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**Preliminary Simulation of Contaminant
Migration in Ground Water at the
Lawrence Livermore National Laboratory**

June 1995

Technical Editors

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Summary

This report reviews a set of two-dimensional ground water flow and contaminant transport simulations in the upper aquifer materials beneath Lawrence Livermore National Laboratory (LLNL). The steady-state flow simulations complement those made in an earlier study (Tompson *et al.*, 1991) and are based upon several improvements in the conceptualization of the hydrogeologic system beneath LLNL. The transport simulations focus on the migration, dilution, extraction, and potential degradation of existing aqueous volatile organic compounds (VOCs) in ground water, under both ambient flow and remedial pumping conditions. Simulations are used to show how, where, and at what rate vertically-averaged concentrations decrease to acceptable levels. Both the flow and transport calculations are made with a slightly modified version of the CFEST finite-element code.

The hydrogeologic study area is defined to be the upper 200 feet of the saturated sediments within a 25 square mile area surrounding LLNL. The mathematical models used in the computer code represent steady, saturated ground water flow and contaminant transport as two-dimensional, vertically averaged processes. Available hydrogeologic data include numerous well-test measurements of hydraulic conductivity, observations of water levels and water chemistry in local and regional monitor wells, borehole logs of soil type, chemical composition, and bulk physical properties, as well as measurements of surface topography and stream flow rates.

Both previous and current flow simulations have been based upon water table conditions and a variety of areal boundary conditions and known source and sink phenomena. Migration calculations focus on a single surrogate total-VOC (TVOC), equal to the sum of all VOC concentrations. Simulations were performed under both ambient (natural flow) and remedial pumping conditions.

Under natural flow conditions, and in the absence of intrinsic contaminant degradation, the results indicate that 800 y are required for the vertically-averaged TVOC concentrations to reduce to 5 parts per billion (ppb) or less in all parts of the study area. Although contaminant levels at several nearby agricultural wells may exceed 5 ppb during this time, levels at the municipal pumping wells in downtown Livermore never exceed 1 ppb. Under non-remedial conditions with an assumed linear TVOC degradation model corresponding to a 50 y half-life, simulation results indicate that all concentrations reduce to 5 ppb in 160 y, with very little impact on water quality at neighboring agricultural or municipal wells.

Results of three additional simulations of TVOC migration under the influence of remedial pumping wells indicate that vertically-averaged TVOC concentrations uniformly reach 5 ppb (or below) within 50 to 75 y with little or no impact on water quality at nearby agricultural and municipal wells. The results were dependent upon the number of wells used, their spatial locations, their time of use, and the assumed state of intrinsic contaminant degradation.

Suggestions for improved accuracy, versatility, and reliability in the simulation approach include moving to a three-dimensional framework and focusing on the migration and extraction of individual contaminant species. Additional suggestions and future directions are included in the final section of the report.

1. Introduction

A two-dimensional, regional ground water modeling study is being conducted as part of the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) Remedial Investigations at Lawrence Livermore National Laboratory (LLNL). The goals of the study are to

- Gain a better understanding of the regional hydrogeological system near LLNL including geologic structure, fluid mass balance, and regional ground water flows.
- Determine gross rates and patterns of transport and transformation of dissolved volatile organic compounds (VOCs) within the saturated zone beneath LLNL.
- Evaluate the basic impacts of remedial pumping (*e.g.*, pump-and-treat) on ground water flow, VOC migration, and VOC extraction.
- Aid in the placement and management of remediation wells and pumping rates.

This study involves the application of a finite-element flow and transport model (CFEST) to a two-dimensional conceptualization of the saturated zone flow system beneath LLNL. The study continues the preliminary work summarized in Thompson *et al.* (1991), and complements earlier modeling efforts that employed the PLUME (In-Situ, 1986) and CAPTURE (McEdwards, 1986) models (Layton *et al.*, 1990; Thorpe *et al.*, 1990).

A brief description of the model study area and regional hydrogeology around LLNL is presented in Section 2. A synopsis of contaminants detected in the saturated zone is also provided. The conceptual models of two-dimensional flow and transport developed for this study are reviewed in Section 3. We also discuss the mathematical equations that form the basis of the computational model. Section 4 includes a summary of the preliminary simulations discussed in Thompson *et al.* (1991) and a review of the hydraulic parameter values. Modifications to the current model are also presented. Results of preliminary VOC transport simulations based upon the ambient flow field are presented in Section 5. These calculations focus on a "no-action" scenario and use an estimate of the current VOC distribution as an initial condition. Discussions of the assigned dispersion parameters and assumed transformation processes are also included. In Section 6, additional results of the migration of contaminants under remedial pumping conditions are presented. Several remedial well field configurations are employed to illustrate the effect of the number of wells, their locations, and their pumping rates on the overall contaminant mass removal rate over time. Finally, in Section 7, our efforts to date are summarized, and recommendations for refinements and improvements in future modeling activities are discussed.

2. Study Area and Regional Hydrogeology

2.1. Study Area

The roughly 25 mi² (65 km²) study area is bounded on the east by the Altamont foothills, on the south by an uplifted zone and recharge area near the Las Positas Fault, and on the west by downtown Livermore (Figs. 1 through 3). In a preliminary set of simulations (Tompson *et al.*, 1991), an inferred horizontal ground water flow line in the Springtown area was chosen as the northern boundary. During more recent calculations, this boundary was expanded further north to the foothills of the Springtown area (Section 4.2). The boundaries were chosen to be hydraulically remote from LLNL and, ultimately, to facilitate specification of the model boundary conditions.

The aquifer of interest is comprised of the saturated alluvial sediments overlying a ubiquitous blue-green clay layer of the Lower Member of the Livermore Formation (Carpenter *et al.*, 1984). In the preliminary simulations, the clay layer formed the lower boundary of the entire study area, and the study area's thickness varied from less than 50 ft near the southeast corner of LLNL to over 500 ft in some areas west of LLNL. In the more recent calculations, saturated alluvial sediments more than about 150 ft below the water table were assumed to have limited impact on the overall horizontal flow field and were excluded from the study area (see Section 4.2). In all instances, the simulated aquifer is known to completely contain the known VOC mass in the saturated zone.

2.2. Regional Hydrogeology

For descriptive purposes, the study area was broken into several distinct material zones (Figs. 2 and 3; Table 1) comprised of:

- Two large regions of saturated alluvium that extend from the northeast to the west of the modeling domain, and include portions of the Altamont, Spring, May, Mocho I, and Mocho II subbasins (DWR, 1966, 1974).
- Areas of topographically higher surface elevations associated with several uplifted zones of generally older sediments (Figs. 1 and 2).
- An elongated fault zone surrounding the Las Positas Fault (Fig. 3).
- A small "toe" zone that represents a hypothesized subsurface uplifted area near the southwest corner of LLNL (Figs. 2 and 3).

The alluvial sediments are the most conductive (water-bearing) zones, whereas the uplifted, fault, and toe zones are considered to be much less permeable. These zones and their hydraulic properties are summarized in Section 4 and Table 1, and are discussed in more detail in Tompson *et al.* (1991).

A map of the potentiometric surface interpolated from spring 1989 LLNL and Alameda County Flood Control and Water Conservation District (Zone 7) (Zone 7, 1989) ground water data is presented in Figure 4. As seen in Figures 2 to 4, ground water enters the

Table 1. Hydrologic flow areas in current model^a.

Area	Description
1. Saturated alluvium	Principal water-bearing sediments in the valley area
a. Mocho I, Spring, May subbasins	
b. Altamont subbasin	
c. Mocho II subbasin	
2. Toe zone	Hypothesized (buried) uplifted area west-southwest of LLNL
3. Las Positas Fault zone	Narrow region surrounding Las Positas Fault south of LLNL
4. SE Upland zone	Uplifted materials south and east of the Las Positas Fault ^b
5. NE Upland zone	Uplifted materials near the Altamont Foothills
6. Western Upland zone	Uplifted materials north and south of downtown Livermore

^a Refer to Figures 5, 6, and 10.

^b As described in Section 4.2, this zone now includes a small less-permeable area near the southeast corner of LLNL.

Mocho II alluvial subbasin south of the Las Positas Fault zone and beneath Arroyo Mocho, and flows west toward downtown Livermore. Smaller amounts of ground water enter the Altamont, May, and Spring alluvial subbasins from the northern and eastern foothills, and exit to the west through a "gap" adjacent to the toe zone at the boundary of the Mocho I and Mocho II subbasins (Figs. 2 and 3). As shown in Figure 3, the Las Positas fault zone apparently separates these two flow regions. Some ground water may exit the region in shallow deposits underlying Arroyo Las Positas and Altamont Creek and discharge as surface flow. The two streams, which are mainly ephemeral upstream of these discharge points, cut through an uplifted and exposed portion of the Lower Livermore Formation along Interstate 580 between First Street and North Livermore Avenue (Fig. 4).

In general, ground water flow in this modeling study is considered to be steady. Short-term fluctuations associated with seasonal variations in ground water extraction rates from municipal and agricultural wells may occur. Longer term trends have been observed as a result of artificial aquifer recharge, reduced ground water extraction from former agricultural wells, and increased pumping from municipal wells associated with the recent drought.

Significant surface recharge in the study area occurs along a portion of Arroyo Mocho, downstream of the South Bay aqueduct. Zone 7 releases water from the aqueduct to Arroyo Mocho for aquifer recharge purposes. Recharge to the aquifer may also occur as precipitation and storm runoff infiltrate through the unsaturated zone. Precipitation in the Livermore Valley occurs primarily in the winter months at an average rate of about 12 to 14 in/y.

Ground water is removed from the alluvial aquifer at several municipal and agricultural wells within the study area. California Water Service Company (CWSC) operates municipal water supply wells near downtown Livermore, and a few agricultural wells exist southwest of LLNL (Figs. 3 and 4). Discharge from the shallow ground water system also occurs along gaining reaches of Arroyo Las Positas and Altamont Creek, west of the intersection of First

Street and Interstate 580 (Fig. 2). Other portions of these streams, including the Arroyo Seco, are ephemeral.

2.3. Occurrence of Contaminants

Several hazardous compounds associated with past activities at the LLNL site have been detected in sediments and ground water beneath the study area (Thorpe *et al.*, 1990). The compounds include a variety of VOCs, fuel hydrocarbons (FHCs), and some localized chromium, tritium, and perhaps lead (Thorpe *et al.*, 1990; USDOE, 1992). This report will be concerned with eight specific "target" VOCs that have been detected in ground water beneath LLNL at concentrations exceeding Federal and State of California Maximum Contaminant Levels (MCLs). These include trichloroethylene (TCE), perchloroethylene (PCE), 1,1-dichloroethylene (1,1-DCE), 1,2-dichloroethylene (both *cis* 1,2-DCE and *trans* 1,2-DCE), 1,1-dichloroethane (1,1-DCA), 1,2-dichloroethane (1,2-DCA), carbon tetrachloride, and trihalomethanes composed of chloroform, bromoform, chlorodibromomethane, and bromodichloromethane (referred to as total trihalomethanes, or THMs). In the saturated zone, the target VOCs have been detected as far as 300 ft below ground surface and as far as 2,000 ft west and 500 ft south of LLNL. These contaminants are believed to have originated in large part from maintenance operations at a former naval installation on the LLNL site (Thorpe *et al.*, 1990). The most likely surface infiltration locations are in the east-central portion of the site near a former aircraft parking ramp, and in the southwest corner of the site near a storm sewer drain into the Arroyo Seco. Most of the target VOCs have also been detected in the unsaturated zone (roughly 30 to 130 ft in depth) beneath the LLNL site. To date, all aqueous concentrations of the target VOCs measured are well below solubility limits (USDOE, 1992), and no free product VOC phases have been detected in the subsurface.

Many of the FHCs in the LLNL subsurface may also be considered as VOCs. These include benzene, ethyl benzene, toluene, several forms of xylene, and ethylene dibromide. These five compounds are known to exist only in a small area near a gasoline spill at the southern boundary of LLNL, in separate aqueous and free fuel product phases, above and below the water table. The modeling studies described in this report will only consider the migration, transformation, and recovery of the eight target VOCs in the saturated zone near LLNL (Section 5.1). Modeling studies focused on the fate of FHCs, heavy metals, or tritium may be described in separate publications.

Regulatory Standards. MCLs have been established to maintain safe drinking water standards for *in-situ* ground waters that may eventually be extracted and used for municipal or private supplies. Separate MCLs have been defined by Federal and State regulators for each target VOC discussed above, as well as for tritium, individual FHCs, and metals (USDOE, 1992). For a given compound, California and Federal MCL values may differ, with the state values usually being more stringent. For the target VOCs, State MCL values range from 0.5 ppb for 1,2-DCA and carbon tetrachloride to 100 ppb for THMs (USDOE, 1992). As discussed below, ground water cleanup strategies typically focus on reducing *in-situ* contaminant levels to the lower of the Federal and State MCL limits through extraction and surface treatment, *in-situ* bioremediation, or other technologies.

Another regulatory constraint involves specific Discharge Limits (DLs) for contaminants in treated ground water. These limits are established in accordance with Federal and State authorities to restrict residual levels of contaminants in waters discharged into lakes, streams, infiltration ponds, injection wells, or trenches. These limits govern the output of treatment facilities as opposed to reducing existing contaminant concentrations in ground water. Individual discharge limits have been established by Federal and State authorities for most of the aforementioned contaminant compounds (except tritium). Although DLs are usually similar in magnitude to MCLs, they can be different for specific compounds or may be applied to groups of compounds (USDOE, 1992). At LLNL, specific DLs have been established for PCE, benzene, and ethylene dibromide (USDOE, 1992), as well as a separate DL of 5 ppb for the total VOC (TVOC) concentration (including the eight target VOCs, five FHC VOCs, and THMs). For example, the 5 ppb discharge limit for THMs at LLNL (assuming it makes up the total VOC discharge) is much lower than the Federal and State 100 ppb MCL for THMs. This means that water extracted from the ground with an *in-situ* THM concentration less than the THM MCL may still have to be treated before it is discharged. In cases like this, both MCLs and DLs may affect strategies for reducing *in-situ* contaminant concentrations.

Text continues on page 10.

Figure 1. LLNL modeling study area and topography.

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Figure 2. LLNL modeling study area showing inferred basin boundaries.

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Figure 3. Perspective conceptualization of the upper aquifer within the LLNL modeling study area.

ERD-CFEST-93/F04

Figure 4. Potentiometric surface based on ground water data from spring 1989.

3. Conceptual and Mathematical Models

The model simulations discussed in this report are based on a two-dimensional conceptualization of flow and transport processes within the study area. In many hydrogeologic settings, the horizontal extent of an aquifer or flow region of interest is typically much greater than its vertical thickness, and the principal flow and transport phenomena occur in horizontal directions. In these cases, it is both practically useful and convenient to base initial model calculations on a set of two-dimensional balance equations expressed in terms of depth-averaged hydraulic quantities or bulk coefficients representative of vertically-integrated behavior (*e.g.*, Bear, 1977; Pinder and Gray, 1977; Gray, 1982).

The physical system within the study area is considered a two-phase porous medium composed of a stationary, nondeforming solid porous matrix saturated with an aqueous liquid. The VOCs are assumed to be totally soluble in the liquid phase, may possibly sorb onto portions of the solid phase or potentially react with other compounds, and will not significantly change the bulk density of the fluid or solid phases or the natural porosity and permeability of the medium. Balance equations for the total fluid mass and momentum are used to determine the flow field (Section 3.1). Separate mass balances are used to describe the migration and transformation of specific components within the liquid and solid phases (Section 3.2).

3.1. Two-Dimensional Flow Equations

The two-dimensional balances of fluid mass and fluid momentum are given most generally by

$$\frac{\partial(b\epsilon\rho)}{\partial t} + \nabla \cdot (b\epsilon\rho\mathbf{v}) + \sum_w^{N_w} \rho Q_w \delta(x - x_w) \delta(y - y_w) + \rho(q^t - q^b) = 0 \quad (1)$$

and

$$\epsilon\mathbf{v} + \mathbf{K} \cdot \nabla h = 0, \quad (2)$$

respectively. Here $\mathbf{v}(x, y)$ is the depth-averaged ground water velocity (L/T), $\rho(x, y)$ is the fluid density (M/L³), $h(x, y)$ is the depth-averaged hydraulic head (L), $\epsilon(x, y)$ is the porosity, $b(x, y; h)$ is the saturated aquifer thickness (L) over which the depth averaging takes place, $\mathbf{K}(x, y)$ is a bulk hydraulic conductivity tensor (L/T) representative of vertically-averaged behavior, ∇ is a two-dimensional (x, y) gradient operator (1/L), and δ is the Dirac delta function. The quantities involving Q_w , q^t , and q^b represent external sources or sinks of fluid mass from wells or surface recharge. The summation term represents the depth-averaged fluid flux (M/L²T) injected or extracted from a series of N_w wells, where Q_w is the pumping (> 0) or injection (< 0) rate (L³/T) of well w located at x_w, y_w . The quantities q^t and q^b represent the volumetric fluid flux (positive upwards) per unit area (L/T) crossing the top and bottom boundaries of the flow unit via natural recharge or discharge, respectively.

Because these expressions were developed under the assumption that the vertical variation of head is small, water table elevations may be used as an indicator of the hydraulic head. When the upper boundary of the averaging unit represents the water table, the thickness

b will become a function of the head h , making the system (1-2) nonlinear and possibly time dependent. In the applications below, both ρ and ϵ are assumed homogeneous and constant, and only steady flow will be considered. Initial solution of these model equations for the LLNL study area was described by Thompson *et al.* (1991). These and more recent steady-state flow simulations are discussed in Section 4.

3.2. Two-Dimensional Transport Equations

The two-dimensional balance of mass for a specific, neutrally buoyant component dissolved in the liquid phase is

$$\frac{\partial(b\epsilon c)}{\partial t} + \nabla \cdot (b\epsilon c \mathbf{v}) - \nabla \cdot (b\epsilon \mathbf{D} \cdot \nabla c) - b\epsilon(R + r) + \sum_w^{N_w} C^w Q_w \delta(x - x_w) \delta(y - y_w) + (q^t C^t - q^b C^b) = 0. \quad (3)$$

Here, $c(x, y, t)$ is the depth-averaged aqueous concentration (M/L^3)¹, $\mathbf{D}(x, y)$ is an effective, two-dimensional dispersion tensor (L^2/T), $r(x, y, t)$ and $R(x, y, t)$ are rates of vertically-averaged mass accumulation or loss (M/L^3T) arising from heterogeneous or homogeneous reactions, respectively (Section 3.2), while b , $\mathbf{v}$, and ϵ are defined as above. As above, the terms involving Q_w , q^t , and q^b represent external sources of solute mass from wells or surface recharge (see Section 3.2).

The dispersion tensor is expressed as

$$\mathbf{D} \approx (A_{11}|\mathbf{v}| + \mathcal{D})\mathbf{I} + (A_{11} - A_{22})\frac{\mathbf{v}\mathbf{v}}{|\mathbf{v}|}, \quad (4)$$

where A_{11} and A_{22} are effective longitudinal and transverse macrodispersivities (L) (Gray, 1982; Thompson, 1990), and $\mathcal{D}$ is an effective molecular diffusivity (L^2/T) for the particular solute in the porous medium of interest.

The two-dimensional balance of mass for the same component in the solid phase is

$$\frac{\partial(b\epsilon^s s)}{\partial t} - b\epsilon^s(R^s + r^s) = 0, \quad (5)$$

where $s(x, y, t)$ is the depth-averaged concentration found on the solid matrix (M/L^3), $\epsilon^s(x, y)$ is a depth-averaged solid phase volume fraction (equal to $1 - \epsilon$, a constant here), and $R^s(x, y, t)$ and $r^s(x, y, t)$ are the associated source and sink terms in the solid phase (M/TL^3). No-flux terms appear because the matrix is assumed stationary and solid phase diffusion is neglected.

External Mass Fluxes. In Eq. (3), the summation term represents the solute flux (M/L^2T) injected ($Q_w < 0$) or extracted ($Q_w > 0$) from the same series of N_w wells introduced above. For a pumping well, the quantity C^w represents the depth-averaged

¹Note that if the liquid and solid solutions are dilute and their phase densities are assumed constant, then any measure of concentration (M/L^3) may be converted to any measure of mass fraction (M/M) through division by a phase density expressed in the appropriate units.

concentration $c(x_w, y_w)$ at the well; for an injection well, it represents the depth-averaged concentration of injected fluid. The pumping and injection behavior represented in Eq. (3) is assumed to be evenly applied over the entire depth of the flow unit so that use of depth-averaged concentrations is valid. The quantities C^t and C^b represent the local concentrations of the solute in the top and bottom surface fluxes q^t and q^b (L/T), respectively. In these simulations, contaminant flux across the top and bottom boundaries of the system will not be considered, so that $C^t \approx C^b \approx 0$. Additionally, the contaminant concentration in water introduced by injection wells is assumed to be zero.

Homogeneous Reactions. Homogeneous reaction processes include in-phase loss or gain of contaminant mass arising from chemical reactions, such as radioactive or biological decay, mineral complexing, or redox processes. In our applications, the relationships

$$R = -\lambda c \quad (6)$$

$$R^s = -\lambda s \quad (7)$$

will be used to represent a simple first-order decay mechanism for contaminants in either phase (λ being a decay rate, 1/T). The decay term is meant to account in a gross fashion for a generic loss due to bacterial or other chemical reactions. More sophisticated approaches are available (*e.g.*, Cederberg *et al.*, 1985; Yeh and Tripathi, 1989; Liu and Narasimhan, 1989; Kindred and Celia, 1989) and may be used in the future to include phenomenological models for specific processes of interest as well as to more systematically track the abundance of all relevant product and source constituents.

Heterogeneous Reactions. Heterogeneous exchange processes involve transfer of contaminant mass across phase boundaries arising from ion exchange or precipitation-dissolution reactions, or other phase-change phenomena. In our applications, reversible sorption processes will be considered. In a liquid-solid system, the mass exchange rates satisfy

$$\epsilon^s r^s + \epsilon r = 0. \quad (8)$$

In many cases, these rates are fast enough to justify use of an equilibrium relationship that describes how chemical mass partitions among the solid and liquid phases. In general, such a relationship will depend on the material and the thermodynamic conditions at a particular location $\mathbf{x}$, and is often expressed phenomenologically as a function of the type and concentration of all dissolved chemical components present at $\mathbf{x}$, the type and abundance of minerals found there, as well as the temperature, pH, and Eh (*e.g.*, Weber *et al.*, 1991).

Normally, partitioning mechanisms are studied under small-scale laboratory conditions for idealized binary systems involving a single chemical and porous medium. In practical problems, these relationships are commonly extrapolated (often in an *ad hoc* fashion) for use in nonideal field systems. Simple phenomenological rules of the form

$$s = \mathcal{F}(c; \mathbf{x}) \quad (9)$$

are widely used, expressed here in terms of vertically-integrated quantities. These effects are normally accounted for by adding Eqs. (3) and (5) to obtain a balance law for the *total mass*

$c^* = \epsilon c + \epsilon^s s$ and then using Eq. (9) to replace Eq. (5). The added equations take the form

$$\frac{\partial(bc^*)}{\partial t} + \nabla \cdot (b\epsilon cv) - \nabla \cdot (b\epsilon \mathbf{D} \cdot \nabla c) + \lambda bc^* + \sum_w^{N_w} C^w Q_w \delta(x - x_w) \delta(y - y_w) = 0, \quad (10)$$

where Eqs. (6-7) have been substituted and C^t and C^b are set to 0. The partition relationship in Eq. (9) can be used to relate c^* to c via

$$c^* = \epsilon c \mathcal{R} \quad (11)$$

where $\mathcal{R}$ is a generalized retardation coefficient defined by

$$\mathcal{R} = 1 + (\epsilon^s \mathcal{F}(c; \mathbf{x}) / \epsilon c). \quad (12)$$

Use of Eq. (11) in Eq. (10) yields

$$\frac{\partial(\mathcal{R} \epsilon b c)}{\partial t} + \nabla \cdot (b \epsilon c v) - \nabla \cdot (b \epsilon \mathbf{D} \cdot \nabla c) + \lambda \mathcal{R} b \epsilon c + \sum_w^{N_w} C^w Q_w \delta(x - x_w) \delta(y - y_w) = 0. \quad (13)$$

Solutions of this equation for VOC concentrations within the LLNL study area are described in Sections 5 and 6. Initial calculations will assume a linear equilibrium partitioning relationship of the form

$$s = K_d(\mathbf{x})c, \quad (14)$$

where $K_d(\mathbf{x})$ is a dimensionless partition coefficient. In this case, $\mathcal{R}$ reduces to $1 + \epsilon^s K_d(\mathbf{x}) / \epsilon$ and is independent of c . The partition coefficient K_d can be related to the more common, mass-based form, $k_{d,m}$ (L^3/M) via $K_d = \rho_b k_{d,m} / (1 - \epsilon)$, where ρ_b is the bulk density of the solid phase material (M/L^3). In this case, $\mathcal{R}$ is expressed as $1 + \rho_b k_{d,m} / \epsilon$. Note that if $\mathcal{R}$ is *spatially constant*, then division of Eq. (13) by $\mathcal{R}$ yields the more familiar mass balance equation for c , expressed in terms of a modified (or retarded) velocity, dispersion tensor, and set of pumping rates.

3.3. A Remark on the Depth-Averaged Conceptualization

It is important to note that the solutions to depth-averaged equations can only be compared with depth-averaged field measurements. As mentioned earlier, ground water pressures are commonly assumed to be hydrostatic over the vertical. By assuming the head is vertically constant, water table elevations can be equated to depth-averaged hydraulic head values. However, point concentration measurements collected at a particular depth may not necessarily be compared with model results unless some effort has been made to integrate a series of point measurements over the vertical. Moreover, if the solute is only located over a fraction of the vertical depth as in a finger of mass moving through a stratified medium, then a vertical average will be "diluted" in some sense and may underestimate what is actually measured at a point. In other words, although a vertically-averaged concentration may be less than some action limit, a point concentration measured at some depth may still be above the limit.

4. Ground Water Flow Simulations

The two-dimensional model of steady ground water flow beneath LLNL has been used to support calculations of contaminant transport described in Sections 5 and 6. The current model has been developed from a set of preliminary calculations that are reviewed below. Several modifications to the first model have been incorporated into the current version, including: (1) an increased grid node density near the contaminant plume; (2) an expanded northern boundary of the simulation domain; (3) a thinner flow domain restricted to approximately the uppermost 150 ft of the aquifer; and (4) certain refinements of material values near the Las Positas Fault zone.

4.1. Review of Previous Simulations

Development and calibration of the original two-dimensional regional ground water flow model was described in detail by Thompson *et al.* (1991). The initial computational flow mesh developed for the study area (Fig. 5) used an inferred ground water flow line as the original northern boundary. Steady forms of Eqs. (1) and (2) were solved on this mesh with a two-dimensional, bilinear implementation of the CFEST finite-element code (Gupta *et al.*, 1987), modified to treat (nonlinear) water table conditions. In this case, the aquifer thickness (b) was considered dependent on the water table elevation (*i.e.*, the hydraulic head). A provisional solution $h^*(x, y)$ is provided to facilitate an iterative process that leads to a series of intermediate solutions h^k , h^{k+1} , and so on, until a final, steady-state solution is found (Pinder and Gray, 1977). Convergence is achieved when the difference (or relative difference) between two sequential iterate solutions is bounded at all nodal points by a specified tolerance factor. The final solution represents the steady-state water table elevation that corresponds to the applied boundary conditions and source terms, and may be used to compute an updated aquifer thickness.

Measurements of water table elevations in local wells from the spring of 1989 were used to estimate the regional distribution of hydraulic head in the study area under ambient (non-remedial) conditions (Fig. 4). We used this distribution of head to specify the initial (provisional) solution for h within the code, as well as specify values of h along domain boundaries that corresponded to the principal inflow and outflow areas. In the original simulations, influx boundaries were located along a small zone in the Altamont Foothills east of LLNL (flux boundary 1 in Fig. 5) and along two segments intersecting more southern stretches of the Mocho II province (flux boundaries 3 and 4 in Fig. 5). The principal outflow boundary was located along the western portion of the domain (flux boundary 2 in Fig. 5). No-flow conditions were specified on other sections of the boundary, corresponding either to impermeable conditions or inferred ground water flow lines.

In one of the better calibrated preliminary simulations (Run 17A in Thompson *et al.*, 1991), a single hydraulic conductivity value of 10 ft/day (3 m/day) was assigned to all simulated alluvial materials. This hydraulic conductivity was determined from pumping test analyses and core sample measurements obtained from wells at the LLNL site. Additional information was also available from other areas within the model domain (Thompson, 1990; Thompson *et al.*, 1991).

Although limited information is available in the highland areas, the existing geologic information and water level data suggest that ground water flow through these sediments is significantly impeded. The hydraulic conductivity for the highlands was estimated to be three orders of magnitude less than that of the alluvial basin (*i.e.*, 0.01 ft/day). The use of these hydraulic conductivity values provided the closest match to the potentiometric contours during the initial calibration (Fig. 4).

Two areas of measured discharge within the domain were included in Run 17A. The first area of discharge was a municipal water well field located near downtown Livermore and operated by CWSC (Fig. 4). An aggregate pumping rate of 2.9 cubic feet per second (cfs) was distributed among three principal water supply wells: 9P1, 9Q1, and 16B1. This extraction rate was estimated from the average pumping rates of these wells during the spring of 1989, the time the calibration water levels were measured.

The second area of discharge included in Run 17A was a gaining reach of Arroyo Las Positas (at element 266 in Fig. 5). A discharge of 1.2 cfs, specified at a single location, was used in many of the preliminary calculations. The streamflow along Arroyo Las Positas is monitored by Zone 7 with a series of stream gauging stations (Zone 7, 1988b), and in recent years the base flow rates varied between 1.2 and 1.4 cfs.

Because areal recharge from precipitation has been estimated to be about 10% of the annual precipitation rate (Zone 7, 1988a), a recharge rate of 0.1 ft/y was applied uniformly over only the alluvial basin elements. The uniform application of infiltration over the entire basin was assumed to account for localized recharge points, such as agricultural and landscape irrigation. It will not account for any concentrated recharge into the basin along the hillslope fronts produced by precipitation runoff from the slopes, infiltration from ephemeral streams, nor infiltration from the nearby South Bay Aqueduct. At this time, it is not clear whether these conditions are needed, but their inclusion should be considered in future simulations.

4.2. Modifications to the Original Flow Model

Several modifications have been made to the original flow model, based in part on the closing recommendations in Thompson *et al.* (1991). The modifications include: (1) slight refinements in the definition of the study area, material zones, and material properties; (2) an increased resolution of the computational mesh; and (3) adjustment of imposed boundary conditions and external, non-remedial source terms. Below, we summarize many of these adjustments as used in calibrated runs of the updated model.

Study Area. Originally, the northern boundary of the study area paralleled an inferred flow line in the Spring subbasin and was treated as a no-flow boundary in the flow model. Subsequent simulations indicated that the position of the flow line (and thus the integrity of the no-flow assumption) would be disturbed under remedial pumping conditions. Hence, the northern boundary of the study area was moved further northward toward the alluvial basin boundary along the Altamont and Tassajara Foothills. The new model mesh is shown in Figures 6 and 7.

As a result, boundary conditions were adjusted to account for recharge that enters along two portions of the new northern boundary segment (Table 2 and Fig. 6). The new northern

Table 2. Flux boundary descriptions in modified flow model.

Boundary segment ^a (flux)	Description
1	Small zone in the Altamont Hills east of LLNL (inflow)
2	Portion of northern alluvium boundary occupied by Altamont Creek (inflow)
3	Portion of northern alluvium boundary occupied by May Subbasin (inflow)
4	Western portion of the study area near downtown Livermore, crossing the lower Mocho II Province (outflow)
5	Small area south of the Toe zone bisecting an arm of the upper Mocho II Province (inflow)
6	Boundary between the Las Positas Fault zone and the upper Mocho II Province (inflow)

^aRefer to Figures 2 and 6 for locations of subbasins and boundary segments.

boundary encircles a region where Altamont Creek and areal recharge enter the alluvial basin from the Altamont Foothills in the east (Flux boundary 2, Fig.6). The May subbasin recharge boundary represents ground water flow into the domain from the north and west of the grid boundary (Flux boundary 3, Fig.6). These inflow boundaries are simulated as regions of constant head. The nodal head values were obtained from interpolations of water levels measured in the spring of 1989 by Zone 7. Topographic and hydrogeologic data suggest that no significant sources of ground water enter the domain along the remainder of the northern boundary. Conditions specified along all boundaries of the expanded study area are summarized in Tables 2 and 3.

The lower boundary of the study area has also been modified in some areas to provide for improved flow field calibration. The alluvial basin sediments are largely made up of shallowly dipping, layered materials that tend to preserve large-scale horizontal flows. As a result, ground water flow in isolated, deeper parts of the basin may be small compared to (or virtually disconnected from) flow in the relatively continuous upper sediments. This assumption is supported by other regional ground water studies (Toth, 1963; Freeze and Witherspoon, 1967), which have shown that the majority of flow takes place near the surface, and only a small percentage of the flow occurs in the deeper parts of the basin. Therefore, we raised parts of the original lower boundary of the study area (formerly along the blue clay layer of the Lower Member of the Livermore Formation) where the total aquifer thickness exceeded 150 ft. As a result, the overall thickness of the simulated aquifer was reduced in these areas. However, the general topography of the aquifer bottom was preserved, yet attenuated in the thickest regions, by including an arbitrary 10% of the residual thickness in excess of 150 ft. Revised distributions of base elevations and simulated aquifer thicknesses are shown in Figures 8 and 9, respectively. This change has had a minor effect on the simulated flow field, and actually resulted in a closer calibration to observed ground water levels. The remaining portions of the study area boundaries are unchanged from those used

Table 3. No-flux boundary descriptions in modified flow model.

Boundary segment ^a (no-flux)	Description
7	Portion of northern alluvium boundary not covered in Table 2
8	Northwestern boundary of the study area inside the Northwest Upland area
9	Southwestern boundary of the study area inside the Southwest Upland area
10	Eastern boundary of the study area inside the Southeast Upland areas (excluding the small recharge segment 1)
11	Eastern boundary of the study area inside the Northeast Upland areas (excluding the small recharge segment 1)

^aRefer to Figure 6 for location of boundary segments.

in the original flow simulations.

Hydrologic Zones and Material Properties. A minor modification in the distribution of basin and highland material types was made south and east of LLNL, in an area where the aquifer thickness is very small. Here, a small region of lower conductivity was "inserted" along Greenville Road in what was previously considered high conductivity alluvial material (Figs. 5 and 6, and Table 1) to be consistent with Zone 7 maps of this area. The hydraulic conductivity in this area was set to the value associated with all other highland zones (0.1 ft/day). This change improved the simulation of observed ground water levels in the southeast corner of LLNL.

In the new simulations, the alluvial materials were broken into three separate regions of differing hydraulic conductivity (Fig. 10). In the Mocho I, Spring, and May Subbasins (which include most materials beneath LLNL), we used an effective value of 10 ft/day; the same value as in the previous simulations. This value is strongly supported by the relatively abundant permeability data collected and analyzed at LLNL (Tompson, 1990; Tompson *et al.*, 1991). In light of finer grained materials and lower well yields found in the Altamont subbasin area east of LLNL, a lower hydraulic conductivity of 5.3 ft/day was used in this region, as suggested by calibration simulations. In the Mocho II subbasin south of LLNL, a slightly reduced conductivity of 8 ft/day was used to better reproduce observed gradients here. Remaining zones and material properties are unchanged from those used in the original flow simulations.

External Nonremedial Sources. The specified discharge of ground water into the Arroyo Las Positas was reduced from 1.2 to 0.9 cfs and distributed evenly among five adjacent elements along the gaining length of the arroyo shown in Figure 6. The applied discharge was reduced from the measured value to compensate for the reduction in simulated aquifer thickness near the reach (section 4.2). The actual alluvial thickness (from which most of the discharge emanates) varies from over 300 ft east of the reach to 50 ft near the reach, and reflects the increasing proximity of the Lower Livermore Formation to the ground surface in

this area. In addition, a measured discharge of 0.4 cfs into Altamont Creek (from the new part of the study area) was distributed over three elements representing the gaining reach of the creek (see Fig. 6). Because the aquifer is relatively thin in this area (less than 150 ft), no compensation for reduced thickness was made.

The applied aggregate pumping rate at the CWSC municipal wells in downtown Livermore was reduced from 2.9 cfs to 1.8 cfs to compensate for the reduction in simulated aquifer thickness (Fig. 9). The simulated aquifer intersects roughly 60% of the screen length of the municipal supply wells, from which the 2.9 cfs was produced.

Two agricultural pumping wells associated with the Wente Brothers Vineyards and the Davey Tree Farm, located southwest of LLNL, were added to the model because records indicated minor rates of ground water extraction during the calibration period. Because they are located near a low-permeability region to the south, significant drawdowns are observed near these wells (Fig. 4). Pumping records for the two wells were incomplete, but an estimated extraction rate of 0.056 cfs for each well was used for these simulations². Addition of these two wells improved the match of simulated and observed ground water levels in this area.

Records show that Zone 7 artificially recharges the upper aquifer materials in the Livermore Valley by discharging water from the South Bay aqueduct into upper reaches of the Arroyo Mocho. In April 1989, stream gauge measurements indicated a loss of about 1.5 cfs in Arroyo Mocho base flow across the modeled domain (Zone 7, 1990). The lost flow can be attributed to irrigation demands and evapotranspiration, as well as direct recharge. Here, a recharge rate of 0.75 cfs was assumed and distributed along 21 elements that correspond to the portion of Arroyo Mocho within the modeling domain. In the new simulations, this additional recharge increased ground water levels along the southwestern boundary of the Mocho II subbasin and more closely represented the observed ground water levels in this region.

Recharge applied to account for rainfall infiltration was not changed from the previous simulations. The addition of remedial pumping wells as a fluid sink is discussed in Sections 4.4 and 6, and in Tompson *et al.* (1991).

Grid Refinements. Because the same computational mesh would be used for contaminant transport calculations (Sections 5 and 6), the node spacing was reduced in the central portion of the study area to minimize the occurrence of numerical artifacts associated with larger grid Peclet numbers (Pinder and Gray, 1977). This refinement also improved the accuracy of simulated drawdowns resulting from remedial pumping. The nodal spacing in the vicinity of the LLNL was reduced from 520 ft to 260 ft (compare Figs. 5 and 6). South of LLNL, a limited number of triangular elements were introduced to allow for smaller elements and to provide a smoother transition of elements across the Las Positas Fault region.

²This corresponds to 25 gallons per minute (gpm). Henceforth, smaller pumping rates (less than 1 cfs) will be expressed in units of gpm for clarity.

4.3. New Flow Solution under Ambient Conditions

Based upon the above considerations, a steady-state potentiometric surface (water table) under ambient (non-remedial) conditions was computed from the new model and is shown in Figure 11. Characteristics of this and other flow simulations discussed in this report are summarized in the Appendix. This particular simulation is Run 24, and continues the sequence of flow model runs initiated in the previous report (Tompson *et al.*, 1991).

Because of the nonlinear nature of a water table solution, about 50 iterations were required to reach an absolute error tolerance of 1.0 ft (based on an initial estimate of observed water levels). Visual comparison of the observed surface (Fig. 4) with the calculated surface (Fig. 11) shows that we obtained a close match in the primary area of interest near the LLNL site. Figure 12 shows a contour map of the differences between the measured and simulated water levels from Run 24. In addition, reasonably good agreement was found in the Mocho II subbasin where the Livermore municipal wells are located. A significant discrepancy is located in the steep-gradient area south and east of LLNL near the Los Positas Fault. Because the sediments in this area are considered essentially impermeable and significant amounts of ground water are not transmitted through this region, a greater margin of error was tolerated here. In addition, actual water level data in this region are scarce and add uncertainty to the interpolated potentiometric surface.

An additional measure of calibration between the simulation and observations can be developed by calculating the difference or root-mean-squared (RMS) difference between the model solution and measurements, as averaged over all nodal points. In terms of the RMS difference, the current solution had an RMS error of 7.5 ft; the best of the previous calibrated solutions (Tompson *et al.*, 1991) had an RMS error of 10 ft.

4.4. Alterations for Simulations under Remedial Conditions

Following application and calibration of the new model under ambient, steady-state conditions, some of the boundary conditions and external discharge specifications were modified further to better represent the actual physics under remedial pumping and contaminant transport conditions. Similar modifications were made and tested in Runs 18 and 19 of Tompson *et al.* (1991). In Run 25, conditions along the Altamont Foothill boundary in the east, Altamont Creek watershed in the northeast, and May recharge basin boundary in the north were changed from constant head to constant flux conditions (as determined from the Run 24 solution; Table A-2, Appendix). Ground water influx at these locations is considered to be insensitive to changes in basin water levels that may be created by remedial pumping; *i.e.*, the watersheds outside the simulated domain are assumed to contribute fixed quantities of ground water to the basin, regardless of what happens within the basin. Thus, maintaining fixed head levels (as in Run 24) along these boundaries could potentially create erroneously steep hydraulic gradients if high pumping conditions were specified in the basin. This, in turn, would produce an erroneously large ground water flux into the basin through these boundaries. We note that the solution of Run 25 (with the modified flux conditions) reproduced the Run 24 solution (with the head solutions).

Using similar arguments, the specification of aquifer discharge into the Altamont Creek

and Arroyo Las Positas was modified beginning with Run 25 (Table A-3, Appendix). Instead of prescribing a fixed discharge along a series of elements as determined from measurements under ambient conditions, constant head conditions, corresponding roughly to the elevation of the arroyo bottoms, were specified along a series of nodes paralleling the streambeds. In reality, lower basin water levels created from remedial pumping could reduce or eliminate the amount of ground water discharging into these streams. If constant discharge conditions are maintained while ground water levels are lowered by remedial extraction, unrealistically low ground water levels may be simulated in these areas. Instead, heads along the source areas were made equal to values derived from the previous calibration run. The heads are, in fact, similar to the topographic elevation of the discharge areas. These conditions should be maintained as long as the neighboring heads remained high enough to support discharge. Otherwise, the conditions would be removed to prevent the streams from acting as unrealistic sources of aquifer recharge. Note that this modification does not apply to aquifer recharge along the Arroyo Mocho.

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Figure 5. Computational mesh for the initial LLNL flow simulations (Tompson *et al.*, 1991).

Figure 6. Improved computational mesh for flow and transport simulations.

Figure 7. Overlay of the improved computational mesh on a topographic map.

Figure 8. Base elevation of the simulated aquifer for the updated model.

ERD-CFEST-93.F9

Figure 10. Distribution of hydraulic conductivity specified on the computational mesh for the updated model.

Figure 11. Simulated potentiometric surface of the LLNL study area from Run 24.

ERD-CFEST-93.F04a

Figure 12. Difference between measured and simulated water levels from Run 24.

5. Migration Simulations Under Ambient Conditions

All chemical transport simulations described in this report focus on estimating the future, two-dimensional spatial distribution of VOCs as they evolve from current conditions (hereinafter referred to as time $t = 0$). Initial concentration distributions specified in the model are determined from current measurements and observations, as opposed to predictions based upon uncertain and inferred VOC releases in the past (Rogers, 1992). In Sections 5.3 and 5.4, we discuss two transport simulations under ambient flow conditions, defined in Flow Runs 24 and 25. These simulations constitute a series of "no-action" scenarios that describe how contaminants may migrate in the absence of remedial action. Later, in Section 6, we consider the impacts of remedial pumping. In particular, the notion of a carefully managed pump-and-treat strategy will be reviewed, in which a sequence of different pumping configurations (well locations and pumping rates) is used to more efficiently reduce concentrations of VOCs to desired levels within a specified time period.

Attention is initially focused on determining the current ($t = 0$) two-dimensional distribution of VOC mass within the LLNL study area. This distribution will be used to initialize all transport simulations in Sections 5 and 6. Essentially, this distribution is determined by integrating a corresponding three-dimensional mass distribution (interpolated directly from point observations and measurements) over the vertical extent of the aquifer.

5.1. Initial Mass Distribution

The initial distributions of VOC component mass were developed from ground water and sediment concentration measurements collected through January 1990 from approximately 270 boreholes and monitor wells at LLNL and in surrounding areas. For convenience, the concentrations of the eight target VOC components (Section 2.3) in the upper saturated sediments have been added to form a surrogate "total" (TVOC) which is considered a single constituent in these modeling calculations³. The surrogate compound has been assigned transport properties that are approximately representative of the eight VOCs of concern. Its liquid, solid, and aggregate concentrations are denoted by c_T , s_T , and c_T^* , respectively.

Three-Dimensional Distribution of VOCs. Measurements of local pore water concentrations in monitor wells, soil concentrations in boreholes, and other geological constraints were used to estimate the initial three-dimensional distribution of individual VOCs and the surrogate TVOC in the alluvial sediments at LLNL. From this distribution, we estimated the total mass of all VOCs in ground water and computed the two-dimensional, depth-averaged concentrations to initialize the chemical transport simulations.

Pore water measurements reflect the average VOC concentrations in ground water near the screened interval of a monitor well at the time of sampling. Because monitor wells are not installed or screened in all VOC-bearing layers or typically in zones of clay and silt, chemical data obtained from wells are insufficient to accurately represent the spatial distribution of VOCs in the ground water system at a given time. However, relatively continuous sediment core samples are collected during the drilling of individual boreholes, and measured soil concentrations may be used to infer liquid concentrations in adjacent ground waters by

³As used here, this TVOC will not include VOCs from FHCs

employing a partitioning relationship like Eq. (14). Unlike the pore water measurements, soil concentrations are not repeatedly measured at the same location over time, and cannot be used to estimate VOC distributions long after the installation of the well.

Systematic "depth sampling" allows the vertical distribution of VOCs to be estimated each time a borehole is drilled (Hoffman and Dresen, 1990). Ground water concentration data from a monitor well located at x_w, y_w were used to approximate the local liquid-phase TVOC concentration over the length of the screened interval centered at z_s (denoted here by $C_T(x_w, y_w, z_s, t = 0)$, the capital letter referring to a measurement). In addition, soil samples from other water-bearing zones were used to determine solid phase concentrations ($S_T(x_w, y_w, z, t = 0)$), which were then used to assign ground water concentrations to the corresponding water-bearing zone using the empirical relation $S_T = 0.2 \cdot C_T$. This relationship was empirically derived from comparisons of hundreds of soil and ground water samples from LLNL monitor wells, and loosely corresponds to use of Eq. (14) with $K_d \approx 0.2$ (Bishop *et al.*, 1990). If the porosity is assumed to be 0.3, $K_d \approx 0.2$ equates to a retardation factor $\mathcal{R}_T \approx 1.5$. In layers of silt and clay where no soil samples were collected, liquid concentrations were set to zero, based upon additional geological and chemical evidence that suggest that VOCs away from source areas at LLNL occur in discrete layers of higher permeability separated by "cleaner" intervals of lower permeability. Altogether, this algorithm provided roughly 45,000 concentration data points along the 270 boreholes from which data were obtained or estimated.

The resulting set of scattered, three-dimensional aqueous TVOC measurements and estimates were then used within the Interactive Volume Modeling (IVM) contouring package developed by Dynamic Graphics, Inc (DGI, 1989). Here, a biharmonic cubic spline function was used to interpolate the scattered data onto a regular, three-dimensional, user-specified grid. A so-called "Z-influence factor" equal to 0.1 was used to provide a forced anisotropy bias in internal distance weighting interpolation calculations (Devany *et al.*, 1990). Following this, a quantitative display of user-specified isocontour surfaces in three dimensions may be interactively displayed, rotated, and sliced. In this procedure, the zero-concentration values discussed above helped prevent erroneous extrapolation that would have otherwise occurred due to the lack of data in fine-grained sediments or in remote locations. The results were compared with geologic cross sections, and the grid was refined to minimize interpolation artifacts. This method produced a three-dimensional representation of TVOCs in ground water that represents *current* or *initial* conditions (Fig. 13). Here, logarithmic contour intervals produced multiple three-dimensional surfaces that correspond to TVOC mass fractions of 1, 10, 100, and 1,000 ppb, respectively.

Mass Within and Volume of TVOC Plume. The mass of TVOCs in the study area (based upon data collected between 1986 and 1990) may be estimated by sequentially integrating the mass distribution within a series of isocontour shells like those shown in Figure 13. For example, the liquid phase TVOC mass within a series of N_k shells may be approximated by

$$M \approx \rho \epsilon \sum_{k=1}^{N_k} \omega_T^k (V_k - V_{k+1}), \quad (15)$$

where ρ is the density of the solution (water), ϵ is the porosity, ω_T^k is an average mass fraction

of TVOCs between shells k and $k+1$, V_k is the raw volume of shell k (easily computed with the IVM software), and $V_{N_k+1} = 0$. If, as in the case of Figure 13, the shells represent a logarithmic scaling of mass fractions, geometric averages should be used to compute ω_T^k . In the present case, using $\epsilon \approx 0.30$, the four shells in Figure 13 were used to compute a mass of 890 kg TVOC present in ground water at the site, as previously reported in the LLNL Feasibility Study (Isherwood *et al.*, 1990). If the notion of a constant retardation factor $R_T \approx 1.5$ suggested above is correct, then roughly 1,330 kg TVOC exist within the liquid and solid phases in the study area.

As part of this calculation, the bulk volume, V_1 , within the 1-ppb outer shell was estimated to be approximately $2.0 \times 10^9 \text{ ft}^3$. This will be used as a rough measure of the TVOC plume's overall volume. Using $\epsilon \approx 0.30$, the volume of fluid contained within the plume (regardless of concentration) is roughly $V_f \approx \epsilon V_1 = 6.0 \times 10^8 \text{ ft}^3$. This volume will be referred to as one "pore volume" and will later be compared with the gross number of equivalent pore volumes of water to be extracted via pumping within each of the proposed remedial pumping schemes.

Two-Dimensional Distribution of TVOCs. Using a similar integration technique, the three-dimensional distribution of mass shown in Figure 13 may be vertically-averaged to provide an initial two-dimensional concentration distribution for our migration studies. When the computational mesh (Fig. 6) is superimposed over the three-dimensional representation (Fig. 13), a vertical volumetric column (with a polygon cross section) may be associated with (and centered on) each node of the computational mesh, such that the union of all columns covers the entire study area, and no two columns share any volume element. Each polygon connects the element centroids around each node. The top and bottom of each column are the water table and lower boundary of the study area, respectively. Within each column, we estimated the liquid phase TVOC mass using a modified version of Eq. (15) and divided it by the volume of pores in the column. This result was assigned to the grid node associated with the column as the initial vertically-integrated concentration $c_T(x_g, y_g, t = 0)$. The simulated distribution of $c_T(x, y, t = 0)$ is shown in Figure 14. The maximum aqueous, vertically-averaged total concentration is about 800 ppb. Values of the corresponding quantities s_T and c_T^* may be derived from partitioning relationships as discussed in Section 3.2.

5.2. Flow and Migration Processes

All transport simulations discussed in this report are based upon solving Eq. (13) for the liquid phase concentration c_T on the new computational mesh (Fig. 6), using a two-dimensional implementation of the CFEST finite-element code (Gupta *et al.*, 1987). When analyzing TVOC migration under steady, ambient conditions (below), the initial TVOC distribution determined above (Fig. 14) have been used to initiate the simulation. This assumes the simulated aquifer thickness from the flow solution is equal to that used in determining the initial concentrations. When analyzing transport under remedial conditions (Section 6), periodic corrections may be needed in the concentration distribution to account for free surface, water-table conditions. In these cases, as discussed in Section 4.1, the active thickness of the simulated aquifer may change with the solution, whether or not steady-state

conditions are considered. If the solute mass within a vertical column of aquifer remains constant while the saturated thickness changes, then the vertically-integrated concentrations must be modified to reflect the change in integration thickness. Although this effect is accounted for by the inclusion of aquifer thickness (b) in the time derivative in Eq. (13), our particular CFEST implementation has assumed b to be constant in time, corresponding to confined aquifer conditions.

As outlined in Section 6, sequences of different steady flow fields, corresponding to different remedial pumping configurations, were used to study TVOC removal from the aquifer (transient effects between flow fields are not considered). When a new (steady) flow field is incorporated into an ongoing transport simulation, the vertically-averaged concentrations must be scaled to account for the changes in saturated (averaging) thickness. Although this effect may seem to arbitrarily change the concentrations (as a byproduct of the two-dimensional conceptualization), it is required to conserve the VOC mass during a flow field transition.

Flow and Dispersion Processes. In Eq. (13), the flux of contaminants is controlled by ground water flow and dispersion processes. The ambient regional ground water flow field produced as described in Section 4.3 (flow Run 25) is used as the basis for the "no-action" transport simulations. The "no-action" flow field is influenced by all existing recharge and discharge processes (from municipal and commercial pumping wells, rainfall recharge, etc.), but not by remedial pumping. The magnitude of contaminant dispersion is dependent on ground water velocity, aquifer dispersivities, and chemical diffusivity, as reflected in the dispersion tensor $\mathbf{D}$ in Eq. (4). In these simulations, chemical diffusion is assumed to be insignificant relative to physical dispersion; therefore, the diffusivity is set equal to zero. Based upon the data analyses of Tompson (1990), a longitudinal dispersivity $A_{11} \approx 260$ ft was chosen, and following Freeze and Cherry (1979), the transverse dispersivity A_{22} was assumed to be one-tenth of A_{11} (≈ 26 ft). For a problem scale on the order of 3,000 ft in length, these values are also consistent with the data tabulated in Gelhar *et al.* (1992). In addition, the dispersivities were assumed to be constant and uniform over the simulation domain. These values are summarized in the Appendix.

Sorption and Decay Processes. In these simulations, the sorption reactions associated with the surrogate TVOC are assumed to follow a simple linear partitioning relationship (Eq. 14), as discussed in Section 3.2. The effect of this process is to retard contaminant advection and dispersion relative to ground water flow, as shown in Eq. (13). The retardation is quantified by the factor $\mathcal{R}_T$, (Eq. 12), assumed here to be a constant value of 1.5. This value is roughly consistent with a myriad of local measurements (Bishop *et al.*, 1990), as well as various history matching analyses (Tompson, 1990; Rogers, 1992).

At the time of these simulations, little work has been done to systematically identify mechanisms for bacterial or abiotic degradation of VOCs in the LLNL study area, much less quantify the potential rates of decay. However, some PCE and TCE degradation byproducts, such as 1,1-DCE, have been detected in ground water beneath the site (Thorpe *et al.*, 1990), and various VOC degradation pathways have certainly been identified in other subsurface systems (Vogel *et al.*, 1987). Examination of concentration measurements for losses or accumulation of decay products over the past 6 y do not suggest any type of "fast" reaction consistent with a half-life of less than 10 y (McNab and Narasimhan, 1994).

Some have suggested that apparent discrepancies between the current mass of TVOCs in the saturated zone and original usage inventories of these compounds 50 y ago may be partially indicative of a loss due to one or more transformation or decay mechanisms. At the simplest level, this might warrant the use of a 50-y half-life to represent biological and/or chemical degradation. However, this argument fails to include potentially large losses due to surface or vadose zone volatilization or unidentified VOC mass in the subsurface, and cannot really justify how or whether all original VOC inventories were released onto the ground surface. Because of these uncertainties, we have incorporated the linear decay models Eqs. (6-7) within our simulations, using a half-life of 50 y ($\lambda = \ln 2/50 \text{ y}^{-1}$), and also report the results of companion simulations based on no-degradation ($\lambda = 0$) to show the relatively large impacts that this assumption has on the model predictions.

Pumping and Other External Sources of Contaminants. The only pumping wells in the ambient-condition simulations are associated with municipal and agricultural extraction (see Run 25, Appendix), and are not located within the plume. The initial contaminant mass distribution is assumed to be completely encapsulated by the water table and lower no-flow boundary. As discussed in Section 3.2, contaminant flux across the top and bottom aquifer boundaries will not be considered, except for extraction through pumping wells.

5.3. "No-Action" Transport Simulation

This section presents the results of a "no-action" transport simulation with degradation (transport run T1, Table A-7, Appendix). Future TVOC concentrations calculated under ambient flow conditions are shown after 50, 160, and 250 y in Figures 15, 16, and 17, respectively. These simulations are based upon the initial condition shown in Figure 14 (Section 5.1), the flow field from Run 25 (Appendix), and a 50-y degradation half-life. The results represent vertically-averaged concentrations. Results of a similar "no-action" simulation without degradation are presented in Section 5.4.

Calculated Conditions after 50 y. As seen in Figures 14 and 15, the VOC plume has migrated to the south and southwest under natural flow processes. Uncontaminated ground water flowing from the east and northeast has caused contaminants from most upgradient portions of the study area to flow west and southwest. The effects of hydrodynamic dispersion have smoothed the steeper concentration gradients and promoted plume dilution. The calculated maximum TVOC concentration after 50 y has decreased from over 800 ppb to 58 ppb, and is located about 1,300 ft south of the initial maximum concentration (Fig. 15). The apparent dilution effect has also been hastened by the assumed degradation process, which has resulted in a 50% reduction of the initial mass by this time. In other words, in the absence of degradation, contour values would be twice as large as indicated in Figure 15 (see also Section 5.4).

After 50 y, calculated TVOC concentrations no longer exceed 10 ppb in the southwest corner of LLNL. The leading edge of the plume, defined here as the 1-ppb isoconcentration contour, is located about 3,600 ft west of Vasco Road; about 1,600 ft further downgradient as compared to the initial conditions (Figs. 14 and 15). The calculated TVOC concentration

at the Wentle Vineyards well (14C3) is about 3 ppb. The simulation results indicate VOCs have not migrated to agricultural well 14K1 at the Davey Tree Farm at this time.

Calculated Conditions after 160 y. As seen in Figure 16, calculated TVOC concentrations are uniformly less than 5 ppb. The 1-ppb isoconcentration contour extends up to 3,200 ft west of Vasco Road and 1,600 ft south of East Avenue. The effects of dispersion and degradation are again significant. The eastern 1-ppb contour of the plume has moved upgradient of its position after 50 y by about 400 ft (compare Figs. 15 and 16). This is most likely an artifact of the dispersion model and large value of dispersivity used.

At this time, the maximum calculated TVOC concentration is less than 5 ppb and is located just south of East Avenue near the Arroyo Seco, more than 3,000 ft southwest of the initial maximum concentration at $t = 0$ (Fig. 14). The 1-ppb TVOC isoconcentration contour is close to Wentle Vineyard agricultural supply well 14C3. The calculated TVOC concentration at Davey Tree Farm well 14K1 is close to 0.1 ppb. Pumping at these wells has likely influenced the position of the 1-ppb contour.

The results in Figure 16 may be used in an approximate sense to indicate a potential state of compliance with current regulations governing allowable VOC concentrations. Clearly, because the TVOC concentration has been calculated to be less than 5 ppb (on a depth-averaged basis) throughout the study area after 160 y, then depth-averaged concentrations of the individual VOC compounds that comprise the total should also be less than 5 ppb. Thus, it would appear that compliance with MCLs of 5 ppb is suggested by the calculations. However, if the VOCs are not uniformly distributed over the vertical dimension of the aquifer, it is possible that concentrations at some depth may exceed an MCL, while still satisfying the limit in an average, vertical sense (Section 3.3). More focus on these issues may be obtained by using three-dimensional simulations to predict concentrations with more spatial detail, or by calculating migration patterns of each VOC constituent. In addition, all cited concentrations or indicated isoconcentration values at $t = 160$ y will be higher by an amount equal to $\exp(160 \cdot \ln 2/50) = 9.2$ (3.2 half lives) in the absence of degradation. Thus, the 1-ppb contour at $t = 160$ y would approximately correspond to a 9 ppb contour, and would negate any previous conclusions regarding MCL compliance. As discussed in Section 5.4, the maximum (vertically-averaged) TVOC concentration in the absence of degradation is not calculated to drop below 5 ppb until almost 800 y.

Calculated Conditions after 250 y. Figure 17 shows calculated TVOC isoconcentration contours after 250 y under the assumed degradation conditions. The position of the leading 0.1-ppb contour of the plume has not moved appreciably from $t = 160$ y to $t = 250$ y, indicating an interesting near-balance between advection and degradation processes. The maximum concentration is roughly 0.9 ppb. The calculated 0.5 ppb TVOC contour intersects the Wentle Vineyard well (14C3). The calculated TVOC concentration at Davey Tree Farm well 14K1 is less than 0.1 ppb. The calculations also suggest that the (vertically-averaged) TVOC level in the downtown Livermore CWSC municipal supply wells (9P1, 9Q1, and 16B1) never exceeds 0.01 ppb under the assumptions of "no-action" and a 50-y degradation half-life. Similarly, no significant concentrations (> 0.01 ppb) are detected at the Arroyo Las Positas discharge area. Again, in the absence of degradation, all cited concentrations or indicated concentrations at $t = 250$ y will be higher by an amount equal to $\exp(250 \cdot \ln 2/50) = 32$ (or five half-lives).

Summary of Transport Run T1. In summary, results of the "no-action" transport simulation indicate significant west-southwesterly migration of the TVOC plume, generally in the direction of natural ground water flow. Over time, the total mass within the plume (as indicated by its areal extent or diameter of a closed isoconcentration contour) is significantly reduced. This is caused by the aggregate losses produced by the assumed degradation process, and not to direct mass extraction by any remedial means.

Under the assumed degradation conditions, results indicate the TVOC plume reaches the CWSC municipal supply wells located in downtown Livermore at extremely low depth-averaged concentrations (0.01 ppb). Figure 18 shows calculated concentrations versus time at Wentle Vineyards well 14C3, Davey Tree Farm well 14K1, and downtown municipal wells 9P1, 9Q1, and 16B1. The results also suggest the maximum total concentration will fall below 5 ppb after 160 y (Fig. 16) and below 1 ppb after 250 y (Fig. 17). By comparison, under no-degradation conditions, the calculated maximum depth-averaged total aqueous VOC concentration is about 28 ppb after 250 y (see Section 5.4). These results stress the importance of clarifying the presently uncertain nature of VOC degradation in the LLNL system. In addition, use of the two-dimensional, depth-averaged conceptualization and surrogate TVOC may limit the degree to which our results may be compared with MCLs for specific VOCs.

5.4. "No-Action, No-Degradation" Transport Simulation

This section presents results of a "no-action, no-degradation" transport simulation (transport run T2, Table A-7, Appendix). Future TVOC concentrations calculated under ambient flow conditions in the absence of degradation ($\lambda = 0$) are shown after 50, 500, and 800 y in Figures 19, 20, and 21, respectively. This simulation is based upon the initial condition shown in Figure 14 (Section 5.1) and the flow field from Run 25 (Appendix). The results represent vertically-averaged concentrations. Reduction of TVOC concentrations will only occur through dispersive dilution, small amounts of VOC removal at non-remedial pumping wells, or minor surface discharges. This simulation represents a more conservative view of TVOC migration under natural flow conditions.

Calculated Conditions after 50 y. Calculated TVOC isoconcentration contours after 50 y are shown in Figure 19. Comparison of Figures 15 and 19 shows, as expected, that at similar times, the calculated distribution of TVOC mass in the no-degradation case at 50 y is twice that found in the degradation case (Section 5.3). As above, the plume moves generally in a southwesterly direction. The maximum aqueous TVOC concentration reaches 116 ppb (as compared with 58 ppb in the degradation case), and is again located about 1,300 ft southwest of the initial high concentration point at $t = 0$ (Fig. 14). The position of the 1-ppb contour is more than 1,000 ft downgradient (southwest) of its initial position. Contaminants are not calculated to reach Davey Tree Farm well 14K1, the CWSC wells in downtown Livermore, or the Arroyo Las Positas discharge area. The calculated TVOC concentration at Wentle Vineyards well 14C3 is about 6 ppb after 50 y.

Calculated Conditions after 500 y. After 500 y of migration under ambient flow conditions with no-degradation, the VOCs have migrated away from LLNL, and TVOC concentrations beneath the site are all less than 1 ppb (Fig. 20). In addition,

TVOC concentrations are greater than 1 ppb near downtown Livermore. However, TVOC concentrations do not exceed 1 ppb at any of the CWSC municipal supply wells during the simulation. TVOC concentrations in ground water discharging to the Arroyo Las Positas north of Livermore are about 2 ppb. The TVOC concentration at Wente Vineyards agricultural well 14C3 is about 7 ppb, while that at Davey Tree Farm well 14K1 is about 10 ppb. Higher concentrations, as delineated by the 10-ppb contour, have migrated past well 14C3 and are approaching well 14K1. Results suggest the maximum TVOC concentration after 300 y at well 14C3 will be about 18 ppb at well 14C3 and about 6 ppb at well 14K1.

Calculated Conditions after 800 y. After 800 y of migration under ambient flow conditions with no-degradation, results suggest the TVOC concentrations fall below 5 ppb throughout the entire domain (Fig. 21). The furthest westward location of the 1-ppb contour is calculated to be about 12,000 ft west of Vasco Road. Calculated TVOC concentrations at Davey Tree Farm well 14K1 and Wente Vineyards well 14C3 at this time are 2 ppb and 0.3 ppb, respectively. The TVOC concentrations at CWSC wells 9P1, 9Q1, and 16B1 are less than 1 ppb. At the Arroyo Las Positas discharge area, the calculated TVOC concentration is about 1.6 ppb.

Summary of Transport Run T2. Results of the "no-action, no-degradation" simulation indicate significant west-southwesterly migration of the TVOC plume, generally in the direction of natural ground water flow. The most notable difference in this case is that the rate of concentration reduction with time is much slower. Only natural dispersion processes contribute to plume dilution. Because degradation has not been included, the mass within the plume remains relatively constant (albeit dispersed) in time, except for minor discharges at local wells or into arroyos. The net result is that the vertically-integrated aqueous TVOC concentrations fail to fall uniformly below 5 ppb until 800 y of migration under the current ambient conditions, and do not fall below 1 ppb until 1,200 y (as compared with 160 y and 250 y, respectively, in the degradation case).

In the no-degradation simulation, the furthest extent of the 1-ppb contour is about 12,000 ft west of Vasco Road, which places portions of the plume under the northeast section of Livermore. The plume also extends northwesterly to the Arroyo Las Positas discharge area. TVOC concentrations at the Arroyo Las Positas discharge area reach a maximum of about 2.4 ppb at 600 y. Results also indicate that TVOC concentrations in ground water extracted by the CWSC wells 9P1, 9Q1, and 16B1 will not exceed 1 ppb over the time frame of the simulation. Concentrations of 0.1 ppb are first detected near well locations 9P1 and 9Q1 after 250 and 350 y, respectively. In the simulation, the maximum TVOC concentrations near well 9P1 are bounded by 0.5 and 1 ppb between years 450 and 850, respectively. Note again that these concentrations represent aqueous TVOC concentrations integrated over the depth of the simulated aquifer. Because all three of the CWSC wells draw water from intervals that intersect and reach further below the simulated unit, actual TVOC concentrations measured in these units would probably be lower than calculated, due to mixing with cleaner waters drawn from the deeper zones. Figure 22 shows calculated concentrations versus time at Wente Vineyards well 14C3, Davey Tree Farm well 14K1, and CWSC municipal downtown wells 9P1, 9Q1, and 16B1.

Text continues on page 47.

ERD-CFEST-93/F11

Figure 13. Three-dimensional representation of the aqueous TVOC distribution beneath the LLNL study area.

Figure 14. Two-dimensional representation of the vertically-integrated, aqueous TVOC distribution beneath the LLNL study area.

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ERD-CFEST-93/F13

Figure 15. Calculated TVOC isoconcentration contours after 50 y; "no-action scenario", 50 y degradation half-life.

ERD-CFEST-93/F14

Figure 16. Calculated TVOC Isoconcentration contours after 160 y; "no-action scenario", 50 y degradation half-life.

ERD-CFEST-93/F15

Figure 17. Calculated TVOC isoconcentration contours after 250 y; "no-action scenario", 50 y degradation half-life.

ERD-CFEST-93/F16

Figure 18. Calculated aqueous, vertically-integrated TVOC concentrations versus time at downgradient ground water supply wells; "no-action" scenario, 50 y degradation half-life.

ERD-CFEST-93/F17

Figure 19. Calculated TVOC Isoconcentration contours after 50 y; "no-action, no-degradation" scenario.

ERD-CFEST-83/F18

Figure 20. Calculated TVOC isoconcentration contours after 500 y; "no-action, no-degradation" scenario.

ERD-CFEST-93/F19

Figure 21. Calculated TVOC Isoconcentration contours after 800 y; "no-action, no-degradation" scenario.

ERD-CFEST-93/F20

Figure 22. Calculated aqueous, vertically-integrated TVOC concentrations versus time at downgradient ground water supply wells; "no-action, no-degradation" scenario.

6. Migration Simulations Under Remedial Conditions

In this section, we consider three separate flow and transport simulations under remedial "pump-and-treat" conditions, and seek to understand how the current two-dimensional contaminant distribution at $t = 0$ can be contained, drawn toward extraction wells, and ultimately removed. All simulations are based upon the same initial VOC mass distribution developed in Section 5.1. Below, we begin by introducing an adaptive pump-and-treat strategy in which a sequence of different extraction and injection well configurations is used over time to maximize removal of VOCs. We then review the initial modeling configuration and associated transport processes. Finally, the three flow and transport simulations are presented and discussed.

6.1. Management-Oriented Simulations

Pump-and-Treat Procedure. The objectives of LLNL pump-and-treat remediation are to arrest further westward migration of the contaminant plume, remove VOC mass at a rate necessary to achieve cleanup within a specified time period, and reduce concentrations to meet regulatory MCLs for each target VOC. The procedure involves the use of extraction wells to remove contaminated ground water, the treatment of this water at the surface, and the possible reintroduction of treated (clean) water into the subsurface via infiltration or injection wells. A set of extraction and injection wells, including their locations, pumping rates, and time of operation, comprises a specific pumping "configuration." As remediation progresses, the pumping configuration may be adjusted or modified to improve efficiency. The wells may be fully or partially screened, and their rates will be bounded by local drawdown and basin safe yield constraints.

The impacts of pump-and-treat remediation have been briefly analyzed in the CERCLA Feasibility Study for the LLNL Livermore Site (Isherwood *et al.*, 1990). In that study, the aggregate contaminant capture zone associated with a proposed pumping configuration was calculated, under conditions of constant westward ground water flow, a confined aquifer of uniform thickness, and no dispersion, sorption, or other chemical degradation, and used to estimate the approximate pumping configuration necessary for containment of the VOC plume. Here, we examine the efficacy of various pump-and-treat procedures using the more detailed CFEST models of flow and transport discussed in the previous sections. Below, we examine how the initial, two-dimensional TVOC distribution, as introduced in Section 5.2 and shown in Figure 14, is reduced in response to various remedial pumping configurations. As above, these simulations focus on vertically-integrated concentrations of the surrogate TVOC compound, and assume that extraction and injection wells are fully screened. Issues regarding plume containment, mass removal rate, concentration reduction, and number of wells required to meet MCL criteria will be addressed.

Adaptive Pump-and-Treat at LLNL. The simulations discussed below are used to analyze an adaptive pump-and-treat strategy for the reduction and removal of contaminants in the LLNL study area. The notion of "adaptive pump-and-treat" involves changing the pumping configuration at selected times in order to enhance cleanup efficiency. Changes may

be made at specified times or in response to a perceived loss in remedial efficiency. Here, models are used to forecast the efficiency of various remedial pumping configurations and plan future configurations.

In the current strategy, an initial well configuration at $t = 0$ is chosen by placing pumping wells in areas of high contamination to force fast, immediate removal of larger amounts of VOC mass, and at downgradient locations to form a hydraulic interception zone to contain VOC mass. A steady flow field corresponding to this well field (and other ambient conditions) is developed and used to calculate contaminant migration and extraction processes under the proposed pumping configuration. After some period of time (*e.g.*, at $t = t_1$), the extraction efficiency may decrease. Unaffected zones of contamination may linger near flow stagnation zones, while original target areas may show reduced concentrations. In response, the flow field may be changed by adjusting the well configuration to target newer areas of high concentration and stop pumping in cleaner zones. Following development of a modified steady flow field, analysis of migration and extraction may continue for another period of time until efficiency is reduced again (*e.g.*, at $t = t_2$), whence the process may be repeated if desired.

Although various sequences of pumping configurations and contaminant reduction scenarios may be explored heuristically with this approach, no particular "optimal" path of configurations is guaranteed.⁴ In Sections 6.3 through 6.5, this approach is used to study three remedial alternatives at LLNL involving cleanup within a 50-y time frame.

6.2. Flow and Migration Processes

Here, attention is focused on the migration and transformation of the surrogate TVOC compound described in Section 5.1 under remedial pumping conditions. Simulations of ground water flow will be based upon solving steady forms of Eqs. (1) and (2) under various pumping configurations. Because of their short duration (weeks), transient phenomena between different steady fields will not be considered. Solutions of the unsteady transport equation (13) that sequentially incorporate the appropriate flow solutions will be used to determine how the aqueous TVOC distribution changes and is reduced with time. As in Section 5, simulations are based on a two-dimensional implementation of the CFEST finite-element code (Gupta *et al.*, 1987), modified for water table conditions, and the new computational mesh (Fig. 6). As discussed in Section 5.2, the vertically-integrated concentration distributions will be rescaled when each new flow field is introduced. This is done to reflect changes in aquifer thickness caused by each new pumping configuration and to conserve solute mass in the model.

Flow Field Configurations. Three remedial transport simulations (Transport Runs T3, T4, and T5; Table A-7, Appendix) are considered below in Sections 6.3, 6.4, and 6.5, respectively. Each simulation involves tracking the migration, transformation, and extraction of TVOC mass under the influence of one or more steady flow fields that correspond to a sequence of different remedial pumping configurations. The first configuration is developed in

⁴As used here, "optimal" may have several definitions; *e.g.*, Dougherty and Marryott (1991), Rogers and Dowla (1994).

each simulation by adding a specific set of extraction and injection wells to the calibrated Run 25 (described in Section 4.4), while subsequent configurations involve adding or deleting wells from previous configurations. As shown in the Appendix, Flow Runs 26, 27, and 28 designate the suite of flow configurations used in each of the three remedial transport simulations.

Initial Mass Distribution. The two-dimensional distribution of TVOCs measured under ambient conditions (Section 5.1 and Fig. 14) are used to initiate each remedial transport simulation. Recall that to conserve solute mass, the vertically-averaged (two-dimensional) concentration distributions must be rescaled to reflect changes in aquifer thickness that arise when the flow field (*i.e.*, pumping configuration) changes (Section 5.2). Thus, the initial TVOC distribution in Figure 14 must be rescaled after the first, and all subsequent remedial flow configurations are computed in each transport problem.

Dispersion, Sorption, and Decay Processes. In all transport simulations, the magnitudes of aquifer dispersivity and chemical diffusivity (as used in the dispersion tensor **D**) are unchanged from those used and described in Section 5 and the Appendix (Table A-7). As reviewed in Section 5.2, the sorption reactions associated with the surrogate TVOC compound are assumed to follow a simple linear partitioning relationship Eq. (14), and a constant retardation factor R_T of 1.5 is used. The linear-degradation model is used in the remedial simulation T3 discussed in Section 6.3. No-degradation is assumed in remedial simulations T4 and T5 discussed in Sections 6.4 and 6.5, respectively.

Pumping and Other External Sources of Water and Contaminants. Pumping wells associated with municipal and agricultural extraction are included in all flow field configurations (Table A-3, Appendix), in addition to specified sequences of extraction or injection wells and other surface discharges associated with remediation (Tables A-4 through A-6, Appendix). These are separately described below. At all times, the contaminant plume is assumed to be encapsulated by the water table and the lower aquifer boundary. Contaminant flux across the top and bottom aquifer boundaries is not considered, except for extraction through pumping wells or discharges to surface streams. In all cases, extracted or discharged waters are assumed to retain their vertically-averaged TVOC concentrations. All treated waters injected or discharged to the surface are assumed to have no TVOC concentrations.

6.3. Fifty-Year Cleanup Simulation with Degradation

Here, we consider a remedial pumping scheme focused on reducing aqueous (vertically-integrated) TVOC concentrations to 5 ppb or less in all parts of the study area within 50 y. We assume degradation processes consistent with a 50-y half-life are occurring. A total of 25 extraction wells, 2 injection wells, and 3 surface discharge areas are used within a series of 12 separate pumping configurations spread out over the 50 y period.

Extraction and Discharge Locations. In all simulations, proposed remedial well locations will be sited near previously identified *extraction* locations (ELs), *discharge* areas, or *treatment facilities* (TFs), either in use or planned, as shown in Figure 23. All extracted ground water will be treated at one of these facilities and either recharged to the aquifer, discharged to the sewer system, or utilized as cooling water within the laboratory's plant engineering system. The particular scheme shown in Figure 23 is what LLNL is obligated to

construct based upon negotiations with regulators as covered in the LLNL Livermore Site Record of Decision (ROD) (USDOE, 1992). The schemes proposed in this and the next two transport simulations (Sections 6.4 and 6.5) build upon this basic plan, and involve the use of additional extraction and injection wells that are not part of the Record of Decision and which LLNL is not committed to build.

As of September 1994, ground water was being extracted from and treated at four of these locations. Extraction well EW-415, located in the southwest corner of LLNL (EL-1), removes ground water that is processed at Treatment Facility A (TFA). Extraction wells EW-704 and MW-357, located along the western LLNL boundary (EL-5), extract ground water that is processed at Treatment Facility B (TFB). Extraction well P-701, located in the northwest portion of LLNL (EL-9), removes ground water that is processed at Treatment Facility C (TFC). In the Gasoline Spill Area, located in the southeastern portion of LLNL (EL-17), gasoline extraction wells GEW-808 and GEW-816 remove ground water containing fuel hydrocarbons and VOCs. Ground water extracted from beneath the Gasoline Spill Area is processed at Treatment Facility F (TFF). All four of these extraction locations are incorporated within the remedial simulations, as well as future Treatment Facilities D, E, G, and T-5475 (TFD, TFE, TFG, and TF5475, respectively).

Ground water processed at TFA is currently being discharged to the Recharge Basin, located approximately 1,000 ft south of LLNL (Fig. 23). In the model, we assume all the ground water processed at TFA is recharged to the aquifer via the Recharge Basin. All of the ground water processed at TFB is discharged to a north-flowing drainage ditch located along Vasco Road. The ditch extends about 2,300 ft north of TFB and ultimately discharges to Arroyo Las Positas. Ground water treated at TFC, located in the northwest portion of LLNL, is discharged to another north-flowing ditch that also drains into the Arroyo Las Positas. Ground water treated at TFF is currently discharged to the sanitary sewer. However, within the simulations, all water treated at TFF is assumed to be recharged to the aquifer via an injection well located southeast of the Gasoline Spill Area. Injection of ground water in this area is extremely important in the model. Small extraction flow rates in this area can quickly dewater the aquifer in the southeast corner of LLNL because the upper saturated zone in this area is thin and is bounded by the Las Positas and Greenville Faults, which are barriers to recharge. By artificially recharging the aquifer in this area, extraction flow rates can be maintained and contaminated ground water can be removed from the southeast corner of LLNL more rapidly. Some of the ground water processed at TFE may also be injected into the aquifer. In the model, the simulated injection point is located in the central portion of LLNL, where total VOC concentrations are less than 5 ppb (Figs. 14 and 23). This injection node provides additional recharge to extraction wells in the southwest corner of LLNL and tends to drive upgradient zones of contamination back toward the eastern and southeastern extraction wells.

Initial Well Configuration. The initial well field configuration for this simulation is composed of 21 extraction locations, 2 injection wells, and 3 surface discharge areas. The extraction wells include the 4 locations operating in September 1994 and 17 others; the injection and discharge areas are as described above. The operation schedule for all wells and discharge areas is summarized in Figure 24, and can be cross-referenced with Figure 28 and a more detailed listing in Table A-4 (Appendix). Note that each entry in Table

A-4 corresponds to a single extraction or injection location as specified at a node in the model; these may, in fact, correspond to a cluster of one or more actual wells in the field. The wells were positioned to maximize contaminant mass removal and prohibit offsite VOC migration. Well placement was based on calculated locations of high VOC concentration, anticipated contaminant migration under the influence of pumping, and the areal extent of individual well capture zones. Simulated rates were based on estimated yields of monitor wells near each location. Figure 25 shows the aggregate rate of extraction and recharge from all remedial wells and discharge locations as a function of time, for this simulation and the others described in Section 6.4 and 6.5. For the initial well configuration, the net steady-state ground water extraction rate is 165 gpm and corresponds to gross extraction and recharge rates of 445 gpm and 280 gpm, respectively. These values may be contrasted with the selected remedial alternative proposed in the Record of Decision (USDOE, 1992) which calls for an net extraction rate of 350 gpm over a 50-y period, with no concurrent reinjection.

The initial head field produced by the first pumping configuration is shown in Figure 28a. Approximate, two-dimensional ground water flow lines produced by this configuration are shown in Figure 26. The calculated thickness of the saturated aquifer has been used to produce the rescaled initial aqueous TVOC distribution shown in Figure 27. The thickness of the aquifer has been reduced most strongly near the areas of pumping and high concentration without changing the VOC mass in the saturated soil column. Hence, the rescaled concentrations in Figure 27 are much higher than those shown in the unpumped field (Fig. 14). The concentration near EL-14 has been raised from 830 to over 1,300 ppb due to the rescaling.

Updated Well Configurations. The initial well configuration is unable to attain the 5-ppb cleanup goal within a 50-y period because the overall extraction efficiency decreased significantly with time. In some cases, continued pumping in "cleaned-up" areas reduced the amount of fresh water available for dilution at downgradient locations; in other locations, stagnation zones in the flow field prevented contaminants in those areas from being removed by extraction wells.

Thus, an adaptive pumping scheme was adopted to improve extraction efficiency. Concentrations were monitored at the end of individual management periods, after which the well locations and pumping rates were modified, if necessary. Initial management periods were 5 y in length; later, 1-y periods were used. Extraction wells not used for plume containment were removed if, at the end of a management period, the aqueous TVOC concentration was below 5 ppb at the extraction node. If an extraction well was removed from the well field, either new wells were added in the remaining areas of high concentration, or the pumping rates of existing wells were increased. In addition, the extraction rate of a well could be increased if the injection rate of an associated well was correspondingly increased. However, to prevent excessive dewatering, the calculated head at simulated extraction wells was examined for each new well field (Fig. 28). Despite the movement of the extraction locations over time, the overall rates of extraction and recharge remained steady for 30 y and slowly reduce to 0 over the final 20 y (Fig. 25).

Selected Results for Transport Run T3. Figures 28a-x present the calculated head for each management period and the calculated distribution of TVOCs at the end of each

period. As seen in these figures, the higher total aqueous VOC concentrations in the eastern portion of LLNL decrease rapidly during the first several management periods. However, lower concentrations in the southwest corner of LLNL and offsite areas persist for much of the simulation.

After the first 5-y management period ($t = 0$ to 5 y), TVOC concentrations near extraction location EL-14a dropped from over 1,300 ppb to about 540 ppb (Fig. 28b). The distribution of aqueous TVOC mass is more uniform. In the eastern portion of LLNL, the calculated plume has moved slightly eastward as a result of an upgradient dispersion flux. Because the concentration of TVOCs is about 5 ppb near extraction location EL-10, pumping at this well was discontinued, and the extraction rates at locations EL-20a and EL-21 were increased accordingly for the next management period (Fig. 28f and Table A-4, Appendix).

Over the next four 5-y management periods ($t = 5$ to 25 y), the calculated distribution of TVOC concentrations did not significantly change. Although no wells were removed, some pumping rates were modified. Pumping at extraction locations EL-11 and EL-12, for instance, was gradually decreased in management periods 3 and 4 ($t = 10$ to 20 y) because of decreasing TVOC concentrations in the northeast corner of LLNL (Figs. 28d and 28f, and Table A-4, Appendix). Pumping rates at EL-14a and EL-19a, now located in an area of relatively higher TVOC concentration, were correspondingly increased. Similarly, the flow rate at EL-21, near the West Traffic Circle, was reduced in the fourth management period ($t = 15$ to 20 y) because of low TVOC concentrations; pumping at EL-20a was increased accordingly (Fig. 28f and Table A-4, Appendix).

In the fifth management period ($t = 20$ to 25y), the flow rates at EL-11 and EL-21 were reduced again, and extraction at EL-20a is reduced to its original flow rate. After 25 y, EL-20a was replaced by EL-20b during management period 6. Because EL-20b was located downgradient of the former EL-20a, it is more effective at capturing a larger portion of the TVOC plume (Figs. 28h and 28j). The flow rate at EL-19a was also increased during this management period. After 30 y, extraction locations EL-11, EL-12, EL-18, and EL-21 were removed from operation, because calculated TVOC concentrations at these nodes were less than 5 ppb (Fig. 28l). The flow rates at EL-13, EL-14a, and EL-17 were increased as more ground water became available (Table A-4, Appendix). After 35 y, extraction from locations EL-16 and EL-17 was stopped.

After 40 y, extraction from locations EL-13, EL-14a, and EL-19a was stopped. New wells EL-14b and EL-19b were placed in the areas containing higher VOC concentrations (Fig. 28p). Injection of treated ground water at IW-2 is discontinued. Extraction from locations EL-1 (EW-415) and EL-2 (at the Detailed Study Area (DSA) cluster) was also stopped, as TVOC concentrations dropped below 5 ppb near these wells. Because ground water extracted from these locations is treated at TFA, the discharge flow rate to the Recharge Basin was reduced accordingly.

At this stage in the simulations, we began examining the results at 1-y intervals. As a result, and to reduce the TVOC concentrations below 5 ppb within 50 y, three different well fields were used during final 5 y of simulations. After 45 y (management period 9), the extraction well EL-4 (EW-712) was shut down, and the discharge to the Recharge Basin was decreased accordingly. The flow rate at EL-14b was also reduced at this time because this

well is located near the perimeter of the 5-ppb isoconcentration contour (Fig. 28r). After 47 y (management period 10), extraction ceased at EL-20b; after 49 y, ground water extraction at EL-14b and EL-19b ceased and injection at IW-1 is discontinued. A new well, EL-14c, was placed within the area where aqueous TVOCs remain at concentrations greater than 5 ppb (Fig. 28v). The final aqueous TVOC distribution (Fig. 28x) shows all vertically-integrated concentrations less than 5 ppb.

As shown in the full sequence of plume figures (Fig. 28a-x), the distribution of aqueous TVOC mass is fairly well contained over the 50 y of pumping. No portions of the plume approach the downtown municipal wells, Arroyo Las Positas discharge area, or any of the nearby agricultural wells. In fact, the 1-ppb TVOC contour remains separated by several hundred feet or more from Wentz Vineyards well 14C3, the closest of all to the contamination, for the duration of the pumping. Figure 29 shows calculated concentrations versus time at Wentz Vineyards well 14C3, Davey Tree Farm well 14K1, and downtown CWSC municipal wells 9P1, 9Q1, and 16B1. By integrating the data in Figure 25, we find that the gross volume of ground water extracted over the lifetime of this simulation is $V_{T3} \approx 1.4 \times 10^9 \text{ ft}^3$. This corresponds to roughly $V_{T3}/V_f \approx 2.4$ pore volumes of fluid that have been removed or flushed from the system to meet the remediation goal. Simultaneously, roughly 1.6 pore volumes of fluid were reinjected into the system to minimize dewatering and improve TVOC extraction efficiency.

In Figure 30, the maximum depth-averaged aqueous TVOC concentration found anywhere in the simulation region is plotted as a function of time. Similar results are plotted for Transport Runs T1 and T2 (made under non-remedial conditions) as well as for runs T4 and T5 discussed in the next sections. For run T3, the maximum observed aqueous TVOC level reaches 5 ppb in 50 y, certainly much faster than would occur in the absence of remedial pumping (compare with 160 y in run T1).

Although the approach used here was able to remove a substantial amount of TVOC mass, the ability to reduce the maximum aqueous TVOC concentration to below 5 ppb within 50 y was aided by the inclusion of the 50-y degradation half-life. The simulations indicate that approximately 940 kg of aqueous TVOC mass was removed from the system over the 50 y of pumping, while some 110 kg remained afterwards in the ground water or on the soil. As the TVOC mass (aqueous plus sorbed) was initially 1,330 kg (Section 5.1), roughly 280 kg of TVOC (or 21% of the initial amount) were removed by the assumed degradation pathway. In the next section, a similar remedial simulation is pursued in which no degradation is assumed.

Text continues on page 85.

ERD-CFEST-93/F21

Figure 23. Planned initial ground water extraction, recharge, and treatment facility locations (from Dresen *et al.*, 1993).

ERD-CFEST-93/F22

Figure 24. Timeline of extraction, injection, and surface discharge for the 50 y cleanup scenario with degradation (Flow Run 26).

ERD-CFEST-93/F23

Figure 25. Aggregate rate of fluid extraction and recharge from all remedial wells and discharge locations as a function of time for Flow Runs 26-28 and Transport Runs T3-T5.

ERD-LSR-93-0136/26

Figure 26. Two-dimensional (vertically-integrated) flow lines and hydraulic capture zones associated with the first pumping configuration of Flow Run 26 (50-y cleanup scenario with degradation).

Figure 27. Two-dimensional (vertically-integrated) representation of the aqueous TVOC distribution beneath the LLNL study area after the first pumping configuration of Flow Run 26 (50-y cleanup scenario with degradation).

ERD-CFEST-93/F19b

Figure 28a. Calculated head: management period 1 (t = 0-5y) (50-y cleanup scenario with degradation).

Figure 28c. Predicted head: management period 2 ($t = 5-10$ y) (50-y cleanup scenario with degradation).

Figure 28d. Calculated TVOC isoconcentration contours after 10 y (50-y cleanup scenario with degradation).

ERD-CFEST-93/F19f

Figure 28e. Calculated head: management period 3 ($t = 10-15$ y) (50-y cleanup scenario with degradation).

ERD-CFEST-93/F19g

Figure 28f. Calculated TVOC isoconcentration contours after 15 y (50-y cleanup scenario with degradation).

ERD-CFEST-93/F18h

Figure 28g. Calculated head: management period 4 ($t = 15-20$ y) (50-y cleanup scenario with degradation).

ERD-CFEST-93/F191

Figure 28h. Calculated TVOC isoconcentration contours after 20 y (50-y cleanup scenario with degradation).

ERD-CFEST-93/F10j

Figure 28i. Calculated head: management period 5 ($t = 20-25$ y) (50-y cleanup scenario with degradation).

ERD-CFEST-93/F19k

Figure 28j. Calculated TVOC isoconcentration contours after 25 y (50-y cleanup scenario with degradation).

ERD-CFEST-93/F191

Figure 28k. Calculated head: management period 6 ($t = 25-30$ y) (50-y cleanup scenario with degradation).

ERD-CFEST-93/F19m

Figure 28I. Calculated TVOC isoconcentration contours after 30 y (50-y cleanup scenario with degradation).

Figure 28m. Calculated head: management period 7 ($t = 30-35$ y) (50-y cleanup scenario with degradation).

ERD-CFEST-93/F18n

ERD-CFEST-93/F19r

Figure 28q. Calculated head: management period 9 ($t = 40-45$ y) (50-y cleanup scenario with degradation).

ERD-CFEST-93/F19s

Figure 28r. Calculated TVOC isoconcentration contours after 45 y (50-y cleanup scenario with degradation).

Figure 28s. Calculated head: management period 10 ($t = 45-47$ y) (50-y cleanup scenario with degradation).

ERD-CFEST-93/F19u

Figure 28t. Calculated TVOC isoconcentration contours after 47 y (50-y cleanup scenario with degradation).

ERD-CFEST-93/F19v

Figure 28u. Calculated head: management period 11 ($t = 47-49$ y) (50-y cleanup scenario with degradation).

Figure 28w. Calculated head: management period 12 (t = 49-50 y) (50-y cleanup scenario with degradation).

ERD-CFEST-93/F26

Figure 29. Calculated aqueous, vertically-integrated TVOC concentrations versus time at downgradient ground water supply wells (50-y cleanup scenario with degradation).

ERD-CFEST-93/F27

Figure 30. Maximum calculated, depth-averaged, aqueous TVOC concentration as a function of time under no-action and remedial conditions.

6.4. Seventy-Five-Year Cleanup Simulation without Degradation

Although degradation was shown in the previous section to have a significant impact on remedial effectiveness, existing data suggest little or no degradation may be occurring in the LLNL subsurface (McNab and Narasimhan, 1994). Therefore, we now consider an analogous remedial pumping scheme in which the effects of degradation are not considered. Except for a few modifications, a similar approach based upon 25 extraction wells, 2 injection wells, and 3 surface discharge areas will be used within a series of 13 separate pumping configurations, spread out over a 75-y period. As discussed below, it was not possible to reduce aqueous TVOC concentrations to less than 5 ppb throughout the study area within 50 y with this set of wells; a more aggressive approach to meet this target is discussed in Section 6.5.

Initial Well Configuration. The initial well field configuration for this simulation was composed of 21 extraction locations, 2 injection wells, and 3 surface discharge areas. The extraction wells include the 4 locations in operation in September 1994 and 17 others; the injection and discharge areas were described above. The operation schedule for all wells and discharge areas is summarized in Figure 31, and can be cross-referenced with Figure 32b and a more detailed listing of flow rates in Table A-5 (Appendix). The initial extraction, injection, and recharge configuration used here is the same as used in the degradation case; hence, the initial aqueous TVOC distribution shown in Figure 32a is the same as indicated at $t = 0$ in Figure 27.

Updated Well Configurations. Paralleling the approach in the previous simulation, 5-y management periods were chosen to observe and adjust the pumping configuration. However, the final two management periods were 4 and 1 y in length, respectively. Over the first four periods, up to $t = 20$ y, the same schedule of pumping and recharge was used as in the previous simulation. Calculated heads and aqueous TVOC concentrations at the end of each management period are shown in Figures 32b through 32i. Because degradation was not included, the effective rate of TVOC mass removal was reduced in comparison with the previous simulation, which becomes quite apparent after 20 y. Hence, the operation of most extraction wells was extended in time (up to $t = 75$ y), and reductions in their extraction rates was slowed in many cases (Fig. 31 and Table A-5, Appendix). To illustrate, Figure 25 shows the aggregate rate of extraction and recharge from all remedial wells and discharge locations as a function of time. Particular changes in the pumping schedule from run T3 include the addition of extraction location EL-20c at $t = 50$ y, and the elimination of the former extraction location EL-19c. Note again that the overall rates of extraction and recharge remain close to 445 gpm and 280 gpm, respectively, for the first 45 y of remediation (Fig. 25). Over the next 30 y, the rates slowly decrease to zero.

Selected Results for Transport Run T4. The final calculated aqueous TVOC distribution shows all vertically-integrated concentrations less than 5 ppb (Fig. 32aa). Over the 75-y pumping sequence, the distribution of aqueous TVOC mass remains fairly well contained. No portions of the plume approach the downtown CWSC municipal wells (16B1, 9P1, and 9Q1), Arroyo Las Positas discharge area, or Davey Tree Farm well 14K1. The 1-ppb contour skirts Wentle Vineyards well 14C3 from years 60 to 70, but higher concentrations are not expected. Figure 33 shows calculated concentrations versus time at the downtown municipal wells, the Wentle Vineyards well, and the Davey Tree Farm well.

Although the areal extent of the TVOC plume at 75 y (Fig. 32aa) is similar to that calculated at the end of the previous simulation ($t = 50$ y, Run T3, Fig. 28), we estimated that it contains an additional 30 kg of TVOC mass. The simulations indicate that pumping has removed roughly 1,190 kg of TVOC mass after 75 y of operation, leaving 140 kg distributed within the system. Compared with the previous simulation, the additional 25 y of pumping has extracted an additional 250 kg of TVOC mass previously removed through the assumed degradation. Integration of the results in Figure 25 also indicate that the volume of ground water extracted over the lifetime of this simulation is $V_{T4} \approx 2.1 \times 10^9$ ft³. This corresponds to roughly $V_{T4}/V_f \approx 3.5$ pore volumes of fluid that have been removed or flushed from the system to meet the remediation goal. Simultaneously, roughly 2.4 pore volumes of fluid were reinjected into the system to minimize dewatering problems and improve TVOC extraction efficiency.

In Figure 30, the maximum depth-averaged aqueous TVOC concentration found anywhere in the simulation region is plotted as a function of time. Although 25 more years are required to reach the maximum aqueous TVOC level of 5 ppb in Run T4, the elapsed time (75 y) is still much less than the time required without remedial pumping (800 y in Run T2).

Text continues on page 116.

ERD-CFEST-93/F28

Figure 31. Timeline of extraction, injection, and surface discharge for the 75-y cleanup scenario without degradation (Flow Run 27).

ERD-CFEST-93.F29a

Figure 32a. Initial TVOC isoconcentration contours ($t = 0$ y) (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29b

Figure 32b. Calculated head: management period 1 ($t = 0-5$ y) (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29c

Figure 32c. Calculated TVOC isoconcentration contours after 5 y (75-y cleanup scenario without degradation).

Figure 32d. Calculated head: management period 2 (t=5-10 y) (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29a

Figure 32e. Calculated TVOC isoconcentration contours after 10 y (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29f

Figure 32f. Calculated head: management period 3 ($t = 10-15$ y) (75-y cleanup scenario without degradation).

Figure 32g. Calculated TVOC isoconcentration contours after 15 y (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29h

Figure 32h. Calculated head: management period 4 (t=15-20 y) (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29i

Figure 32i. Calculated TVOC isoconcentration contours after 20 y (75-y cleanup scenario without degradation).

Figure 32j. Calculated head: management period 5 (t=20-25 y) (75-y cleanup scenario without degradation).

Figure 32k. Calculated total VOC isoconcentration contours after 25 y (75-y cleanup scenario without degradation).

Figure 32I. Calculated head: management period 6 ($t = 25-30$ y) (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29m

Figure 32m. Calculated TVOC isoconcentration contours after 30 y (75-y cleanup scenario without degradation).

Figure 32n. Calculated head: management period 7 ($t = 30-35$ y) (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29o

Figure 32o. Calculated TVOC isoconcentration contours after 35 y (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29p

Figure 32p. Calculated head: management period 8 ($t = 35-45$ y) (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29q

Figure 32q. Calculated TVOC isoconcentration contours after 45 y (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29r

Figure 32r. Calculated head: management period 9 ($t = 45-50$ y) (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29a

Figure 32s. Calculated TVOC isoconcentration contours after 50 y (75-y cleanup scenario without degradation).

Figure 32t. Calculated head: management period 10 (t=50-65 y) (75-y cleanup scenario without degradation).

ERD-CFEST-93/F29u

Figure 32u. Calculated TVOC isoconcentration contours after 65 y (75-y cleanup scenario without degradation).

Figure 32v. Calculated head: management period 11 ($t=65-70$ y) (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29w

Figure 32w. Calculated TVOC isoconcentration contours after 70 y (75-y cleanup scenario without degradation).

Figure 32x. Calculated head: management period 12 (t=70-74 y) (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29y

Figure 32y. Calculated TVOC isoconcentration contours after 74 y (75-y cleanup scenario without degradation).

Figure 32z. Calculated head: management period 13 (t=74-75 y) (75-y cleanup scenario without degradation).

ERD-CFEST-93.F29aa

Figure 32aa. Calculated TVOC isoconcentration contours after 75 y (75-y cleanup scenario without degradation).

ERD-CFEST-83/F30

Figure 33. Calculated aqueous, vertically-integrated TVOC concentrations versus time at downgradient ground water supply wells (75-y cleanup scenario without degradation).

6.5. "Aggressive" Cleanup Simulation without Degradation

This section describes a different remediation approach designed to reduce vertically-integrated aqueous TVOC concentrations to 5 ppb or below within 50 y, in the absence of degradation. To do this, an "aggressive" pumping scheme composed of 63 extraction locations, 40 injection wells, and 3 surface discharge areas was designed and implemented in simulation T5 over 8 management periods. The relatively large number of wells was used to increase the overall efficiency of extraction by targeting removal efforts in numerous small, interconnected areas.

Initial Well Configuration. The initial well field configuration for this simulation was composed of 35 extraction locations, 15 injection wells, and 3 surface discharge areas (Fig. 35). The initial extraction locations include two of the currently operating clusters (EW-415 and MW-357/EW-704), as well as 33 other closely spaced locations selectively placed in areas of high or areally extensive VOCs in the eastern, north-central, and southwestern portions of LLNL. Use of the third currently operating cluster (GEW-808, GEW-816), which is considered to be screened in deeper sediments in the simulation, was postponed until $t = 20$ y. The fourth currently-operating location (P-701) was not used. The relatively large number of injection wells in eastern part of the laboratory was used to balance the larger, more densely distributed extraction wells and minimize potential dewatering problems. The overall rates of extraction and recharge from all remedial wells and discharge locations are shown in Figure 25. The net steady-state ground water extraction rate for the initial well configuration is 167 gpm, corresponding to a total extraction rate of 726 gpm and a total recharge rate of 559 gpm.

Because most of the VOC mass is currently in eastern LLNL near Greenville Road, a relatively large cluster of extraction and injection wells was used in this area (Fig. 35). In this region, the modeled aquifer thickness ranges from 3 ft in the southeast corner to over 140 ft near the central area, resulting in a wide range of transmissivity values and allowable extraction and reinjection rates. Larger extraction rates (16 gpm) were assigned to wells in the northeast corner of LLNL where the aquifer is thicker and is recharged via underflow from the east. Smaller rates (10 gpm) were assigned to the extraction wells in the southeast, along with a series of reinjection wells to support accelerated flow-through efficiency. Many of the injection wells were used in extraction/injection pairs, while others such as 18b and 18c were single wells in the extreme southeast corner of LLNL. Ground water was also removed by a few extraction wells in the north-central LLNL area, near the West Traffic Circle (Fig. 35). Here, the modeled aquifer thickness exceeds 130 ft and may sustain extraction rates of up to 16 gpm. No reinjection wells were used in this area in the initial configuration.

A sizable fraction of the TVOC mass is located in the southwest area of LLNL, and portions have migrated past the western LLNL boundary. In this region, the modeled saturated aquifer thickness exceeds 150 ft, and allows for relatively large extraction rates (near 50 gpm). In this simulation, several extraction wells were initially placed inside of the zone defined by the closed 5-ppb TVOC contour near TFA and TFB; several others were placed west of Vasco Road to remove contaminants that have moved off-site and to arrest further migration. Reinjection at a central LLNL location (well 13g, 31 gpm, Fig. 36a) was used to increase flow and contaminant migration toward the southwest extraction wells, and

to arrest further westward migration of contaminants from the eastern and north central areas of LLNL.

In this simulation, recharge was also promoted at three other surface discharge areas, including the Recharge Basin and TFB drainage ditch, as in previous simulations, and a new north-south recharge trench located in the south-central part of LLNL (Fig. 35). Recharge in this trench was used to promote separation between the major zones of contamination in the eastern and western parts of the laboratory (Fig. 35). The operation schedule for all wells and discharge areas is summarized in Figure 34, and can be cross-referenced with a more detailed listing of flow rates in Table A-6 (Appendix) and Figure 36. The initial aqueous TVOC distribution, rescaled to reflect the aquifer thickness produced by the first pumping configuration, is shown in Figure 35.

Updated Well Configurations. In contrast with previous simulations, the first management period lasted 15 y. Figure 36b shows the calculated aqueous TVOC concentration contours at the end of this period. Residual TVOC concentrations have been reduced to less than 100 ppb (Fig. 30) and are much smaller than at the 15-y point in the 75-y simulation (Fig. 32g). At this point, about 1,200 kg of TVOC mass has been removed, representing over 90% of the original estimated amount. This is roughly the same amount of mass removed over the entire 75-y simulation discussed in Section 6.4.

Nevertheless, to reduce aqueous TVOC concentrations to 5 ppb or below in 50 y, new extraction and injection wells were required. For the next 5-y management period, several new extraction and reinjection wells were added in higher concentration areas in the eastern part of LLNL (Table A-6, Appendix, and Fig. 34). Solo injection at locations 18c and 18d was discontinued in favor of these new pairs. One extraction/injection pair (19b/19l) was discontinued because of low concentrations. In the southwest area, two new extraction wells were added in the center of the plume (4b and 23, Fig. 36c), while two others (15 and 16) were discontinued because of low concentrations. Several additional extraction and injection wells were also added in the vicinity of the West Traffic Circle. Note that the overall rate of extraction and recharge from all remedial wells and discharge locations (Fig. 25) grows considerably to extremes of 940 gpm and 833 gpm, respectively, after $t = 20$ y.

Figure 36d shows aqueous TVOC isoconcentration contours after 20 y. The maximum concentration is about 50 ppb, and more than 99% of the VOC mass has been extracted from the aquifer. Note that the central recharge trench has helped create a large area of low concentration (less than 1 ppb) in the southcentral part of LLNL. Recharge in this area, in combination with upgradient extraction, has prevented ground water in the east containing larger amounts of TVOC mass from migrating westward toward central LLNL.

Selected Results for Transport Run T5. Over the next six 5-y management periods between $t = 20$ and 50 y, the distribution of wells and their pumping rates were modified according to the same type of heuristic procedure described in Section 6.2, targeting remaining higher concentration areas and eliminating extraction in zones where cleanup standards were achieved. Table A-6 (Appendix) and Figures 25 and 34 summarize the well operation schedule, and Figures 36a-p show the resulting head and aqueous TVOC distributions at the end of each management period. As seen in these figures, extraction rates peak at about $t = 25$ y, but only a very small number of wells are operating in the eastern part of LLNL in the last 10 y.

The final calculated aqueous TVOC distribution shown in Figure 36p shows all vertically-integrated concentrations to be less than 5 ppb. Over the 50-y pumping sequence, the distribution of aqueous TVOC mass is fairly well contained. No portions of the plume approach the downtown CWSC municipal supply wells 9P1, 9Q1, and 16B1, Arroyo Las Positas discharge area, Davey Tree Farm well 14K1, or Wente Vineyards well 14C3. Figure 37 shows calculated concentrations versus time at the CWSC wells, the Wente Vineyards well, and the Davey Tree Farm well. The areal extent of the TVOC plume at 50 y is a bit larger than that calculated at the end of the previous simulation ($t = 75$ y, Run T4, Fig. 32aa), yet is estimated to contain much less mass. Pumping in the 50-y "aggressive" simulation has been estimated to remove over 99% of the TVOC mass after 20 y. Analysis of Figure 25 indicates that roughly $V_{T5} \approx 2.2 \times 10^9$ ft³ have been extracted over the lifetime of this run, or approximately $V_{T5}/V_f \approx 3.8$ pore volumes of fluid. Simultaneously, about 3.1 pore volumes of fluid were reinjected into the system to minimize dewatering and improve TVOC extraction efficiency. The maximum depth-averaged aqueous TVOC concentration found anywhere in the simulation region is plotted as a function of time in Figure 30.

Compared with the previous simulations, the accelerated pumping schedule used in the early years of this simulation produces the most rapid rate of mass extraction and concentration reduction. The "adaptive pump-and-treat" strategy contributed significantly toward decreasing the total cleanup time, preventing the spread of contaminants and decreasing localized aquifer drawdown. Overall, the pumping schedule used here appears to provide the most promising basis for meeting the remediation goals in Section 6.1. Although this aggressive strategy maximizes the removal rate of TVOC mass, the costs associated with building and operating the larger number of wells and associated pipeline systems may not represent the most economically feasible approach.

Text continues on page 138.

ERD-CFEST-93/F31

Figure 34. Timeline of extraction, injection, and surface discharge for the aggressive cleanup scenario without degradation (Flow Run 28).

Figure 35. Two-dimensional (vertically-integrated) representation of the aqueous TVOC distribution beneath the LNL study area after the first pumping configuration of Flow Run 28 (aggressive cleanup scenario without degradation).

ERD-CFEST-93/F32

ERD-CFEST-93/F33a

Figure 36a. Calculated head: management period 1 (t=0 y) (aggressive cleanup scenario without degradation).

Figure 36b. Calculated TVOC isoconcentration contours after 15 y (aggressive cleanup scenario without degradation).

ERD-CFEST-93/F33C

Figure 36c. Calculated head: management period 2 ($t = 15-20$ y) (aggressive cleanup scenario without degradation).

ERD-CFEST-93/F33d

ERD-CFEST-93/F339

Figure 36e. Calculated head: management period 3 (t = 20-25 y) (aggressive cleanup scenario without degradation).

Figure 36f. Calculated TVOC isoconcentration contours after 25 y (aggressive cleanup scenario without degradation).

Figure 36g. Calculated head: management period 4 ($t = 25-30$ y) (aggressive cleanup scenario without degradation).

ERD-CFEST-89/F33h

Figure 36h. Calculated TVOC isoconcentration contours after 30 y (aggressive cleanup scenario without degradation).

Figure 36i. Calculated head: management period 5 (t = 30-35 y) (aggressive cleanup scenario without degradation).

ERD-CFEST-93/F33j

Figure 36j. Calculated TVOC isoconcentration contours after 35 y (aggressive cleanup scenario without degradation).

Figure 36k. Calculated head: management period 6 ($t = 35-40$ y) (aggressive cleanup scenario without degradation).

Figure 36I. Calculated TVOC isoconcentration contours after 40 y (aggressive cleanup scenario without degradation).

Figure 36m. Calculated head: management period 7 ($t = 40-45$ y) (aggressive cleanup scenario without degradation).

Figure 36n. Calculated TVOC isoconcentration contours after 45 y (aggressive cleanup scenario without degradation).

Figure 36o. Calculated head: management period 8 ($t = 45-50$ y) (aggressive cleanup scenario without degradation).

Figure 36p. Calculated TVOC isoconcentration contours after 50 y (aggressive cleanup scenario without degradation).

ERD-CFEST-83/F34

Figure 37. Calculated aqueous, vertically-integrated TVOC concentrations versus time at downgradient ground water supply wells (aggressive cleanup scenario without degradation).

7. Interpretations and Recommendations

7.1. Summary

We have described the application of a two-dimensional finite-element model to simulate ground water flow and contaminant mass transport in the saturated aquifer beneath LLNL. The study region encompasses the upper 200 ft of saturated sediments in a roughly 25-mi² (65 km²) region of the eastern Livermore Valley in California. The flow simulations complement earlier work summarized by Tompson (1990) and Tompson *et al.* (1991), and are the basis for the mass transport studies. For simplicity, the transport simulations focused on the migration of a single surrogate TVOC. TVOC concentrations represent the aggregate concentrations of eight separate aqueous VOC contaminants (excluding FHC VOCs) found in the study area.

Five separate two-dimensional transport simulations were conducted. For simplicity, contaminant distributions were considered well-mixed over the vertical dimension of the aquifer such that a two-dimensional conceptualization could be used in the model. Transport Runs T1 and T2 were conducted under non-remedial ("no-action") conditions. Results of these simulations indicate that the TVOC plume may migrate eastward toward downtown Livermore under existing natural flow patterns. Run T1 employed a questionable model of TVOC degradation and showed that natural dilution and assumed degradation processes would result in concentrations uniformly below 5 ppb in 160 y, and 1 ppb in 250 y. Run T2 showed that natural dilution alone without degradation would cause concentrations to fall uniformly below 5 ppb after 800 y and 1 ppb in 1,200 y. Although contaminant mass is calculated to reach CWSC municipal supply wells 9P1, 9Q1, and 16B1 in both simulations, TVOC concentrations at the wells were shown to be bounded by 0.01 ppb in Run T1 and 1.0 ppb in Run T2, far below current cleanup levels. Concentrations above 5 ppb are calculated to reach only Wente Vineyards well 14C3 in Run T2; concentrations at Davey Tree Farm well 14K1 and at the Arroyo Las Positas discharge area were calculated to be below 5 ppb in both runs.

Transport Runs T3, T4, and T5 were conducted under remedial pumping conditions. Results of these simulations indicated that all three remedial strategies would reduce the vertically-integrated, aqueous TVOC concentrations to 5 ppb or below within a 50- to 75-y time frame, with negligible impact on surrounding ground water use. Although this may seem long from an economic or public policy perspective, it is comparable to the evolution time of the existing contamination distribution itself, and is quite short when compared with the cleanup time under natural dilution (non-remedial) conditions (*i.e.*, Runs T1-T2). In all cases, the extraction efficiency is larger at early times when more confined zones of higher concentration can be easily targeted for cleanup. Efficiency diminishes significantly at later times when remaining areas of low concentration above regulatory limits are widely dispersed. This is a common malady of most pump-and-treat applications. The "adaptive" approach used here allows some improvement in efficiency at most times, yet will only work to a limited degree within certain operational constraints, and it will certainly increase costs.

In addition, the Simulations T3, T4, and, T5 suggest that between 2.4 and 3.8 equivalent pore volumes of ground water need to be pumped out of the system to lower TVOC levels

and meet remediation goals with a corresponding 1.6 to 3.1 pore volumes of treated water being simultaneously recharged. In all runs, gross extraction rates in excess of the 350 gpm level suggested in the selected alternative in the ROD (USDOE, 1992) were required, as well as significant amounts of aquifer recharge. Nevertheless, the net ground water extraction rate remained at or below 165 gpm in all cases.

Simulations T3 and T4 used a relatively small number of wells (25 to 30) over the cleanup period. The first run (T3) employed a model of TVOC degradation to achieve cleanup in 50 y; the second (T4) assumed no degradation and achieved cleanup over a 75-y period. On the other hand, the final simulation (T5) used a more aggressive strategy based upon 62 extraction and 40 injection wells to achieve cleanup without degradation within 50 y. Although some 99% of the TVOC mass was extracted in the first 20 y, the distribution of the remaining amount still exceeded regulatory concentration limits over a wide area and required 30 more years of pumping to reach compliance. Given this, it seems that more cost-effective remedial technologies or more flexible regulatory guidelines may be necessary for dealing with dilute, widespread zones of contamination that exceed MCLs.

7.2. Interpretation of Results

Although the current simulations incorporate more realism than previous modeling efforts (*e.g.*, Layton *et al.*, 1990; Thorpe *et al.*, 1990), interpretation of the new results must still be qualified with respect to the conceptual assumptions and physical and chemical models used to represent the system.

Use of the two-dimensional conceptualization (Section 3.3) and surrogate TVOC (Section 5.1), for example, provided ways to simplify several aspects of the flow and migration calculations. In the two-dimensional approach, explicit description of hydraulic variables over the vertical dimension of an aquifer was dismissed in favor of vertically-averaged quantities. In the case of solute concentration, this procedure implicitly distributes solute mass over the entire aquifer column and imparts an added degree of dilution. Because measurements along the vertical dimension in an aquifer may show significant variability about their average value, two-dimensional model results could be misinterpreted to imply premature compliance with regulatory limits.

On the other hand, extraction wells are actually screened in primarily highly contaminated and more permeable zones, and, consequently, may remove contaminant mass more rapidly than is calculated by the two-dimensional model results. In addition, comparison of surrogate TVOC concentrations with a single regulatory MCL may be too conservative. For example, if TCE makes up one-third of all initial TVOC concentrations at all locations, then, all other things being equal, concentrations at any future time and location and will be one third of the TVOC concentration. Thus, utilizing the aggressive cleanup scenario (Fig. 36h), the aqueous TCE concentration in year 30 will likely be bounded by 5 ppb, possibly indicating an earlier compliance with a 5-ppb MCL for TCE. This suggests that the proposed remediation schemes may, in general, require less time and smaller quantities of extracted ground water to reach regulatory compliance.

Other issues to consider when interpreting the results include justifying the representation of simulated aquifer thickness, overall aquifer boundaries, and effective hydraulic properties

in the model, especially in more remote areas of the study area where field data are sparse. In addition, the extent to which flow conditions or sources of fluid mass remain constant over the study periods may also affect the results. Oversimplified representations of chemical phenomena may also limit or qualify interpretation of the results. We have already seen how potential VOC degradation through microbial or abiotic pathways can impact the simulation results. Certainly, a clearer understanding of individual VOC sorption phenomena and the impacts of the natural background geochemistry may further improve the reliability of the simulations.

7.3. Recommendations

In response to the important list of caveats just reviewed, we conclude by proposing several activities that will expand, complement, or supplement the reliability of current and future simulations. Progress in these areas will be discussed in future reports.

1. *Pursue the development of flow and transport models that incorporate three-dimensional behavior.* The simplest approach would involve defining a layered, three-dimensional study area similar to that shown in Figure 3, minimally incorporating two layers to represent the permeable sediments and upper part of the Lower Livermore Formation, respectively. Within the permeable sediments, the same "bulk" parameters used in the two-dimensional model could be vertically extrapolated, while lower values could be specified in the lower confining unit. The three-dimensional TVOC plume shown in Figure 13 could then be directly used as the initial TVOC distribution. This approach would incorporate basic three-dimensional flow effects, eliminate the dilution produced by vertical integration in the two-dimensional case, and provide a more realistic view of the vertical TVOC distribution at future times.

An intermediate approach might also be pursued in which major conductive zones and features of the permeable sediments are resolved as a more complicated system of layers and lenses. In this case, the actual well screening and production from the more permeable zones should be more accurately represented.

Alternatively, a more detailed three-dimensional modeling approach could also be followed in which local aquifer heterogeneity is directly represented at a fine scale within the model. This would be accomplished by producing plausible statistical realizations that preserve observed structural characteristics of the aquifer (*e.g.*, *Tompson et al.*, 1993). Although this approach would be more computationally intensive, the resulting simulations would naturally reproduce dilution and dispersion effects accounted for earlier by effective macrodispersion coefficients (Section 3.2 and *Tompson*, 1990). Here, deviations away from the effective dispersion model created by boundary effects, pumping wells, or short travel distances would be accounted for, and the resulting small-scale spatial variability in concentration should be closer to what is actually observed in the field.

2. *Develop migration simulations of the eight specific target VOCs instead of the single surrogate TVOC compound.* Using this approach, confusion in cleanup times

estimated with the surrogate model would be eliminated and focus should be placed on remediation based upon the evolution of each individual VOC plume. It is likely that the overall calculated cleanup time and equivalent pore volumes of ground water extracted will be significantly reduced, even if the same 2-D conceptualization and remedial scenarios discussed above are used.

3. *Clarify or formally justify potential bacterial or abiotic transformation mechanisms for specific LLNL VOCs.* This includes determination of plausible degradation rates, geochemical or other limiting constraints, as well as whether any toxic byproducts may be produced (*e.g.*, McNab and Narasimhan, 1994).
4. *Quantify the fate of VOCs in the unsaturated zone.* Although VOCs infiltrated to the ground water from the surface, relatively little is known about the current distribution of VOCs in the vadose zone, and to what extent they may act as a future source of additional contamination in the saturated zone. The VOC cycle in unsaturated sediments may include advective and dispersive flows with infiltrating water, or as a separate phase; adsorption to the sediments; possible degradation; evaporation; eventual recondensation; or even venting to the atmosphere at the ground surface. Understanding this cycle better may contribute to a better understanding of the overall VOC mass balance between the surface and ground water over the last 50 y.
5. *Development of more efficient remedial pumping schemes.* Clearly, the adaptive approach used here to improve TVOC extraction efficiency over time was heuristic; application of more formalized optimization methods (*e.g.*, Dougherty and Marryott, 1991; Rogers and Dowla, 1994) may lead to overall reduction in well costs and requisite pumping times. Alternatively, different remedial strategies may be studied; for example, those that maximize mass removal by pumping over shorter (*e.g.*, 10- to 20-y) periods, the remainder being treated by another method, such as bioremediation or natural dilution under ambient (no pumping) conditions.
6. *Development of compliance monitoring strategies.* This issue involves comparison of simulated concentrations with future concentration measurements to determine whether remedial behavior calculated by a model is being realized in the field. Certainly, elements of model validation and calibration over the long term will be relevant; however, there will be additional considerations. In the future, determining the three-dimensional distribution of VOCs from aqueous well samples alone will be more difficult than the method used in Section 5.1. This is mainly because down-hole sediment samples will not be available as they were when the wells were drilled; the abundant soil concentration data used in Section 5.1 will be absent. Thus, how can the rather spotty and locally variable aqueous concentration measurements be effectively compared with results from simulations? One approach is to develop a rational, dynamic measure of concentration variance that can be used to compare measurements to smoother simulation results (*e.g.*, Kabala and Sposito, 1994; Kapoor and Gelhar, 1994).
7. *Continuously improve and calibrate flow model boundaries, boundary conditions, effective flow parameters, and sources and sinks of ground water recharge or*

discharge. This type of activity must continually be pursued to improve the conceptual understanding of the geologic system, and to provide new interpretations and information for three-dimensional simulations of the real physical system.

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References

- Bear, J. (1977), "On the Aquifer's Integrated Balance Equations", *Advances in Water Resources* 1, 15-23.
- Bishop, D., D. Rice, L. Rogers, and C. Webster-Scholten (1990), *Comparison of Field-Based Distribution Coefficients (K_d 's) and Retardation Factors (R's) to Laboratory and other Determinations of K_d 's*, Lawrence Livermore National Laboratory, Livermore, Calif. (UCRL-AR-105002).
- Carpenter, D. W., J. J. Sweeney, P. W. Kasameyer, N. R. Burkhard, K. G. Knauss, and R. J. Shlemon (1984), *Geology of the Lawrence Livermore National Laboratory Site and Adjacent Areas*, Lawrence Livermore National Laboratory, Livermore, Calif. (UCRL-53316).
- Cederberg, G. A., R. L. Street, and J. O. Leckie (1985), "A Groundwater Mass Transport and Equilibrium Chemistry Model for Multicomponent Systems", *Water Resources Research*, 21(8), 1095-1104.
- DGI, (1989), *Interactive Volume Modeling, User's Guide*, Dynamic Graphics Inc., Alameda, Calif.
- Devany, R. O., B. J. Qualheim, and V. Johnson (1990), "Computer-Assisted Development of a Three-Dimensional Contaminant Volume Model in an Alluvial Aquifer", *EOS*, 71(43), p. 1316 (abs)
- Dougherty, D. E., and R. A. Marryott (1991), "Optimal groundwater management, 1, Simulated Annealing", *Water Resources Research*, 27(10), 2493-2508.
- Dresen, M. D., J. P. Ziagos, A. J. Boegel, E. M. Nichols, and J. K. Macdonald, Eds. (1993), *Remedial Action Implementation Plan for the LLNL Livermore Site, Livermore, California*, Lawrence Livermore National Laboratory, Livermore, Calif. (UCRL-AR-110532).
- DWR (1966), *Evaluation of Ground Water Resources: Livermore and Sunol Valleys: Appendix A: Geology*, California Department of Water Resources, Sacramento, Calif. (Bulletin No. 118-2).
- DWR (1974), *Evaluation of Ground Water Resources: Livermore and Sunol Valleys*, California Department of Water Resources, Sacramento, Calif. (Bulletin No. 118-2).
- Freeze, R. A., and J. A. Cherry (1979), *Groundwater* (Prentice Hall, Englewood Cliffs, N.J.).
- Freeze, R. A., and P. A. Witherspoon (1967), "Theoretical Analysis of Regional Groundwater Flow. 2. Effect of Water-Table Configuration and Subsurface Permeability Variation", *Water Resources Research*, 3(2), 623-634.
- Gelhar, L. W., C. Welty, and K. R. Rehfeldt (1992), "A Critical Review of Data on Field-Scale Dispersion in Aquifers", *Water Resources Research*, 28(7), 1955-1974.
- Gray, W. G. (1982), "Derivation of Vertically Averaged Equations Describing Multiphase Flow in Porous Media", *Water Resources Research*, 18(6), 1705-1712.

Gupta, S. K., C. R. Cole, C. T. Kincaid, and A. M. Monti (1987), *Coupled Fluid, Energy, and Solute Transport (CFEST) Model: Formulation and User's Manual*, Report BMI/ONWI-660, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio (Report BMI/ONWI-660).

Hoffman, F., and M.D. Dresen (1990), "A Method to Evaluate the Vertical Distribution of VOCs in Ground Water in a Single Borehole", *Ground Water Monitoring Review*, 10(2), 95-100.

In-Situ, Inc., (1986) "Plume Contaminant Migration", In-Situ, Inc., Laramie, Wyo.

Isherwood, W. F., C. H. Hall, and M. D. Dresen, Eds. (1990), *CERCLA Feasibility Study for the LLNL-Livermore Site*, Lawrence Livermore National Laboratory, Livermore, Calif. (UCAR-AR-104040).

Kabala, Z. J., and G. Sposito, "Statistical Moments of Reactive Solute Concentration in a Heterogeneous Aquifer", *Water Resources Research*, 30(3), 759-768.

Kapoor, V., and L. W. Gelhar (1994), "Transport in Three-dimensionally Heterogeneous Aquifers, 1. Dynamics of Concentration Fluctuations", *Water Resources Research*, 30(6), 1775-1788.

Kindred, J. S., and M. A. Celia (1989), "Contaminant Transport and Biodegradation, 2. Conceptual Model and Test Simulations", *Water Resources Research*, 25(6), 1149-1159.

Layton, D. W., J. I. Daniels, and W. F. Isherwood, Eds. (1990), *Baseline Public Health Assessment for CERCLA Investigations at the LLNL Livermore Site*, Lawrence Livermore National Laboratory, Livermore, Calif. (UCRL-53953).

Liu, C. W., and T. N. Narasimhan (1989), "Redox-Controlled Multiple-Species Reactive Chemical Transport 2. Verification and Application", *Water Resources Research*, 25(5), 883-910.

McEdwards, D. G. (1986), "CAPTURE: A Program for Generating Ground Water Flow Lines for Extraction Wells and Trenches in Uniform Ground Water Flow", Data Services, Petaluma, Calif.

McNab, W. W., and T. N. Narasimhan (1994), "Degradation of Chlorinated Hydrocarbons and Groundwater Geochemistry: A Field Study", *Environmental Science and Technology*, 28(5), 769-775.

Pinder, G. F., and W. G. Gray (1977), *Finite Element Simulation in Surface and Subsurface Hydrology* (Academic Press, New York NY).

Rogers, L. L., and F. U. Dowla (1994), "Optimization of Groundwater Remediation Using Solute Transport Modeling and Artificial Neural Networks", *Water Resources Research*, 30(2), 457-481.

- Rogers, L. L. (1992), "History Matching to Determine the Retardation of PCE in Ground Water", *Ground Water*, 30(1), 50-60.
- Thorpe, R. K., W. F. Isherwood, M. D. Dresen, and C. P. Webster-Scholten, Eds. (1990), *CERCLA Remedial Investigations Report for the LLNL Livermore Site*, Lawrence Livermore National Laboratory, Livermore, Calif. (UCAR-10299).
- Tompson, A. F. B. (1990), *Flow and Transport within the Saturated Zone Beneath Lawrence Livermore National Laboratory: Modeling Considerations for Heterogeneous Media*, Lawrence Livermore National Laboratory, Livermore, Calif. (UCID 21828).
- Tompson, A. F. B., E. M. Nichols, P. F. McKereghan, and M. C. Small (1991), *Summary of Preliminary Ground Water Simulations in the Livermore Regional Modeling Study - CFEST Finite Element Code*, Lawrence Livermore National Laboratory, Livermore, Calif. (UCRL-AR-107049).
- Tompson, A. F. B., S. Ashby, R. Falgout, and S. Smith (1993), *On the Role of High Performance Computing for Simulating Subsurface Flow and Chemical Migration*, Lawrence Livermore National Laboratory, Livermore, Calif. (UCRL-JC-114179).
- Toth, J. (1963), "A Theoretical Analysis of Groundwater Flow in Small Drainage Basins", *Journal of Geophysical Research*, 68(16), 4795-4812.
- U. S. Department of Energy (USDOE) (1992), *Record of Decision for the Lawrence Livermore National Laboratory Livermore Site*, Lawrence Livermore National Laboratory, Livermore, Calif. (UCRL-AR-109105).
- Vogel, T. M., C. S. Criddle and P. L. McCarty (1987), "Transformations of Halogenated Aliphatic Compounds", *Environmental Science & Technology*, 21(8), 722-736.
- Weber, W. J., P. M. McGinley, and L. E. Katz (1991), "Sorption Phenomena in Subsurface Systems: Concepts, Models, and Effects on Contaminant Fate and Transport", *Water Research*, 25(5), 499-528.
- Yeh, G. T., and V. S. Tripathi (1989), "A Critical Evaluation of Recent Developments in Hydrogeochemical Transport Models of Reactive Multichemical Components", *Water Resources Research*, 25(1), 93-108.
- Zone 7 (1988a), *Memorandum: Rainfall and Applied Water Recharge Model*, Alameda County Flood Control and Water Conservation District, Pleasanton, Calif. (February 9).
- Zone 7 (1988b), *Memorandum: Synoptic Streamflow Data through 1988 Water Year*, Alameda County Flood Control and Water Conservation District, Pleasanton, Calif. (December 15).
- Zone 7 (1989), *Memorandum: Spring 1989 Groundwater Level Report*, Alameda County Flood Control and Water Conservation District, Pleasanton, Calif.
- Zone 7 (1990), *Memorandum: Surface Water Annual Report 1989 Water Year*, Alameda County Flood Control and Water Conservation District, Pleasanton, Calif.

Appendix: Characteristics of Flow and Transport Runs

Tables A-1 and A-2 summarize the hydraulic conductivities and boundary conditions specified in all of the flow simulations. Table A-3 summarizes all the natural and existing (*e.g.*, non-remedial) sources and sinks of fluid mass specified in Flow Runs 24 through 28. Note that the numbering scheme continues the sequence begun in Thompson *et al.* (1991). Tables A-4 through A-6 summarize all of the extraction and injection wells and other discharge areas used in the three remedial simulations defined by Flow Runs 26, 27, and 28 and Transport Runs T3, T4, and T5. Included in the lists are the proposed extraction locations, well names (if existing), times of operation, and specified flow rates. As discussed in Section 6.3, these simulations are based upon the ROD, but are not part of the formally negotiated remediation activity. Wells indicated in the tables for a given extraction location are either in existence now or "proposed" for the purposes of the simulations. LLNL is not committed to building the proposed wells, or necessarily operating the existing wells in the manner shown. Finally, Table A-7 reviews several specific mass transport characteristics of Transport Runs T1 through T5.

Table A-1. Regional hydraulic conductivities specified in flow simulations.

Flow run(s)	Flow region ^a	Conductivity <i>K</i> (ft/day)	Comments
24-28	1a	10.0	Basic, low-range effective value estimated for Main Basin materials
	1b	5.3	Reduced effective value for Altamont Subbasin
	1c	8.0	Reduced effective value for Mocho II alluvium
	2-6	0.01	Lower permeability by factor of 1,000

^a Refer to Figure 10 for illustration of flow regions.

Table A-2. Boundary conditions applied in flow simulations.

Flow run(s)	Boundary segment ^a	Condition	Comments
24	1-6	Flux	Specified head measured from Fig. 6
	7-11	No-flux	Specified no-flux
25-28	1-3	Flux	Specified normal flux as evaluated along boundary in Run 24
	4-6	Flux	Specified head measured from Fig. 6
	5-11	No-flux	Specified no-flux

^a Refer to Figure 6 for location of boundary segments.

Table A-4. Remedial wells and pumping rates used in Flow Run 26 (50-y cleanup scenario with degradation)^a.

Extraction location	Well(s) ^b	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
1	EW-415 ^c (A)	0-40	40	Operating
		40-50	0	
2	MW-262, MW-520	0-40	30	Detailed Study Area
	P-601, P-522 (A)	40-50	0	
3	MW-109, MW-408 (A)	0-50	25	Offsite (Arroyo Seco)
4	EW-712 (A)	0-45	30	
		45-50	0	
23	MW-457 (A)	0-50	25	Offsite (Arroyo Seco)
5	MW-357 ^c , EW-704 ^c (B)	0-50	20	Operating
6	MW-610 (B)	0-50	10	
7	MW-655 (B)	0-50	10	
8	MW-454 (C)	0-50	10	
9	P-701 (C)	0-50	10	Operating
10	MW-319/320/487 (C/D)	0-5	20	West Traffic Circle
		5-50	0	
21	MW-114/315/317 (C/D)	0-5	25	West Traffic Circle
		5-15	40	
		15-20	30	
		20-30	20	
		30-50	0	
11	MW-351 (D)	0-10	35	Drainage Retention Basin
		10-15	30	
		15-20	15	
		20-30	10	
		30-50	0	
12	MW-142/220/561 (D)	0-10	25	East Traffic Circle
		10-15	20	
		15-30	10	
		30-50	0	

Table A-4. (continued)

Extraction location	Well(s) ^b	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
20a	MW-361/119 (D)	0-5	40	Drainage Retention Basin
		5-15	45	
		15-20	50	
		20-25	40	
		25-50	0	
20b	proposed (D)	0-25	0	
		25-30	40	
		30-47	50	
		47-50	0	
13	proposed (E)	0-30	15	Special tritium treatment facility
		30-40	20	
		40-50	0	
14a	MW-206 (T-5475)	0-10	15	
		10-15	20	
		15-30	25	
		30-40	30	
14b	proposed (T-5475)	40-50	0	
		0-40	0	
		40-45	40	
		45-49	30	
14c	proposed (E)	49-50	0	
		0-49	0	
19a	MW-257/566 (E)	49-50	50	
		0-10	20	
		10-15	25	
		15-20	30	
		20-25	40	
		25-40	50	
19b	proposed (E)	40-50	0	
		0-40	0	
		40-49	50	
		49-50	0	

Table A-4. (continued)

Extraction location	Well(s) ^b	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
17	GEW-808 ^c , GEW-816 ^c (F)	0-30 30-35 35-50	10 15 0	Gasoline Spill Area (Dynamic Stripping Project)
18	MW-112 (F)	0-30 30-50	10 0	
16	TW-11, TW-11A (G)	0-35 35-50	20 0	
IW-1	proposed (from E)	0-49 49-50	-50 0	Central LLNL
IW-2	EW-SNL-707 (from F)	0-40 40-50	-20 0	Sandia Property
Recharge Basin (from A)		0-40 40-45 45-50	-150 -80 -50	
TFB ditch (from B)		0-50	-40	
TFC ditch (from C)		0-50	-20	

^a Other ambient sources and sinks shown in Table A-3.^b Associated treatment facility shown in parentheses (*i.e.*, A = TFA).^c Currently in operation.

Table A-5. Remedial wells and pumping rates used in Flow Run 27 (75-year cleanup scenario without degradation)^a.

Extraction location	Well(s) ^b	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
1	EW-415 ^c (A)	0-70	40	Operating
		70-75	0	
2	MW-262, MW-520	0-70	30	Detailed study area
	P-601, P-522(A)	70-75	0	
3	MW-109, MW-408 (A)	0-70	25	Offsite (Arroyo Seco)
		70-74	50	
		74-75	0	
4	EW-712 (A)	0-70	30	
		70-75	0	
23	MW-457 (A)	0-70	25	Offsite (Arroyo Seco)
		70-74	50	
		74-75	100	
5	MW-357 ^c , EW-704 ^c (B)	0-70	20	Operating
		70-75	0	
6	MW-610 (B)	0-70	10	
		70-75	0	
7	MW-655 (B)	0-70	10	
		70-75	0	
8	MW-454 (C)	0-75	10	
9	P-701 (C)	0-75	10	Operating
10	MW-319/320/487 (C/D)	0-5	20	West Traffic Circle
		5-75	0	
21	MW-114/315/317 (C/D)	0-5	25	West Traffic Circle
		5-15	40	
		15-45	30	
		45-75	0	
11	MW-351 (D)	0-10	35	Drainage Retention Basin
		10-15	30	
		15-20	15	
		20-30	10	
		30-75	0	

Table A-5. (continued)

Extraction location	Well(s) ^b	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
12	MW-142/220/561 (D)	0-10	25	East Traffic Circle
		10-15	20	
		15-30	10	
		30-75	0	
20a	MW-361/119 (D)	0-5	40	Drainage Retention Basin
		5-15	45	
		15-20	50	
		20-25	40	
20b	proposed (D)	25-75	0	
		0-25	0	
		25-30	40	
		30-50	50	
20c	proposed (D)	50-75	0	
		0-50	0	
		50-65	50	
		65-75	0	
13	proposed (E)	0-30	15	
		30-35	25	
		35-50	30	
		50-75	0	
14a	MW-206 (T-5475)	0-10	15	Special tritium treatment facility
		10-15	20	
		15-35	25	
		35-50	20	
14b	proposed (T-5475)	50-75	0	
		0-50	0	
		50-65	30	
		65-75	0	
19a	MW-257/566 (E)	0-10	20	
		10-15	25	
		15-20	30	
		20-25	40	
		25-50	50	
		50-75	0	

Table A-5. (continued)

Extraction location	Well(s) ^b	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
19b	proposed (E)	0-50 50-65 65-75	0 50 0	
17	GEW-808 ^c , GEW-816 ^c (F)	0-35 35-45 45-75	10 20 0	Gasoline Spill Area (Dynamic Stripping Project)
18	MW-112 (F)	0-35 35-75	10 0	
16	TW-11, TW-11A (G)	0-50 50-75	20 0	
IW-1	proposed	0-65 65-75	-50 0	Central LLNL
IW-2	EW-SNL-707	0-50 50-75	-20 0	Clean Site Area
Recharge Basin (from A)		0-70 70-75	-150 -100	
TFB ditch (from B)		0-70 70-75	-40 0	
TFC ditch (from C)		0-75	-20	

^a Other ambient sources and sinks shown in Table A-3.^b Associated treatment facility shown in parentheses (*i.e.*, A = TFA).^c Currently in operation.

Table A-6. Remedial wells and pumping rates used in Flow Run 28 (aggressive cleanup scenario without degradation)^a.

Extraction location	Well(s) ^b	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
1	EW-415 ^c (A)	0-25	50	Online
		25-50	0	
2	MW-262, MW-520	0-30	50	Detailed Study Area
	P-601, P-522 (A)	30-50	0	
22	EW-903 (A)	0-40	50	Offsite (Arroyo Seco)
		40-50	0	
23	EW-904 (A)	0-15	0	Offsite (Arroyo Seco)
		15-40	50	
		40-50	0	
4a	EW-712 (A)	0-25	50	
		25-50	0	
4b	proposed (A)	0-15	0	
		15-35	50	
		35-50	0	
5	MW-357 ^c , EW-704 ^c (B)	0-40	16	Online
		40-50	0	Building 141 Study Area
6	proposed (B)	0-25	16	
		25-50	0	
7	proposed (B)	0-25	50	
		25-50	0	
10a	proposed (C/D)	0-25	16	West Traffic Circle Study Area
		25-50	0	
10b	proposed (C/D)	0-15	0	
		15-25	-16	
		25-50	0	
21a	proposed (C/D)	0-40	16	West Traffic Circle Study Area
		40-50	0	
21b	proposed (C/D)	0-40	16	
		40-50	0	
21c	proposed (C/D)	0-15	0	
		15-40	16	
		40-50	0	
21d	proposed (C/D)	0-15	0	
		15-45	16	
		45-50	0	

Table A-6. (continued)

Extraction location	Well(s)	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
21e	proposed (C/D)	0-15	0	North of Drainage Retention Basin
		15-35	16	
		35-50	0	
21f	proposed (C/D)	0-40	0	
		40-45	16	
		45-50	0	
21g	proposed (C/D)	0-15	0	
		15-40	-16	
		40-50	0	
21h	proposed (C/D)	0-15	0	
		15-40	-16	
		40-50	0	
21i	proposed (C/D)	0-20	0	
		20-35	-16	
		35-50	0	
11a	proposed (D)	0-35	16	
		35-50	0	
11b	proposed (D)	0-30	16	
		30-50	0	
11c	proposed (D)	0-30	16	
		30-50	0	
11d	proposed (D)	0-15	0	
		15-25	16	
		25-50	0	
11e	proposed (D)	0-15	0	
		15-25	16	
		25-50	0	
11f	proposed (D)	0-15	0	
		15-40	16	
		40-50	0	
11g	proposed (D)	0-15	0	
		15-30	-16	
		30-50	0	
11h	proposed (D)	0-15	0	
		15-35	-16	
		35-50	0	

Table A-6. (continued)

Extraction location	Well(s)	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
12a	proposed (D)	0-20	16	East Traffic Circle Study Area
		20-50	0	
12b	MW-142/220/561 (D)	0-25	16	
		25-50	0	
12c	proposed (D)	0-25	16	
		25-50	0	
12d	proposed (D)	0-25	16	
		25-50	0	
12e	proposed (D)	0-15	0	
		15-20	16	
		20-50	0	
12f	proposed (D)	0-15	0	
		15-30	-16	
		30-50	0	
12g	proposed (D)	0-15	0	
		15-25	-16	
		25-50	0	
12h	proposed (D)	0-25	-16	
		25-50	0	
13a	proposed (E)	0-40	16	
		40-50	0	
13b	proposed (E)	0-40	16	
		40-50	0	
13c	proposed (E)	0-15	0	
		15-40	16	
		40-50	0	
13d	proposed (E)	0-20	0	
		20-40	13	
		40-50	0	
13e	proposed (E)	0-20	0	
		20-45	13	
		45-50	0	
13f	proposed (E)	0-40	0	
		40-45	13	
		45-50	0	

Table A-6. (continued)

Extraction location	Well(s)	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
13g	proposed (E)	0-40	-31	Central LLNL Injection Area
		40-50	0	
13h	proposed (E)	0-15	0	
		15-40	-16	
		40-50	0	
13i	proposed (E)	0-15	0	
		15-35	-16	
		35-50	0	
13j	proposed (E)	0-20	0	
		20-40	-16	
		40-50	0	
13k	proposed (E)	0-20	0	
		20-45	-13	
		45-50	0	
13l	proposed (E)	0-20	0	
		20-35	-13	
		35-50	0	
14a	MW-257/566 (E)	0-35	10	
		35-50	0	
14b	proposed (E)	0-20	10	
		20-50	0	
14c	proposed (E)	0-25	10	
		25-50	0	
14d	proposed (E)	0-20	10	
		20-50	0	
14e	proposed (E)	0-25	10	
		25-50	0	
14f	proposed (E)	0-20	0	
		20-25	13	
		25-50	0	
14g	proposed (E)	0-35	-10	
		35-50	0	
14h	proposed (E)	0-20	-10	
		20-50	0	
14i	proposed (E)	0-25	-10	
		25-50	0	

Table A-6. (continued)

Extraction location	Well(s)	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
14j	proposed (E)	0-20	-10	
		20-50	0	
14k	proposed (E)	0-25	-10	
		25-50	0	
14l	proposed (E)	0-20	0	
		20-25	-13	
		25-50	0	
19a	proposed (E)	0-30	10	Eastern Landing Mat Storage Area
		30-50	0	
19b	proposed (E)	0-15	10	
		15-50	0	
19c	proposed (E)	0-20	10	
		20-30	0	
		30-40	-13	
		40-50	0	
19d	proposed (E)	0-30	10	
		30-50	0	
19e	proposed (E)	0-15	0	
		15-35	16	
		35-50	0	
19f	proposed (E)	0-15	0	
		15-35	16	
		35-50	0	
19g	proposed (E)	0-15	0	
		15-35	16	
		35-50	0	
19h	proposed (E)	0-20	0	
		20-30	13	
		30-50	0	
19i	proposed (E)	0-30	0	
		30-40	13	
		40-50	0	
19j	proposed (E)	0-35	0	
		35-45	16	
		45-50	0	
19k	proposed (E)	0-15	0	
		15-30	-10	
		30-50	0	

Table A-6. (continued)

Extraction location	Well(s)	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
19l	proposed (E)	0-15	-10	
		15-50	0	
19m	proposed (E)	0-20	-10	
		20-50	0	
19n	proposed (E)	0-30	-10	
		30-50	0	
19o	proposed (E)	0-15	0	
		15-35	-16	
		35-50	0	
19p	proposed (E)	0-15	0	
		15-40	-16	
		40-50	0	
19q	proposed (E)	0-15	0	
		15-35	-16	
		35-50	0	
19r	proposed (E)	0-20	0	
		20-30	-13	
		30-50	0	
20a	MW-361/119 (E)	0-35	16	South of Drainage Retention Basin
		35-50	0	
20b	proposed (E)	0-35	16	
		35-50	0	
20c	proposed (E)	0-15	0	
		15-35	16	
		35-50	0	
20d	proposed (E)	0-15	0	
		15-30	13	
		30-50	0	
20e	proposed (E)	0-20	0	
		20-40	13	
		40-50	0	
20f	proposed (E)	0-20	0	
		20-40	-13	
		40-50	0	
20g	proposed (E)	0-15	0	
		15-35	-16	
		35-50	0	

Table A-6. (continued)

Extraction location	Well(s)	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
20h	proposed (E)	0-40	-16	
		40-50	0	
20i	proposed (E)	0-15	0	
		15-35	-16	
		35-50	0	
20j	proposed (E)	0-15	0	
		15-30	-13	
		30-50	0	
17a	proposed (F)	0-25	10	Gasoline Spill Area
		25-50	0	
17b	proposed (F)	0-20	10	
		20-50	0	
17c	proposed (F)	0-20	0	
		20-40	13	
		40-50	0	
17d	GEW-808 ^c , GEW-816 ^c (F)	0-20	0	
		20-35	13	
		35-50	0	
17e	proposed (F)	0-40	0	
		40-50	13	
17f	proposed (F)	0-15	0	
		15-25	-10	
		25-50	0	
17g	proposed (F)	0-20	-10	
		20-50	0	
17h	proposed (F)	0-20	0	
		20-50	-13	
18a	MW-112 (F)	0-25	10	
		25-50	0	
18b	proposed (F)	0-20	-10	
		20-35	-13	
		35-50	0	
18c	proposed (F)	0-15	-23	
		15-50	0	
18d	proposed (F)	0-15	-23	
		15-50	0	

Table A-6. (continued)

Extraction location	Well(s)	Period of operation (y)	Pumping rate Q_w (gpm)	Comments
15	MW-307 (G)	0-15	50	
		15-50	0	
16	TW-11, TW-11A (G)	0-15	50	
		15-50	0	
Recharge Basin (from A)		0-40	-100	
		40-50	0	
TFB ditch (from B)		0-25	-100	
		25-40	-16	
		40-50	0	
New Recharge Trench (from E, F, and G)		0-25	-150	South-central LLNL
		25-30	-115	
		30-35	-65	
		35-40	-29	
		40-50	0	

^a Other ambient sources and sinks shown in Table A-3.

^b Treatment facility shown in parentheses (*i.e.*, A = TFA).

^c Currently in operation.

Table A-7. Characteristics of transport simulations and associated flow configurations.^a

Transport run	Simulation time (y)	Number of flow configurations	Flow run	Dispersivities A_{11} (ft) A_{22} (ft)		Diffusivity $\mathcal{D}$ (ft ² /day)	Retardation $\mathcal{R}$	Decay rate λ (y ⁻¹)	Comments
T1	0-250	1	25	260	26	0	1.5	0.014	"No-action" case with degradation
T2	0-1,200	1	25	260	26	0	1.5	0	"No-action" case without degradation
T3	0-50	12	26	260	26	0	1.5	0.014	50-y cleanup with degradation
T4	0-75	13	27	260	26	0	1.5	0	75-y cleanup without degradation
T5	0-50	8	28	260	26	0	1.5	0	"Aggressive" cleanup without degradation

^a Refer to Figures 13 or 14 for an illustration of the initial total aqueous VOC concentration distribution at $t=0$.