. The time for remediation is proportional to the ratio of hydrocarbon compound mass to volume of air flow through the targeted zone. Thus, air will be flowing to the extraction point inside the entire capture zone, in the outer areas, the flow rate will not be sufficient to achieve the remedial goals, and remediation rates at the "fringes" of the capture zone will be much slower. To increase the rate of remediation, the estimated radius can be reduced based on empirical data or prior experience at similar sites.

4.4.3 SCREENING MODEL ANALYSES

Estimating the recovery of residual LNAPL through venting is another difficult process to model. Johnson et al. [19] have developed a simple program, called HYPERVENTILATE, distributed by USEPA, which is user-friendly software that can guide the use of vapor extraction technology. The software guides the user through a structured thought process that involves the following steps:

a. Identify and characterizing required site-specific data.
b. Decide if soil venting is appropriate at a specific site.
c. Evaluate air permeability test results and conducting aquifer performance tests.
d. Calculate the minimum number of vapor extraction wells needed.
e. Illustrate how the results at a specific site might differ from the ideal case.

Both the mass removal rates and the radius of influence are evaluated so that the number of wells, well spacing, well head vacuum, flow rate, and treatment system requirements can be determined for the system design. This approach is effective in developing a system that will achieve site target levels in a reasonable time frame, be cost-effective, and meet regulatory requirements. The approach requires a higher level of expertise, but can yield more successful results in the long run. A listing of the approaches to SVE optimization and their data requirements are presented in Tables 2, 4, and 5.

4.4.4 DETAILED MODELING ANALYSIS

The detailed modeling approach is generally used on large sites with complex hydrogeology. Models are used to simulate vapor flow paths, flow rates, and removal rates from the subsurface. This approach uses the site assessment, pilot test, and concentration data to develop an optimal design for the vapor extraction and treatment system, and requires the highest level of expertise.

A model, called AIR3D, has been developed by Joss and Baehr (1992). This model uses the MODFLOW model (McDonald and Harbaugh, 1988) to simulate the movement of air in the unsaturated zone. AIR3D is a three-dimensional model that can be used to evaluate the effectiveness of venting wells and trenches in a complex system. AIR3D also contains an optimization module to help the modeler to determine the minimum number of wells and/or trenches needed to contain a certain residual volume. Information on these models and their data requirements are presented in Tables 2, 4, and 5.

Table 5—Summary Matrix of Venting Models (From EPA Workshop, January 1993)

Model Name	Model Type	Developer	Availability	Applications	Output
Hyper Ventilate	Screening	Shell Development Westhollow Research Center	Distributed by EPA/OUST	Feasibility of SVE use; qualitative estimates of cleanup time and some design parameters	Estimates of flow rates; removal rates; residual concentrations; number of wells required
Venting	Screening	Environmental Systems and Technologies, Inc.	Available to public; $300	Feasibility of SVE use; qualitative estimate of cleanup times	Mass removal rate curve for each spill component
CSUGAS	3-D Finite Difference Vapor Flow	Colorado State University Civil Engineering Department	Available to public; $125	Quantitative estimate of design parameters	Soil pressure distribution; total system flow
Airflow	2-D Finite Element Radial Symmetric Airflow	Waterloo Hydrologic Software	Available to public; $700	Quantitative estimate of vapor pressure flow at steady state	Soil pressure distribution, total system flow
Airtest	2-D Analytical radial-symmetric airflow	A. L. Baehr, C. J. Joss Drexel University	Test Phase	Quantitative estimate of pressure and flow estimate	Permeability, pressure distribution and flow
AIR3D	3-D Finite Difference	American Petroleum Institute	Distributed by API	Quantitative estimate of pressure and flow	Permeability, pressure distribution and flow

SECTION 5—ADDITIONAL CONSIDERATIONS

5.1 Coupling of Systems

In each of the above sections, the basic approaches to remediation were discussed separately. In many instances, coupling the various technologies enables site remedial goals and closure be achieved more rapidly. For instance, LNAPL recovery systems and SVE can be implemented together to enhance removal of LNAPLs and begin volatilization of residuals concurrently. In terms of the optimization of combined systems, there are no standard techniques available that take into account dissolved, liquid, and vapor phase remedial evaluation simultaneously. Optimization of these systems is usually evaluated separately, as discussed above; areas where savings on duplication can be realized are then incorporated into the system design. Coupling of systems can be a very effective technique to reduce remedial time frames, and it should be an approach that is evaluated during the design or later evaluation phases of a project.

5.2 Cost Considerations in Optimization

In each of the approaches to optimization presented, one of the key factors to evaluating the optimum solution is the the overall cost of the solution. To adequately evaluate and compare various remedial scenarios on a cost basis, the long-term O&M costs associated with the system over its operational life must also be taken into account with the initial capital costs. Another consideration is that a less expensive approach could be currently taken with the knowledge that an additional expenditure would be required in the future, or a larger sum could be currently spent to correct the problem. The question is: which approach is better from an economic perspective? "Present value" analyses can be used to answer these types of questions. The basic concept in the use of present value is to bring the expenditure of future dollars into today's dollars, that is, the equivalence of any future amount to any present amount.

5.2.1 EXAMPLE #1: PRESENT WORTH OF A FUTURE AMOUNT

An example of a present-worth analysis is to evaluate two remedial alternatives in which one calls for a larger expenditure at a future date. An organization can spend $150,000 now on a system that will remediate a given site. Alternatively, the organization can spend $10,000 now to satisfy initial regulatory requirements deferring installation of a more expensive remedial system costing $200,000 can be installed in five years. Which option is less costly, assuming interest at 6 percent compounded annually?

Option A:

$150,000 0

Present Worth (Option A) = $150,000

Option B:

$10,000 $200,000

Present Worth (Option B) = $10,000 + $200,000 $(P/F_{i,n})$;

Where:
i = interest rate.
n = number of years.

The present worth (P) of a future value (F) $(P/F_{i,n})$ is calculated as follows:

$$P = F\left[\frac{1}{(1+i)^n}\right]$$

$$P = F\,(.747)$$

$$P = 200,000\,(.747)$$

$$P = 149,451$$

$$Present\ Worth = 10,000 + 149,451 = 159,45$$

Based solely on the capital expenditures, Option A would be less expensive.

5.2.2 EXAMPLE #2: PRESENT WORTH OF ANNUAL O&M COSTS

Another common example is the comparison of the capital cost of equipment and the associated O&M costs. A company has the option of purchasing a $10,000 piece of equipment now and maintaining it at a cost of $6,000 per year or paying $30,000 for a lower maintenance piece of equipment and maintaining it at a cost of $1,000 per year. If, at the end of five years, the salvage value is zero and the interest expense is 6 percent compounded annually, which is less expensive?

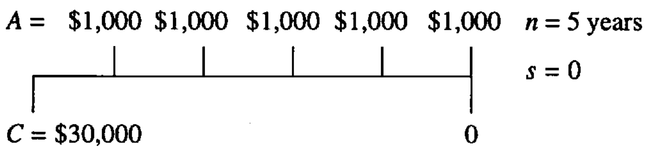
Option A:

A = $6,000 $6,000 $6,000 $6,000 $6,000 $n = 5$ years

$s = 0$

C = $10,000 0

Option B:



This solution requires a uniform series present-worth analysis. The present worth (P) of an annual cost (investment) (A) is calculated as follows ($P/A_{i,n}$):

Option A:

$$P = A\left(\frac{(1+i)^n - 1}{i\,(l+i)^n}\right)$$

$$P = 6,000\left(\frac{(1+.06)^5 - 1}{06\ 1+.06^5}\right)$$

$$P = 6,000\left(\frac{.33}{.08}\right)$$

$$P = 6,000\ (4.212) = \$25{,}272$$

$$Total\ Cost = \$10{,}000 + 25,272 = 35,272$$

Option B:

$$P = A\left(\frac{(1+i)^n - 1}{i\,(l+i)^n}\right)$$

$$P = 1,000\ (4.212) = 4{,}212$$

$$Total\ Cost = \$30{,}000 + 4,212 = 34,212$$

Economically, Option B is the better choice as it has the smallest equivalent present cost.

These are very simple examples of how economic analysis can be used to aid in evaluating remedial options. This is a very important consideration that is often overlooked in evaluating scenarios, although there are many other management criteria that must be considered in addition to these economic considerations. For more information on engineering economic analysis, refer to F. Stermole's book [21].

5.3 Optimization Questions

To determine if the system has been optimized, you should have answers to the following questions:

a. Have remediation goals been established?
  1. End result.
  2. Clean up target levels.
  3. Approach.
  4. Financial resources available.
  5. Time frame.

b. Have evaluation criteria been defined to determine effectiveness/monitoring requirements?

c. Has the level of optimization been determined, based on site complexity, management issues, and exposure (see Section 3.3)?

d. Have data collection requirements been met for selected optimization?

e. Has the method for optimization been selected and implemented?

f. Has the economic cost, capital, and O&M been evaluated?

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