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CONVERSION FACTORS

For those readers interested in using the International System of Units (SI), the following table can be used to convert the inch-pound units of measurement used in this report to SI units:

Multiply	By	To obtain
inch (in.)	25.40	millimeter
foot (ft)	0.3048	meter
foot per second (ft/s)	0.3048	meter per second
foot per day (ft/d)	0.3048	meter per day
foot per second per square foot	3.281	meter per second per square meter
cubic foot per second (ft^3/s)	0.02832	cubic meter per second
cubic foot per day (ft^3/d)	0.02832	cubic meter per day
gallon (gal)	3.785	liter

Sea level: In this report "sea level" refers to the National Geodetic Vertical Datum of 1929 (NGVD of 1929)—a geodetic datum derived from a general adjustment of the first-order level nets of both the United States and Canada, formerly called "Mean Sea Level of 1929."

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Abstract

Hydrogeologic factors influencing leachate movement from an in-situ oil-shale retort near Rock Springs, Wyoming, were investigated through models of ground-water flow and solute transport. Leachate, indicated by the conservative ion thiocyanate, has been observed ½ mile downgradient from the retort. The contaminated aquifer is part of the Green River Formation and consists of thin, permeable layers of tuff and sandstone interbedded with oil shale. Most solute migration has occurred in an 8-foot sandstone at the top of the aquifer. Ground-water flow in the study area is complexly three dimensional and is characterized by large vertical variations in hydraulic head. The solute-transport model was used to predict the concentration of thiocyanate at a point where ground water discharges to the land surface. Leachate with peak concentrations of thiocyanate—45 milligrams per liter or approximately one-half the initial concentration of retort water—was estimated to reach the discharge area during January 1985.

This report describes many of the advantages, as well as the problems, of site-specific studies. Data such as the distribution of thin, permeable beds or fractures might introduce an unmanageable degree of complexity to basin-wide studies but can be incorporated readily into site-specific models. Solute migration in the study area occurs primarily in thin, permeable beds rather than in oil-shale strata. Because of this behavior, leachate traveled far greater distances than might otherwise have been expected. The detail possible in site-specific models permits more accurate prediction of solute transport than is possible with basinwide models. A major problem in site-specific studies is identifying model boundaries that permit the accurate estimation of aquifer properties. If the quantity of water flowing through a study area cannot be determined prior to modeling, the hydraulic conductivity and ground-water velocity will be poorly estimated.

INTRODUCTION

The development of oil-shale resources in Colorado, Utah, and Wyoming presents a variety of potential hydrologic problems. Methods of extracting oil and gas from shale without mining are called in-situ retorting techniques, use of which could result in degradation of ground-water quality both within and adjacent to the retort sites. The in-situ retorting process begins with fracturing of the oil shale to increase its permeability within a carefully delineated volume of rock. The organic matter within the fractured zone or retort chamber is ignited, and combustion is induced through the formation by injected air. The organic matter bound within the rock is converted to oil and gas ahead of the combustion zone. The oil is then pumped to the surface. Significant quantities of water vapor and other gases also are recovered at the surface. Variations of this technique have been developed, but all produce water of very poor quality. Retorting of the oil shale stops when the combustion zone has extended throughout the retort chamber. If the chamber fills with formation water, soluble material can transfer from the burnt shale to the water. This transfer can cause ground-water contamination if the water migrates outside the retort chamber.

Digital models of ground-water flow and solute transport have been suggested as aids in predicting possible impacts of retorting on the ground-water system. Past modeling techniques were not designed for use in rock such as oil shale in which permeability and porosity result from fracturing. To solve this shortcoming, a number of models were developed in the last few years for use in fractured media. However, few oil-shale retorts have been operational for an extended period of time, and well-documented instances of solute migration from these facilities are rare. As a result, digital modeling techniques have not been adequately tested under the unusual geologic conditions present in oil-shale basins.

The experimental oil-shale retorting facility (fig. 1) operated by LETC (Laramie Energy Technology Center) near Rock Springs, Wyo., provides an opportunity to investigate changes in ground-water quality after in- situ retorting of oil shale. This facility was

active from 1969 through 1979, and adequate time has elapsed to permit significant solute migration. This report is one of several that describe a study of ground-water flow and solute transport at the LETC facility. The broad objectives of the study were to identify geologic, hydraulic, and chemical factors that control the process of solute migration in oil shale and, by application to the LETC study area, to develop methods for data collection and interpretation that can be used with confidence at other retort sites.

The specific objectives of this report are to identify geohydrologic factors that are important to the process of solute transport within the LETC study area and to demonstrate the uses and limitations of various modeling techniques in a field problem. Because of the complex chemical nature of oil-shale water, only movement of nonreacting contaminants is considered. Although the oil-shale strata at the LETC facility are not stratigraphic equivalents of the formations being exploited in the Piceance basin of Colorado, the major area of development, the lithology of the two regions is similar. Therefore, modeling techniques used in this study can be applied to other oil-shale basins.

Figure 1. Location of study area, southwestern Wyoming.

DESCRIPTION OF THE STUDY AREA

In-situ fracturing and retorting experiments were conducted by LETC from 1969 through 1979. The location of these experiments is shown in figure 2. The principal experiment of interest in this report occurred during 1976 and was designated by LETC as site 9. The chemical analysis of ground-water samples has indicated the migration of solutes from this site; solute plumes from other experiments either dispersed through the ground-water system or were of such limited areal extent that they were negligible.

The in-situ retort process used by LETC has the potential of recovering vast oil-shale resources from low-grade deposits in contrast to other retort processes that might not be economical. Improvements in the LETC process have been made (Lekas, 1981), but the basic nature of the method has remained unchanged.

The site 9 retort experiment was described in detail by Long and others (1977) and is summarized here. The target shale zone was located in the Tipton Shale Member of the Green River Formation of Eocene age between 137 and 177 ft below land surface. Eight production wells were drilled on the perimeter of a 70 × 70 ft grid. An injection well was drilled in the center of the square pattern.

The formation was hydraulically fractured in three approximately horizontal planes at depths of about 147, 157, and 173 ft. The fractures were filled with sand under pressure. Slurried explosive was injected in the center well with the intention of forcing explosive into the middle fracture for detonation while using the upper and lower fractures to reflect the shock waves and limit the vertical extent of the rubbled zone. Problems with the system resulted in detonation of the explosive in the upper fracture. A second blast was needed to fracture the formation between the middle and lower fractures. Because of this problem, oil shale was fractured from the lower fracture to the top of the Tipton Shale Member where a basal sandstone of the overlying Wilkins Peak Member of the Green River Formation acted to absorb the shock waves.

The retort chamber was ignited April 5, 1976, by placing an electrical resistance heater in the center well to heat injected air and injecting propane into the same well. Propane injection was terminated after 78 days, and air injection continued through 150 days. Formation temperatures measured in wells above and adjacent to the retort chamber indicated that retorting had ceased after 200 days. Material-balance calculations indicated that 45,150 gal of oil were retorted; however, only 2,483 gal were recovered by production wells. The inability to recover oil was attributed to failure of the mechanical lift pumps used during the experiment. Shortly before the retorting experiment was started, LETC began a
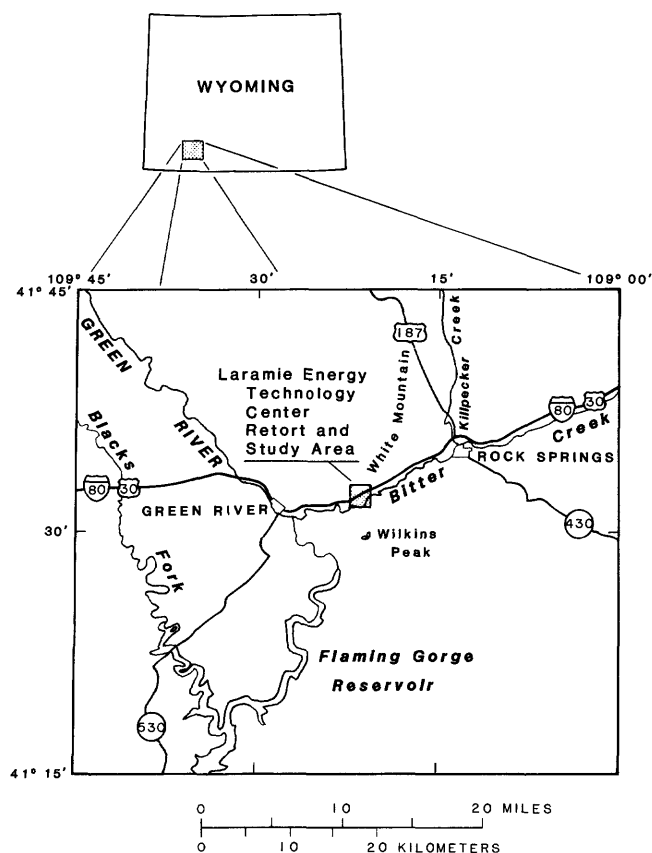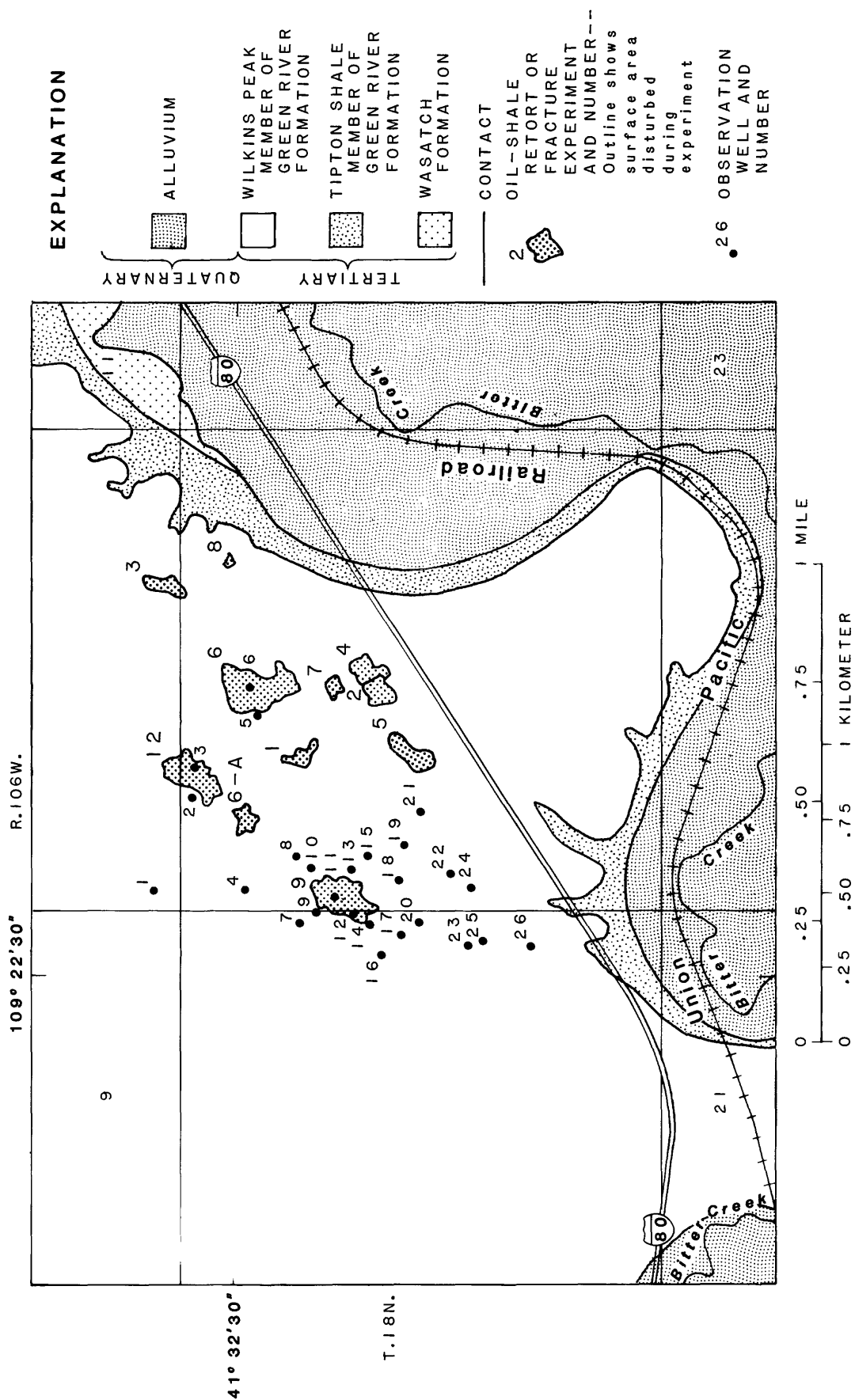
Figure 2. Surface geology, well numbers, and location of oil-shale retort experiments.

program to monitor ground-water levels and water quality in and adjacent to site 9; this program continued through 1983.

STRATIGRAPHY

The oil-shale resource used by LETC near Rock Springs, Wyo., lies within the Tipton Shale Member of the Green River Formation of Eocene age, which conformably overlies the Wasatch Formation of Eocene age throughout the study area. Geologic characteristics of these formations were described basinwide by Bradley (1964) and Culbertson and others (1980). Geologic investigations at the LETC facility were documented by Dana and Smith (1972). The Wasatch Formation consists of fluvial deposits; the Green River Formation is primarily lacustrine. In general, the Green River Formation overlies the Wasatch Formation, but intertonguing of the two formations has been observed throughout the Green River basin. The surface geology of the study area is shown in figure 2. The geohydrologic units, stratigraphic units, and generalized lithology are shown in figure 3.

The basal unit of interest to this study was mapped as the Niland Tongue of the Wasatch Formation by Roehler (1981) from outcrops along White Mountain. However, no evidence for intertonguing of the Wasatch and Green River Formations could be found in the subsurface at the LETC facility. Therefore, in this report the basal unit is simply called the Wasatch Formation. The upper 225 ft of the Wasatch Formation at the LETC facility consists of shale and mudstone sporadically interbedded with thin sandstones. Beneath this part of the formation is 130 ft of sandstone and sandy mudstone and about 100 ft of variegated mudstone containing red sandstone lenses. A major regional aquifer of red, medium-grained sandstone occurs below the mudstone beds. The areal and vertical extent of this aquifer is poorly defined and may include parts of both the Wasatch and Fort Union Formations. The sandstone is interbedded with sandy, gray mudstone and continues well below the section of interest to this study.

The Tipton Shale Member of the Green River Formation can be characterized as fine-grained, brown, flaky shale, ostracode-bearing shale, and low- to medium-grade oil shale. Thin, persistent layers of carbonate-rich volcanic tuff are common in the Tipton Shale Member and range in thickness from ½ to 8 in. Several of these tuffs are used as marker beds because they are readily recognized on geophysical logs. The base of the Tipton Shale Member is sharply defined by beds of oolitic limestone that contain an abundance of snail shells (*Goniobasis* sp.) and freshwater clams (*Unio* sp.). Little horizontal variation in lithology has been noted within

Figure 3. Geohydrologic units, stratigraphic units, and generalized lithology of the Wasatch and Green River Formations at site 9.

the Tipton Shale Member in the study area, but the unit is characterized by vertical changes. A measured section of the Tipton Shale Member is given in table 1.

Core analyses by Pasini and others (1972) showed that the direction of minimum tensile strength of oil shale in undisturbed areas of the Tipton Shale Member is oriented at N. 40° E. This direction is at right angles to the orientation of lineaments observed on areal photographs of the land surface. The reason for this difference is unknown. Pasini and others (1972) concluded that vertical fractures, where present, strike at N. 40° E.

The Wilkins Peak Member of the Green River Formation overlies the Tipton Shale Member at the LETC facility. This unit consists of mudstone, marlstone, and shale with occasional tuff and sandstone beds. The

Table 1. Measured section of the Tipton Shale Member of the Green River Formation

[Modified from Dana and Smith (1972) and Roehler (1981)]

Distance from top of Tipton Shale Member (feet)	Thickness (feet)	Description
0–15.9	15.9	Oil shale, green-gray to sooty black.
15.9–16.0	0.1	Tuff, yellow-brown, very fine grained to fine-grained.
16.0–29.0	13.0	Oil shale, medium-gray to sooty black.
29.0–29.3	0.3	Tuff, gray to brown, very fine grained.
29.3–32.0	2.7	Oil shale, light-brown to black.
32.0–32.1	0.1	Tuff, gray to brown.
32.1–37.2	5.1	Oil shale, medium-gray to black, slightly dolomitic.
37.2–37.3	0.1	Tuff, brown, fine-grained.
37.3–39.8	2.5	Oil shale, medium- to dark-gray.
39.8–40.0	0.2	Tuff, white to gray, very porous, fine-grained.
40.0–47.5	7.5	Oil shale, light-brown to black.
47.5–47.9	0.4	Tuff, dolomitic, tan to buff, very porous.
47.9–49.0	1.1	Oil shale, light-brown to black.
49.0–49.3	0.3	Oil shale, tan to gray, very calcareous.
49.3–49.5	0.2	Tuff, tan.
49.5–52.3	2.8	Oil shale, medium- to dark-gray. Several thin tuff layers.
52.3–52.4	0.1	Tuff, brown, fine-grained. Some massive quartz.
52.4–56.3	3.9	Oil shale, light- to dark-gray, calcareous.
56.3–56.7	0.4	Tuff, white to gray, chalky, very friable.
56.7–58.7	2.0	Oil shale, medium-gray to black.
58.7–58.9	0.2	Dolomite, fossiliferous, silty in part.
58.9–59.3	0.4	Tuff, gray, fine-grained, very calcareous, very porous.
59.3–62.8	3.5	Oil shale, gray to brown, fractured.
62.8–64.9	2.1	Shale and siltstone, sandy in part, porous.
64.9–65.9	1.0	Oil shale, gray, silty, calcareous.
65.9–67.3	1.4	Siltstone and shale, sandy, very porous.
67.3–69.9	2.6	Sandstone, light-gray, fine- to medium-grained.
69.9–71.0	1.1	Shale and siltstone, tan to light-gray.
71.0–71.8	0.8	Oil shale, medium-gray.
71.8–72.5	·0.7	Shale, tan to gray, nearly a dolomite.
72.5–103.0	30.5	Oil shale, gray, some dolomitic shale.
103.0–110.0	7.0	Oil shale, light- to dark-brown.
110.0–114.3	4.3	Oil shale, gray.
114.3–114.4	0.1	Tuff.
114.4–117.1	2.7	Oil shale, brown, flaky.
117.1–117.4	0.3	Tuff.
117.4–122.3	4.9	Oil shale, brown, flaky.
122.3–123.4	1.1	Tuff.
123.4–124.2	0.8	Oil shale, brown, flaky.
124.2–124.3	0.1	Tuff, tan.
124.3–125.9	1.6	Oil shale, brown, flaky.
125.9–126.4	0.5	Tuff, tan, biotite.
126.4–133.4	7.0	Oil shale, gray, papery soft.
133.4–135.1	1.7	Limestone, gray, finely crystalline, sandy, fossiliferous.
135.1–143.2	8.1	Shale, dolomitic to very limy, fossiliferous.

base of the Wilkins Peak Member is marked by an 8-ft-thick limy sandstone that forms a caprock in outcrops. Overlying this basal bed is 207 ft of marlstone. The only permeable bed of significance in this 207-ft section is a 4-in. tuff called the Firehole Bed. The remainder of the Wilkins Peak Member has been eroded throughout the study area.

Alluvial deposits of Quaternary age are present along Bitter Creek. The thickness of these deposits is not known. However, the discharge areas for ground water in the Tipton Shale Member are along outcrops higher than the alluvium. Water in the alluvium is hydraulically isolated from water in the Tipton Member. Therefore, the alluvial deposits are not important to this study.

GEOHYDROLOGY

The geohydrologic system in the vicinity of the retort sites consists of two aquifers and two confining units. The aquifers and confining units are defined on the basis of relative permeabilities and therefore do not coincide exactly with geologic formations and members. The relation of aquifers and confining units to geologic formations and members is shown in figure 3.

Wasatch Aquifer and Upper Wasatch Confining Unit

The basal aquifer in the study area is the Wasatch aquifer. This aquifer consists of medium-grained sandstone and sandy mudstone. The top of the aquifer is located 225 ft below the top of the Wasatch Formation. Few water wells are open to the Wasatch aquifer within the study area, but it is apparent that the potential exists for high-yielding wells. No evidence of secondary permeability exists, but the extensive sand facies within the aquifer indicate that the hydraulic conductivity is large. No reliable aquifer test of the Wasatch aquifer has been conducted within the study area.

The upper Wasatch confining unit overlies the Wasatch aquifer. This confining unit is approximately 232 ft thick and consists of 7-ft-thick massive limestone at the base of the Tipton Shale Member of the Green River Formation overlying 225 ft of mudstone and shale within the upper part of the Wasatch Formation. The top 44 ft of the confining unit is particularly shaly, soft, and erodable and is unlikely to develop fractures or solution channels.

Regional potentiometric-surface maps of the Wasatch aquifer indicate water enters the aquifer in outcrop areas north and east of the study area and discharges to the Flaming Gorge Reservoir, about 30 mi southwest of the study area (E.A. Zimmerman, U.S. Geological Survey, written commun., 1982). Discharge also occurs locally to the alluvium along Bitter Creek. A comparison of regional potentiometric maps with hydraulic-head data collected at deep wells within the study area confirms this interpretation.

Within the study area, the alluvium along Bitter Creek overlies the upper Wasatch confining unit. Therefore, water moving from the Wasatch aquifer into the alluvium moves through the confining unit with a resultant decrease in head. Although no wells penetrate the Wasatch aquifer where covered by alluvium, the vertical variation in hydraulic head near well 16 (fig. 4) clearly shows this trend. Very limited hydraulic-head data for wells open to the top part of the upper Wasatch

confining unit indicate that horizontal-head gradients toward Bitter Creek also exist.

The relation of hydraulic head within the upper Wasatch confining unit to head within the overlying Tipton aquifer near well 16 is shown in figure 4. Although this figure shows the vertical variation in hydraulic head at a single point, similar illustrations can be prepared for other locations within the study area. On the basis of head data at several locations, it appears that there is a potential for movement of water from the lower part of the Tipton aquifer into the upper Wasatch confining unit. Alone, the hydraulic gradient does not indicate how much water moves between the geohydrologic units.

The quality of water in the Tipton aquifer is significantly different from the quality of water in the Wasatch aquifer. Because of the large difference, water-quality data are particularly useful for estimating the relative amount of water in the upper Wasatch confining unit that originates from overlying and underlying aquifers. The dissolved-solid concentration of water in the Tipton aquifer is an order of magnitude greater than the dissolved-solid concentration of water in the Wasatch aquifer. Similar differences exist for individual ions. The dominant ions in water of the Wasatch aquifer are sodium, bicarbonate, and sulfate.

Concentrations of dissolved solids, sodium, and chloride in ground-water samples (table 2) were used to test for ground-water movement between the Tipton aquifer and the upper Wasatch confining unit. Chloride
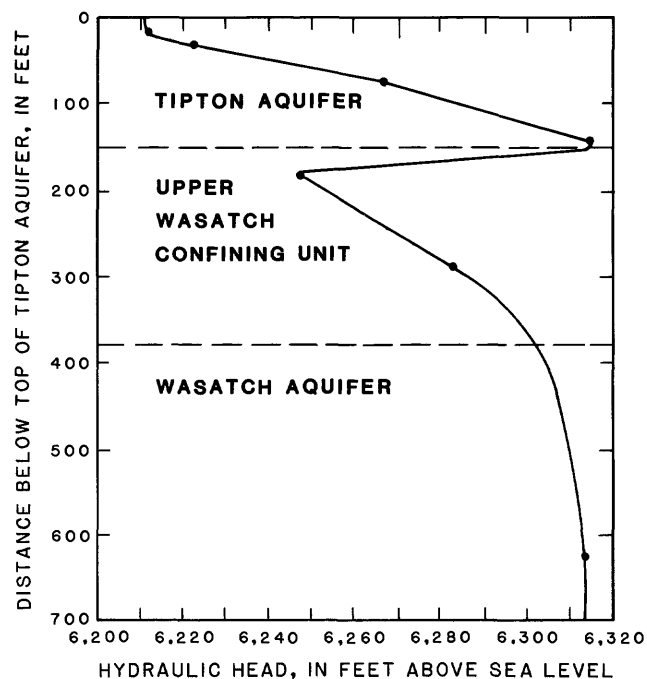

Figure 4. Vertical variation in hydraulic head near well 16.

Table 2. Dissolved-solid, sodium, and chloride concentrations in selected ground-water samples collected during May 1982

[mg/L, milligrams per liter]

Geohydrologic unit	Number of samples	Dissolved-solid concentration (mg/L)		Sodium (mg/L)		Chloride (mg/L)	
		Minimum	Maximum	Minimum	Maximum	Minimum	Maximum
Lower part of Tipton aquifer.	4	6,040	11,100	2,300	4,600	2,900	7,500
Upper Wasatch confining unit.	3	1,040	1,330	400	520	66	170
Wasatch aquifer.	2	1,370	1,620	540	700	81	270

is the most useful of these water-quality constituents because the ion is normally conservative in ground-water systems. Similar tables of water-quality data can be constructed for other dates.

On the basis of mass-balance calculations for the water-quality constituents given in table 2, it can be concluded that virtually all the water in the upper Wasatch confining unit originates in the Wasatch aquifer. Mass-balance calculations are based on the expression

$$C_{UW} = C_W P_W + C_T P_T$$

where C_{UW} is the solute concentration of water in the upper Wasatch confining unit,

C_W is the solute concentration of water in the Wasatch aquifer,

P_W is the fractional part of water in the upper Wasatch confining unit originating in the Wasatch aquifer,

C_T is the solute concentration of water in the Tipton aquifer, and

P_T is the fractional part of water in the upper Wasatch confining unit originating in the Tipton aquifer.

Recognizing that the sum of P_T and P_W equals one, one can solve for P_T. For example, applying the equation to the range of chloride concentrations given in table 2 shows that less than 1 percent of water in the upper Wasatch confining unit originates in the Tipton aquifer. One possible explanation for this conclusion is that the top 44 ft of the upper Wasatch confining unit, a particularly soft, shaly mudstone, is virtually impermeable.

A second possible explanation is that 7 ft of limestone at the contact between the Tipton aquifer and the upper Wasatch confining unit is very permeable, permitting relatively rapid horizontal movement of water from the lower part of the Tipton aquifer toward Bitter Creek and outcrop areas along Bitter Creek. Therefore, water in the limestone would not mix with water in deeper parts of the upper Wasatch confining unit.

Evidence does not exist to support the hypothesis that the limestone at the contact of the Tipton aquifer and the upper Wasatch confining unit is very permeable. Discharge from the limestone at outcrops adjacent to Bitter Creek has not been observed, and in contrast to most permeable limestones, the limestone shows no sign of fractures or solution channels.

On the basis of existing lithologic and water-quality data, it can be concluded that the upper Wasatch confining unit is a relatively impermeable base for the Tipton aquifer. In the flow-model analysis, described later in this report, it is assumed that no water moves between the Tipton aquifer and underlying sediments. Therefore, the remainder of this report is concerned only with ground-water flow and solute transport in the Tipton aquifer.

Tipton Aquifer

The Tipton aquifer overlies the upper Wasatch confining unit and consists of an 8-ft section of sandstone at the base of the Wilkins Peak Member overlying a 135-ft section of shale and tuff in the Tipton Shale Member. Both members are in the Green River Formation. The oil-shale retort experiments were conducted within this aquifer. Most of this report is a discussion of ground-water flow and solute transport within the Tipton aquifer.

The Wilkins Peak confining unit overlies the Tipton aquifer and extends upward to the land surface. Much of this confining unit has been removed by erosion. The unit is about 120 ft thick at site 9. The Wilkins Peak confining unit does not yield water to wells with the exception of wells drilled near site 12. Wells at site 12 are open to the tuff of the Firehole Bed of the Wilkins Peak Member. The Firehole tuff throughout most of the study area has been removed by erosion.

Table 3. Open intervals and steady-state water-level altitudes for wells drilled in the Tipton aquifer, May 1982

Well number (used in figure 2)	Open interval (feet below top of Tipton aquifer)	Water-level altitude (feet above sea level)
1	24–65	6,286
2	65–143	6,327
3	8–65	6,255
4	0–10	6,228
5	8–53	6,256
6	8–49	6,253
7	9–64	6,248
8	2–65	6,226
9	7–65	6,238
10	8–65	6,237
11	5–65	6,226
12	7–65	6,234
13	10–58	6,246
14	4–65	6,236
15	8–65	6,238
16	5–81	6,225
17	18–143	6,284
18	6–99	6,236
19	24–92	6,256
20	3–112	6,236
21	13–139	6,270
22	11–120	6,257
23	8–120	6,255
24	24–127	6,258
25	0–135	6,257
26	2–143	6,223

Hydraulic Head

Water from wells open to the Tipton aquifer is derived from two sources: tuff or sandstone beds, and fractures in shale and marlstone. The quantity of water moving though unfractured shale and marlstone is very small by comparison. For purposes of solute transport, water in the shale and marlstone matrix can be treated as essentially static. Wells open to the 8-ft sandstone at the top of the aquifer have significantly greater yields than wells that are not open to this interval.

The hydraulic-head distribution within the Tipton aquifer indicates that flow within the aquifer is three dimensional. Water-level data from wells open to the Tipton aquifer must be interpreted in light of the vertical-head variation that exists within the aquifer. The open interval and water-level altitudes for wells drilled in the Tipton aquifer are listed in table 3. As indicated in this table, wells open to the Tipton aquifer rarely act as piezometers, and the altitudes of the measured water levels represent average heads for the open intervals.

Where the hydraulic head varies appreciably at different depths in the aquifer, as it does in the Tipton aquifer, a potentiometric surface is meaningful only if it describes the static head along a particular stratum of the aquifer. Therefore, potentiometric data in three dimensions are required to describe the distribution of head. Because there are few wells in the study area, the number of potentiometric maps that can be prepared is limited. The measured potentiometric surface for the interval 13 to 63 ft below the top of the Tipton aquifer is shown in figure 5. The retort chamber at site 9 is within this interval, and it causes a slight depression in the potentiometric surface, indicating that the resistance to vertical movement of water in the retort chamber is less than water in the surrounding undisturbed formation. The potentiometric surface shows that the retort chamber acts as a sink in the mapped interval. Water entering the retort chamber flows vertically upward through the overlying fractured shale into the 8-ft sandstone at the top of the aquifer.

A comparison of measured steady-state water-level altitudes with structure-contour maps of various horizons in the Tipton aquifer indicates that there are several areas where the rock is unsaturated. This feature is most common in the 8-ft sandstone at the top of the Tipton aquifer but also occurs in other beds of the aquifer. These unsaturated areas are delineated in figure 5. Limited test drilling confirms this interpretation.

Water-level changes were measured during and shortly after the operation of the retort at site 9. During the experiment (April 1976 through August 1976), the aquifer was dewatered by production wells drilled around the periphery of the retort chamber. Pumping rates varied over time and included water created as a byproduct of the retort process and water obtained from the aquifer. An average pumping rate of 45 ft^3/d was needed to dewater the retort chamber.

Ground water also was pumped from the aquifer while water-quality samples were obtained from observation wells. Based on discussions with LETC personnel concerning sampling procedures, estimates of the water quantity necessary for sampling were made. The quantity of water pumped for sampling purposes typically exceeded the quantity of water pumped to keep the retort chamber dewatered. Because of the large number of wells sampled for water-quality data, the limited accuracy of estimated pumpage, and the absence of unsampled observation wells, attempts to estimate the hydraulic conductivity and storage coefficient from measured water-level changes were not successful. Attempts to analyze water-level recovery after retorting ceased were also unsuccessful because sampling continued during the recovery period. Water levels in observation wells returned to steady-state levels throughout the study area by October 1976.

Figure 5. Steady-state potentiometric surface for interval 13 to 63 ft below top of the Tipton aquifer, May 1982.

Recharge and Discharge

The source of water recharging the Tipton aquifer is not known. Recharge may occur as precipitation on outcrops along White Mountain or as interformational leakage from the New Fork Tongue of the Wasatch Formation, which intertongues between the Tipton Shale and Wilkins Peak Members of the Green River Formation in the northern Green River basin. The New Fork Tongue thins from the north and is absent in the study area. Regardless of the source of water, the distance between recharge areas and the retort experiments is great.

Because of the distance between recharge areas and the retort experiments, all interpretations in this report use a boundary of specified hydraulic head along the upgradient side of the study area. The upgradient boundary of the study area has been placed 1,850 ft northeast of site 9 to ensure that the hydraulic head near the boundary is not affected by any transient stress.

Discharge from the Tipton aquifer occurs as seepage along outcrops higher than the Bitter Creek alluvial valley (fig. 5). The rate of seepage is not sufficient to permit measurement. Water is used by several species of phreatophytes that grow along these outcrops. The most common phreatophyte is greasewood (*Sarcobatus vermiculatus*). The U.S. Department of Agriculture (1954) described greasewood as very salt and alkali tolerant and stated that it usually grows in a fine-textured, relatively impermeable soil with high salinity, exchangeable sodium, and a shallow water table. This description fits the Tipton aquifer very well. In places where railroad cuts intersect the aquifer, salt deposits and minor seeps have been observed.

The Blaney–Criddle method, modified by Lenfest (1987), was used to estimate discharge from the Tipton aquifer to phreatophytes. The location and density of phreatophytes were mapped by field reconnaissance, and total discharge within the study area from the Tipton aquifer was estimated to be 0.14 ft^3/s. By distributing this flow rate uniformly among the permeable sandstone and tuff beds of the Tipton aquifer, the specific discharge from the 8-ft sandstone bed at the top of the aquifer was estimated to be 1.57 × 10^{-6} ft/s.

Cruff and Thompson (1967) compared several methods of estimating potential evapotranspiration with pan evaporation adjusted to equivalent lake evaporation. The results of this study showed that the evaporation calculated by the Blaney–Criddle method matches the adjusted pan evaporation reasonably well when the water supply to plants is not limited. The standard deviation of the difference between estimates was 9 percent of pan values.

Water Quality

Water from wells open to the Tipton aquifer is derived primarily from permeable beds of tuff and sandstone. The quality of well water is therefore representative of water in the permeable beds. However, molecular diffusion between water in permeable beds and nearly immobile water of the oil-shale matrix also affects measured water quality.

The three-dimensional ground-water flow pattern in the Tipton aquifer is reflected in the quality of water obtained from wells. In water samples taken prior to retorting, dissolved-solid concentration ranged from 12,000 to 19,000 mg/L, and virtually all the cations were sodium. The water samples generally have a pH between 9 and 11.5. The distribution of anions prior to retorting depends on the distance of the sampled interval above the aquifer base. Water obtained from wells that are open to deep intervals is predominantly a sodium chloride type. Water from shallow wells is a sodium bicarbonate type, possibly because of water dissolving bicarbonate from tuff beds as it moves upward from depth in the formation. The tuff beds show a dominance of dolomite and other carbonate minerals (Bradley, 1964). The sodium bicarbonate water might also result from the dissolution of trona and other evaporites.

A wide variety of chemicals have been observed in water produced during the retorting experiment (Fox and others, 1978). Particularly noteworthy are large concentrations of organic carbon and nitrogen; sulfur species; and trace constituents such as arsenic, boron, cyanide, and fluoride. Thiocyanate (SCN⁻) is of particular interest in this report. Leenheer and others (1981) stated that because thiocyanate is essentially nonreactive in the anaerobic environment of the Tipton aquifer and absent prior to retorting, it is an ideal candidate for a tracer of retort-plume migration.

Figure 6 shows the concentration of thiocyanate in water from wells sampled during December 1981, more than 5 years after the site 9 retort experiment. Two points are noteworthy in these data. First, it can be seen that the solute plume is moving within the top sandstone bed of the aquifer. Second, the solute plume has not completely flushed from the retort chamber. This incomplete flushing indicates that the retort chamber acted as a source of solute for some time after retorting. Because data are limited, no attempt has been made to contour thiocyanate concentrations as shown in figure 6.

MODEL OF GROUND-WATER FLOW

An understanding of the ground-water flow system is a necessary prerequisite to considering solute transport. Ground-water velocities, obtained by

Figure 6. Thiocyanate concentrations, December 1981.

modeling ground-water flow, are coefficients in the equation of solute transport. A theory of flow through fractured media was described by Snow (1969). He showed that many fracture-flow problems can be solved using an anisotropic hydraulic-conductivity tensor in conjunction with standard porous-media techniques. This approach can be used if fractures are sufficiently dense to act in a fashion similar to granular media.

Only a brief summary of the ground-water flow theory is presented here. Instead, emphasis is placed on systematically applying knowledge of the geology and hydrology of the study area to determine values of hydraulic conductivity and other model coefficients.

Theory

The basic governing equation for three-dimensional flow is

$$\frac{\partial}{\partial x_i} (K_{ij} \frac{\partial h}{\partial x_j}) + W = S \frac{\partial h}{\partial t} \qquad i, j = 1, 2, 3 \qquad (1)$$

where K_{ij} is the hydraulic-conductivity tensor, LT^{-1} (length/time),

W is the source-sink function, T^{-1},

S is the specific storage, L^{-1}, and

h is hydraulic head, L.

The source-sink term may be distributed areally or may be a point to represent a well. Boundary conditions that can be applied on the periphery of the problem include known specific discharge normal to the boundary and known head. The coefficients K_{ij}, W, and S are approximated by subdividing the region of interest into discrete zones and treating the coefficients as constants within each zone. This method gives rise to internal boundary conditions at zonal discontinuities. Along these boundaries, both head and specific discharge must remain unchanged as the boundary is crossed.

The finite-element method is used in this report to solve equation 1. Details of this method were discussed by Zienkiewicz (1971). Operational aspects of the finite-element method in three-dimensional flow problems were described by Gupta and Tanji (1976). The ground-water system within the Tipton aquifer is modeled under steady-state conditions (for reasons detailed in a later section), a process that is accomplished by setting specific storage in equation 1 to zero.

Direct measurement of all geohydrologic characteristics needed to construct a model of ground-water flow is not possible. As a result, values of model coefficients are adjusted until the difference between measured and calculated water levels is acceptable. During the course of most modeling studies, it becomes apparent that a number of alternate sets of model parameters produce solutions that fit measured head data almost equally well and that some parameters are determined more accurately than others. Cooley (1977) proposed a statistical regression procedure for estimating model parameters, testing model fit, and determining reliability and significance of the model and parameters.

The computer program used in this study (Glover, 1987) is an adaptation of the regression procedure of Cooley (1977) to the analysis of three-dimensional flow in steady-state ground-water systems. The set of optimal model parameters is defined as the set that minimizes the squared difference between measured and calculated hydraulic heads. If the finite- element form of equation 1 was substituted directly into the best-fit criterion, the resulting regression model would be nonlinear with respect to model parameters. Therefore, the finite-element equation is linearized by a Newton–Raphson technique, and the result is substituted. The resulting regression model is linear, but iteration is needed in order to obtain globally optimum estimates of model parameters.

Upon convergence, the regression procedure gives estimates of model parameters, standard errors of parameters, and the error variance of the correlation coefficient of the model. Estimated standard errors of parameters are measures of the range over which the respective parameters can be varied and produce solutions for the head distribution that are similar to the distribution obtained by using optimal estimates. The error variance of the model is the measure of overall goodness of fit. The correlation coefficient is the ratio of explained variation to total variation in hydraulic head. Results of the regression model can be used to construct joint confidence regions for model parameters, computed heads, and predicted heads. The method for constructing confidence regions was described by Cooley (1979). Joint confidence regions are measures of model reliability.

The regression model is based on a number of assumptions. In order to statistically analyze results of the regression model, it is assumed that differences between measured and calculated heads are uncorrelated with zero mean and constant variance. Although nonlinear, the model is assumed to behave in an approximately linear manner. Cooley (1979) presented methods for testing these assumptions, including analysis of residuals and calculation of the degree of nonlinearity of the regression model.

The relation between hydraulic head in the aquifer and the water level measured in a well open to part or all

of the aquifer is governed by aquifer properties, well-bore characteristics, and the vertical-head gradient within the aquifer. An accurate treatment of the relation would require solving the three-dimensional equation of ground-water flow in the close vicinity of the well bore. However, this approach is not practical. Instead, in this study, a relation based on the steady-state conservation of water within the well bore and Darcy's law is used. The result is a weighted average of hydraulic head over the open interval:

$$h_{int} = \frac{\int_{z_1}^{z_2} K_{ii} \, h \, dz}{\int_{z_1}^{z_2} K_{ii} \, dz} \qquad i = 1, 2 \qquad (2)$$

where h_{int} is depth-integrated head, L,

h is piezometric head within the aquifer, L,

z_2 is the upper limit of the open interval, L,

z_1 is the lower limit of the open interval, L, and

K_{ii} is hydraulic conductivity, LT^{-1}.

A derivation of equation 2 was given by Glover (1987). The depth-integrated head is directly comparable to measured water-level data. The regression technique of Cooley (1977) was modified by Glover (1987) to use depth-integrated head.

Application

To construct a model of ground-water flow, all coefficients and boundary conditions incorporated in equation 1 must be defined. The accuracy of these data has an important bearing on the reliability of the model results. Because the flow model of the Tipton aquifer uses the same numerical methods as other areal studies, similarities exist in the data requirements. Reports by Konikow (1977) and Robson and Saulnier (1981), describing other flow and transport models, discussed many of these requirements. Emphasis in this report is given only to those data requirements that are unusual because of the dual-porosity nature of oil- shale aquifers.

Because ground-water velocity is a coefficient in simulations of solute transport, the ground-water flow and solute-transport models of the Tipton aquifer must be operated over the same time period. The ideal time to start a simulation of solute transport is the moment oil and water production from the retort chamber stops, and the formation begins to resaturate with water. Mechanisms for transferring soluble material from retorted shale to formation water can then be simulated. Unfortunately, this approach requires the determination of numerous model coefficients related to mass transfer, the conversion from water-table to confined conditions,

and the variation of hydraulic conductivity because of a large range in temperature. Insufficient data were collected during and shortly after the retort experiment to accurately simulate either ground-water flow or solute transport during the flooding of the formation.

An alternative, practical approach to selecting an initial time for simulation was taken in this study. Simulation began when the ground-water flow system returned to steady-state conditions. (The justification for this simplified approach is given later.) During the course of the retort experiment, the retort chamber was dewatered by pumping. The hydraulic gradient and water-quality data collected from observation wells indicated that no contaminant escaped from the chamber during the experiment, although water produced from the chamber contained large concentrations of numerous chemical constituents. At the end of the retort experiment, dewatering was curtailed, and the retort chamber began to fill with water. However, prevailing hydraulic gradients toward the retort chamber continued to prevent transport of any contaminant outside the retort chamber. The quality of water from wells outside the chamber continued to approximate preretorting conditions, and solute concentration within the chamber remained large.

Water levels in observation wells approached steady-state values during the first week of October 1976; simultaneously, levels of solute concentration within the retort chamber declined, indicating that solute migration had begun. Figure 7 shows this trend for ammonia. For this reason, October 4, 1976, was selected as the starting date for solute- transport simulations. This starting date greatly simplified the development of a flow model because a single steady-state solution could be used throughout the simulation period.
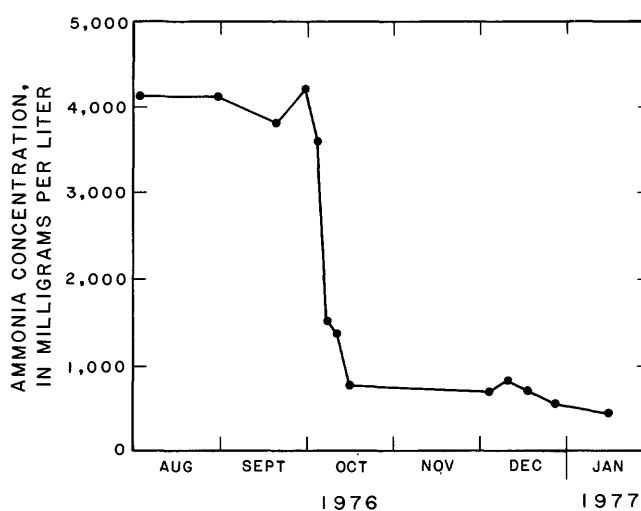

Figure 7. Ammonia concentration in water in well 11 completed in retort chamber, August 1976 to January 1977.

The finite-element method with isoparametric cubes was used in this study. Nodes were located at each corner of an element, and irregularly shaped cubes were used. This distortion in element shape allowed accurate modeling of aquifer geometry and permitted nodes to be placed at well locations. The element network consisted of four layers, including areas hydraulically downgradient from the retort operation where contaminant is likely to spread and areas upgradient to a distance hydraulically unaffected by the retort operation. In areas where the upper part of the Tipton aquifer is dry, the number of layers was reduced accordingly. The horizontal layout of elements is shown in figure 8; the vertical spacing of elements relative to aquifer lithology is shown in figure 9.

A variety of boundary conditions was used in the model of ground-water flow. The northeast boundary was treated as a specified-head condition. Values of hydraulic head were obtained from wells open to various intervals along this boundary. The boundary was oriented normal to the direction of flow. The northwest boundary and parts of the southeast boundary were treated as no-flow boundaries. Water-level data indicate that potentiometric contours for each layer are perpendicular to these boundaries. The base and top of the Tipton aquifer were also treated as no-flow barriers, for reasons discussed previously. Areas where the Tipton aquifer crops out were treated as specified discharge boundaries. Discharge was determined using the Blaney–Criddle method, as discussed previously, and was apportioned to each layer on the basis of relative thickness of permeable beds. The distributed rate of discharge is given in figure 9. Because the rate of discharge is reasonably accurate as estimated using the Blaney–Criddle method, it was not varied during model calibration.

Hydraulic Conductivity

Hydraulic conductivity throughout the model area was assessed by considering the relative distribution of permeable beds and fractures and applying the methods of Snow (1969). This assessment was useful in structuring the flow-model calibration, providing initial estimates of hydraulic conductivity that were subsequently improved during calibration, and in attaching a physical significance to the resultant estimates of hydraulic conductivity. The hydraulic conductivity of the sandstone section in the uppermost layer is probably horizontally isotropic because no fracturing is evident within the unit. The presence of bedding planes, however, indicated that vertical hydraulic conductivity is less than horizontal hydraulic conductivity.

As applied in this study, Snow's (1969) method for evaluating flow through fractured or dual-porosity media entailed several assumptions. Flow in an element of

aquifer occurs through permeable materials—tuffs and sandstones—and through fractures. Shale and oil shale are assumed sufficiently impermeable to be ignored. Each series of tuff beds or fractures is represented by a set of parallel plates. Equations are developed that describe flow along the plates. No flow occurs perpendicular to the plates. The principle of superposition is used to algebraically sum the flow contributed by each set of plates. The resulting expression is manipulated algebraically to give an estimate of hydraulic conductivity that is effective over an entire element of aquifer.

As discussed previously, vertical fractures within the Tipton aquifer are likely to be oriented at N. 40° E. (fig. 8). Designating this orientation as the y direction and treating the fracture system as a series of parallel conduits (fig. 10), one can write the Navier–Stokes equation for flow through fractures and equate it to Darcy's law, giving

$$Q_{fx} = 0$$

$$Q_{fy} = -\frac{2}{3}\frac{1}{\Delta}\frac{1}{n_f}\frac{g}{\nu}w_x w_z I_y \sum_{i=1}^{n_f}(b_i^*)^3 \tag{3}$$

and

$$Q_{fz} = -\frac{2}{3}\frac{1}{\Delta}\frac{1}{n_f}\frac{g}{\nu}w_x w_y I_z \sum_{i=1}^{n_f}(b_i^*)^3$$

where Q_{fx}, Q_{fy}, and Q_{fz} are flow in the x, y, and z directions through fractures in each element, $L^3 T^{-1}$ (cubic length/time);

Δ is the average fracture spacing, L;

n_f is the number of fractures per element;

g is the constant of gravitational acceleration, LT^{-2} ;

ν is the kinematic viscosity of the fluid, $L^2 T^{-1}$;

w_x, w_y, and w_z are element widths in the x, y, and z directions, L;

I_y and I_z are hydraulic-head gradients in the y and z directions, dimensionless; and

b_i^* is the half width of a single fracture, L.

Note that the flow in the x direction, normal to fractures, is zero.

The tuff and sandstone beds within the Tipton aquifer can be viewed as infinite, parallel conduits filled with permeable, granular material. Flow through an element with tuffs and sandstones of variable thickness can be estimated by
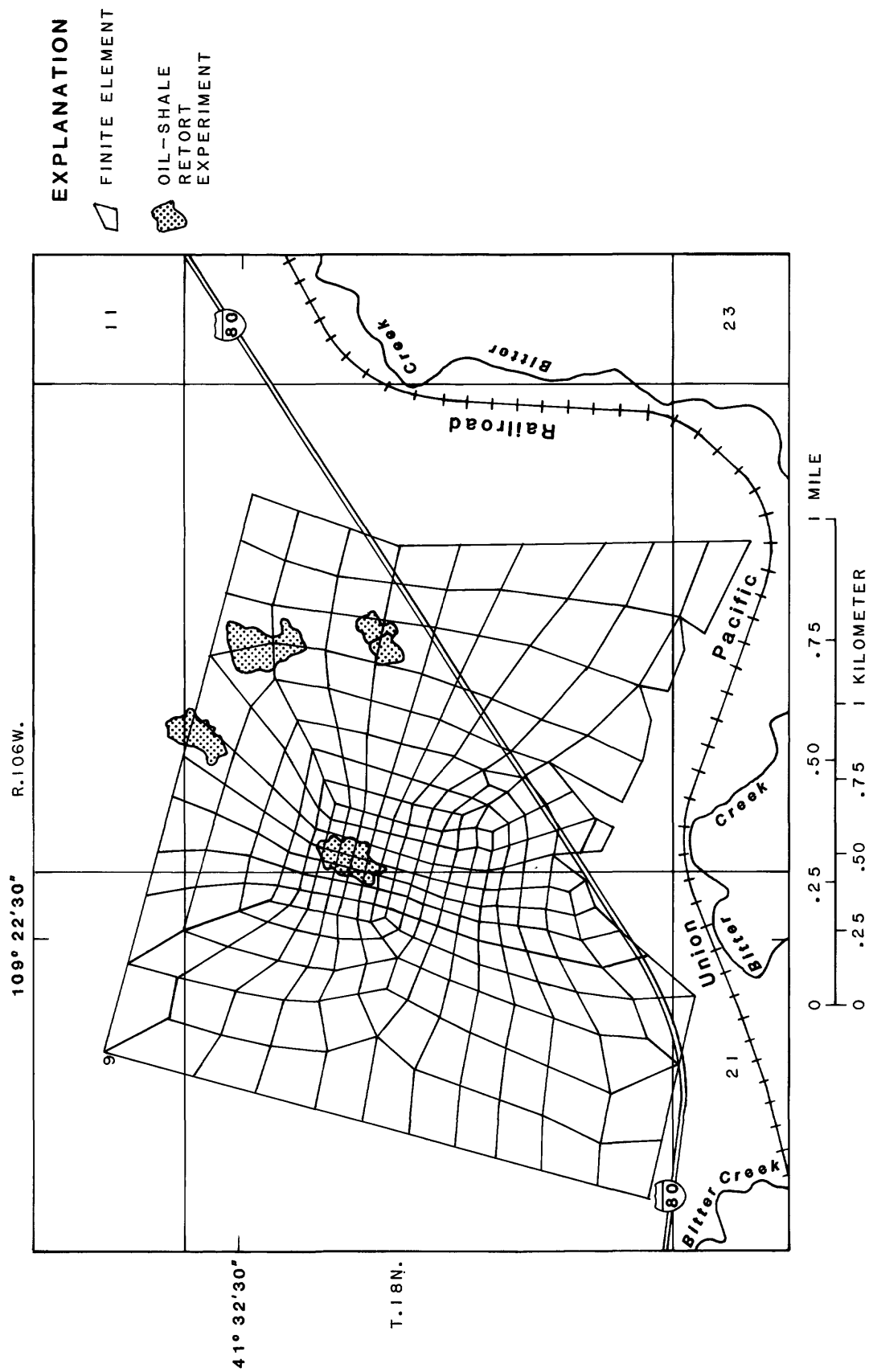
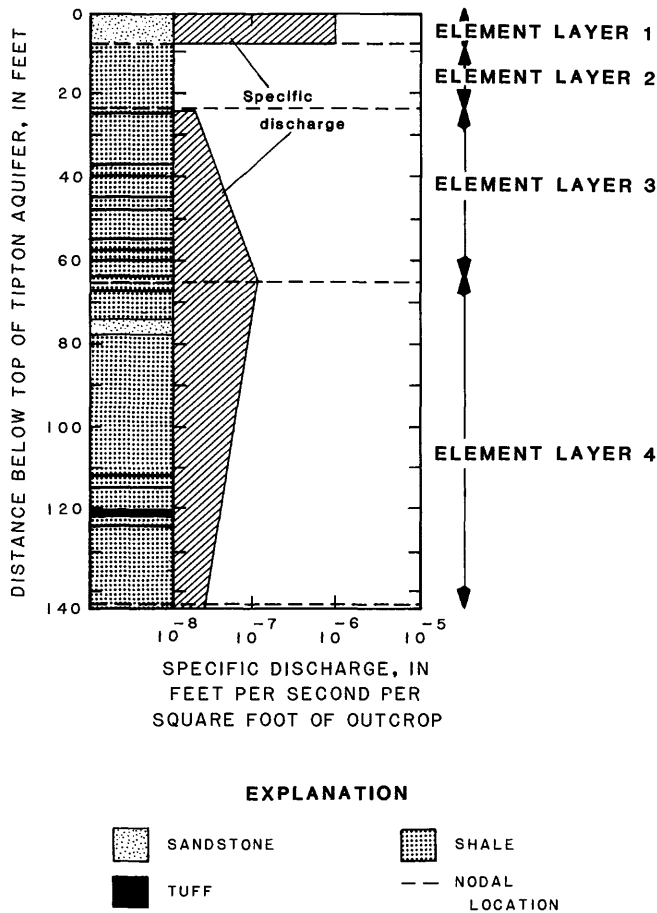**Figure 8.** Finite-element grid used to model study area.

Figure 9. Relation of lithology of Tipton aquifer to vertical spacing of model elements and estimated aquifer discharge.
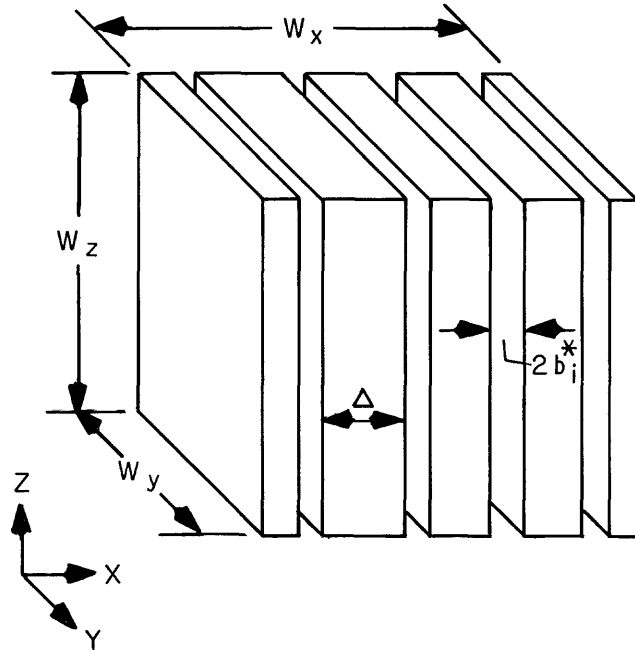

Figure 10. Solid volume cut by parallel-plate conduits.

$$Q_{tx} = -w_y \, K_t \, I_x \sum_{i=1}^{n} b_i$$

$$Q_{ty} = -w_x \, K_t \, I_y \sum_{i=1}^{n} b_i \qquad (4)$$

and

$$Q_{tz} = 0$$

where Q_{tx}, Q_{ty}, and Q_{tz} are flow in the x, y, and z directions through tuff and sandstone beds, $L^3 \, T^{-1}$;

w_x and w_y are element widths in the x and y directions, L;

K_t is the hydraulic conductivity of tuff and sandstone beds, LT^{-1};

I_x and I_y are the hydraulic-head gradients in the x and y directions, dimensionless; and

b_i is the thickness of a single tuff or sandstone bed, L.

Note that vertical flow between permeable beds is ignored and that the permeable beds are treated as isotropic media.

The total flow through an element is the vector sum of the contributions of individual conduits. From this superposition principle, it follows that

$$\bar{K}_x = K_t \, \frac{1}{w_z} \sum_{i=1}^{n} b_i$$

$$\bar{K}_y = K_t \frac{1}{w_z} \sum_{i=1}^{n} b_i + \frac{2}{3} \frac{1}{\Delta} \frac{1}{n_f} \frac{g}{v} \sum_{i=1}^{n_f} (b_i^*)^3 \qquad (5)$$

and

$$\bar{K}_z = \frac{2}{3} \frac{1}{\Delta} \frac{1}{n_f} \frac{g}{v} \sum_{i=1}^{n_f} (b_i^*)^3$$

where $\bar{K}_x$, $\bar{K}_y$, and $\bar{K}_z$ are effective hydraulic conductivity for an element of aquifer in the indicated direction. If evidence of additional fractures existed, then this information could be incorporated. Fractures other than those considered here undoubtedly do exist, but the frequency of fractures probably is small enough to be ignored. Although accurate values of $\bar{K}_x$, $\bar{K}_y$, and $\bar{K}_z$ cannot be determined from field data, the preceding analysis does give an indication of the degree of anisotropy that occurs within the study area.

Table 4. Estimates of hydraulic conductivity and standard errors for each zone used in model of the Tipton aquifer

| Zone | Hydraulic conductivity (feet per day) | | | Standard error (feet per day) | | |
| | Horizontal | | | Horizontal | | |
	N. 50° W.	N. 40° E.	Vertical	N. 50° W.	N. 40° E.	Vertical
1	19.4	19.4	4.30×10^{-4}	1.62	1.62	2.02×10^{-3}
2	0	4.30×10^{-5}	4.30×10^{-5}	0	1.47×10^{-4}	1.47×10^{-4}
3	0.432	0.432	4.30×10^{-7}	0.881	0.881	5.96×10^{-5}
4	.670	.670	1.72×10^{-5}	.475	.475	1.21×10^{-4}
Retort	.436	.436	4.30×10^{-3}	.881	.881	5.62×10^{-3}

The preceding discussion indicated that a rather simple zonal structure could be used to describe hydraulic conductivity. The lateral continuity of tuff beds and the uniform dip of the beds throughout the study area indicated that a single value could be used to describe either $\bar{K}_x$, $\bar{K}_y$, or $\bar{K}_z$ within each horizontal layer of elements. Therefore, zones were defined to coincide with element layers and were numbered consecutively from the top of the aquifer. The zonal numbering scheme in areas unaltered by retorting is shown in figure 9. In addition to the four zones shown in figure 9, a fifth zone was designated as elements at a depth of 24 to 65 ft below the top of the aquifer where hydraulic fracturing and oil-shale retorting significantly changed aquifer properties.

Calibration

Model calibration began with an initial estimate of hydraulic conductivity of 10 ft/d for permeable beds, an average fracture spacing of 5 ft, and an average fracture width of 0.25 in. Equations 5 were used to determine effective hydraulic conductivity for each model zone. Subsequent model runs using the regression technique of Cooley (1977) resulted in best- fit estimates of hydraulic conductivity for each zone given in table 4. The standard-error of estimate for hydraulic head for the calibrated model is 1.5 ft. The maximum deviation between calculated and measured hydraulic head is 2.1 ft and occurs at well 25. No trends were evident in the residuals. The correlation coefficient for the flow model is 0.998. The calculated head configuration along a line S. 15° W. is shown in figure 11. The vertical-head gradient in the upper 65 ft of the aquifer decreased near the retort chamber (1,800 ft from the northwest model boundary). The decreased gradient is the result of decreased resistance to upward movement within the fractured and retorted interval (from 24 to 65 ft below the top of the aquifer).

Estimates of hydraulic conductivity obtained by model calibration can be translated into physically meaningful values by using equations 5. Zone 4, with a total thickness of 78 ft, includes 7.8 ft of permeable tuff, sandstone, and limestone. Using the value of horizontal hydraulic conductivity in zone 4 (table 4) and equations 5, one can estimate the hydraulic conductivity of permeable material, K_t at 6.7 ft/d. In zone 3, K_t is estimated to be 8.1 ft/d. The difference in the two estimates might be due to differences in hydraulic conductivity of tuff beds and other permeable beds. Permeable siltstone and limestone make up a significant part of the permeable material in zone 4 and might have smaller hydraulic conductivity values than tuff beds. The total thickness of tuff in zone 2 is negligible. The horizontal hydraulic conductivity of the 8-ft sandstone at the top of the aquifer (zone 1) is estimated to be 19.4 ft/d. The extremely low values of vertical hydraulic conductivity indicate that open fracturing is not significant outside the retort chamber.

Model Reliability

In most studies of ground-water flow, the distribution of hydraulic head throughout the flow system is not known exactly. Accurate determination of recharge and discharge also is seldom possible. Because of these limitations, it is possible to use differing sets of hydraulic-conductivity estimates to develop several flow models that fit measured data equally well. Therefore, it is important to determine the reliability of any estimate made with a model. The regression method described by Cooley (1977) provides a framework for model development that permits evaluation of model reliability. This regression method was used during flow-model calibration.

The ability to use regression techniques in assessing model reliability is dependent upon the assumption that the model behaves in a linear manner with respect to calibration coefficients. In the present study, the flow model is nonlinear with respect to
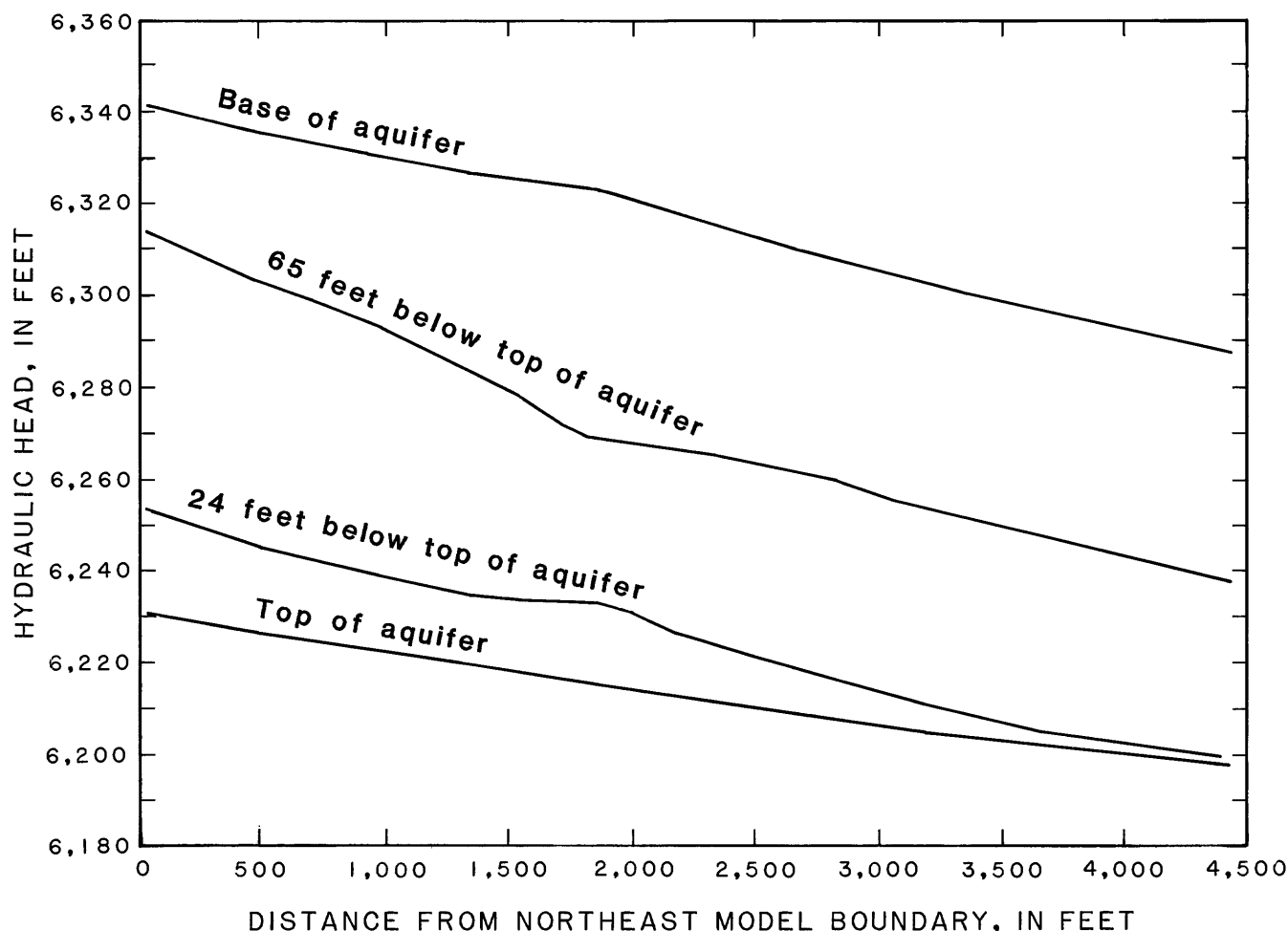
Figure 11. Calculated distribution of hydraulic head within the Tipton aquifer along a line S. 15° W.

hydraulic conductivity, and measures of reliability are only approximately correct. Nevertheless, the discussion that follows gives a useful indication of model reliability and sensitivity.

During model calibration, the rate of discharge was not varied, although it was recognized that the rate is only an estimate. This approach was taken because it is important to keep the number of calibration coefficients small in comparison to the number of measured water levels. The results of the discussion that follows are based on the premise that discharge is known precisely. Therefore, measures of reliability, such as standard errors, are probably low. These measures could be adjusted for error in the discharge estimate by adding the error variance of hydraulic conductivity and an assumed error variance of discharge.

Although the match between calculated and measured water levels is excellent, the standard errors for most estimates of hydraulic conductivity are large. The standard errors of estimated hydraulic conductivity for the flow model are listed in table 4. Large standard

errors relative to estimates of hydraulic conductivity indicate the extreme insensitivity of the solution to variations in hydraulic conductivity.

A precise estimate of horizontal hydraulic conductivity in zone 1 is important to the solute-transport analysis presented later in this report because the largest migration of contaminant from the retort chamber occurs in zone 1. As seen in table 4, the standard error of the hydraulic conductivity is small relative to the estimated horizontal hydraulic conductivity, indicating that coefficient is estimated precisely. If a value of 9 percent is assumed for the standard error of estimated discharge, in keeping with the results of Cruff and Thompson (1967), then the standard error for hydraulic conductivity in zone 1 increases to 2.4 ft/d.

Summary of Flow Model

The preceding sections show that a model of ground-water flow can be developed that accurately describes the flow system within the vicinity of an in-situ

oil-shale retort facility. Furthermore, the model can be calibrated in a physically meaningful fashion by considering detailed geologic and hydraulic data that are often neglected in basinwide studies. Data such as the distribution of thin, permeable beds or fractures may introduce an unmanageable degree of complexity to basinwide studies or may not be available for large parts of a basin. In site-specific studies, these data are usually available because the information is needed to properly design and operate an oil-shale retort. The smaller size of site- specific study areas permits the ready incorporation of detailed data in digital flow models. When these data are collected, they can be used to develop a physically meaningful structure for estimating hydraulic conductivity. Much of the curve matching that occurs in the process of calibrating flow models can be eliminated.

The model of ground-water flow at the LETC retort facility demonstrates some of the problems of site-specific studies. As with all flow models, accurate estimation of hydraulic conductivity and, therefore, ground-water velocity requires a knowledge of the amount of water flowing through the system. In this report, the estimate of discharge along outcrops of the Tipton aquifer is reliable. Water enters the model area along a specified head boundary, and other boundaries are modeled as no-flow barriers. It is not always possible to designate model boundaries that permit the accurate estimation of unknown model coefficients in site-specific studies.

MODEL OF SOLUTE TRANSPORT

Development of a solute-transport model began with a comparatively simple continuum model with few calibration parameters. A sophisticated fracture model, although theoretically correct for applications in oil-shale strata, has the disadvantage of requiring many calibration parameters. In field problems with limited water-quality data, it may be possible to obtain multiple sets of parameter estimates that match measured solute concentrations. The accuracy of predictions with a fracture model may be no better than predictions with a continuum model. The approach taken in developing a solute-transport model for the current study was to calibrate a continuum model, observe deficiencies in the model, and use these observations as a basis for extending the model to more complex solute- transport mechanisms.

A number of models have been suggested for use in studies of ground- water flow and solute transport in oil shale. The most widely used models employ a continuum approach. Robson and Saulnier (1981) provided an example of a study using a continuum model. In this approach, the fractured oil shale is represented by

a corresponding granular, porous medium that acts in a hydraulically similar fashion to the actual ground-water system. This approach may be proper if the fracture spacing is reasonably dense and typically requires the estimation of a minimum number of aquifer properties. The theoretical basis is weak for applying a continuum model to solute transport in fractured media.

Continuum Approach

The transport of a conservative solute in ground water is described by

$$\frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i} (c_i q_i) = \phi \frac{\partial c}{\partial t} - Wc^* \quad i,j = 1,2,3 \quad (6)$$

where D_{ij} is the hydrodynamic-dispersion coefficient, $L^2 T^{-1}$ (square length/time);
ϕ is porosity, dimensionless;
$q_i = -K_i (\partial h/\partial x_i)$ is the Darcian fluid velocity, LT^{-1};
W is a source-sink term, T^{-1};
c is solute concentration, ML^{-3} (mass/cubic length); and
c^* is solute concentration of a fluid source, ML^{-3}.
With a continuum model, it is assumed that the oil shale is hydraulically similar to porous, granular material. The hydrodynamic-dispersion coefficient is related to fluid velocity by

$$D_{ij} = a_{ijmn} \frac{q_m q_n}{|q|} \quad i,j,m,n = 1,2,3$$

where a_{ijmn} is the dispersivity of the aquifer, L;
q_m and q_n are fluid velocity, LT^{-1}; and
$|q|$ is the magnitude of the velocity vector, LT^{-1}.
For isotropic media,
a_{iiii} is α_L, longitudinal dispersivity, L,
$i = 1,2,3$;
a_{iijj} is α_T, transverse dispersivity, L,
$i,j = 1,2,3$;
a_{ijij} is $\frac{1}{2} (\alpha_L - \alpha_T)$ $i,j = 1,2,3$
All other components of dispersivity equal zero.

The form of the transport equation used in this study (equation 6) was also used by Pinder and Gray (1977) and Bibby (1981). Konikow (1977) and most studies of solute transport by the U.S. Geological Survey used a form of equation 6 that is obtained by dividing the equation by porosity and defining the hydrodynamic-dispersion coefficient in terms of interstitial fluid velocity. Either form of the equation can be used successfully; however, when comparing results, one should recognize

that the hydrodynamic- dispersion coefficient of the two equations will differ by the magnitude of porosity. The advantage of using equation 6 as written is that sensitivity coefficients—the rate of change of concentration per unit change in aquifer properties—are easily calculated.

Galerkin's method of weighted residuals with iso-parametric finite elements was used in this study to solve equation 6. The same finite-element grid was used to simulate ground-water flow and solute transport. Details of the finite-element method applied to solute-transport problems can be obtained from Bibby (1981) or Pinder and Gray (1977). The addition of upstream weighting functions in formulating the finite-element solution was described by Noorishad and Mehran (1982). This technique has permitted the accurate simulation of solute transport when such transport is dominated by advection.

The solute concentration of water in a well is related to the solute concentration in the aquifer by the three-dimensional equation of solute transport. It is not practical to solve this problem at each well bore. Assuming steady-state conservation of solute and using Darcy's law, one can obtain a simplified expression:

$$c_{int} = \frac{\int_{z_3}^{z_4} cq_i \, dz}{\int_{z_3}^{z_4} q_i \, dz} \qquad i = 1, 2 \qquad (7)$$

where c_{int} is the depth-integrated solute concentration, ML^{-3};

c is the solute concentration along the well bore, ML^{-3};

z_3 to z_4 is the segment of the well bore where water enters, L; and

q_i is the Darcian velocity K_{ii} $(h-h_{int})$ with dimensions, T^{-1}.

Equation 7 is used to determine the concentration of solute in the well segment, z_3 to z_4.

Initial Conditions

For reasons discussed previously, simulation of solute transport began with solute concentrations observed on October 4, 1976. This beginning date for simulation coincided with a return to steady-state conditions of ground-water flow and marked the beginning of observed solute migration from the retort chamber. Thiocyanate (SCN⁻) was used as a conservative tracer in this modeling study. Leenheer and others (1981) presented evidence that thiocyanate is nonreactive in the anaerobic environment of the Tipton aquifer. Thiocyanate was essentially absent from the ground-water system prior to retorting.

Negligible thiocyanate data are available for the period during and immediately after the retort experiment. Various concentrations of thiocyanate have been reported for site 9 production water ranging from 75 mg/L (Stuber and others, 1978) to 123 mg/L (Fox and others, 1978), but the mean value is probably near 80 mg/L (Leenheer and others, 1981). Stuber and others (1978) also noted that the ratio of the concentration of thiocyanate to the concentration of ammonia in water within the retort chamber remained constant from the time of the retort experiment to October 1977, one year later. No explanation for this observation was given, but it seems reasonable that ammonia acted as a conservative ion during this period. Because the principal mechanism for removing ammonia from retort water is believed to be cation exchange, it may be inferred that all exchange sites within the retort chamber were occupied during the retort experiment. It is unlikely that ammonia would remain conservative outside the retort chamber. Because extensive ammonia data were collected by LETC during and shortly after the retort experiment, the ratio of ammonia to thiocyanate was used to determine an initial thiocyanate concentration of 78 mg/L. Outside the retort chamber a concentration of 0.00 mg/L is assumed.

A knowledge of initial solute concentration within the retort chamber is not sufficient information to ensure a unique set of estimates for calibration parameters. The mass of the solute must be known. The volume of retorted oil shale at site 9 was known (Lawlor and others, 1979), but the porosity of the chamber was not determined prior to calibrating a solute- transport model. Therefore, it was recognized early in the calibration process that no unique set of parameter estimates would be obtained.

The continuum approach allowed a relatively small number of aquifer properties to be estimated during model calibration. In addition to ground- water velocity and, therefore, hydraulic conductivity, aquifer properties considered during calibration were the dispersivity and porosity of the top sandstone strata and the porosity of oil shale in and adjacent to the retort chamber. Because adequate data are not available to determine unique values of dispersivity for both oil shale and sandstone, a single value of longitudinal dispersivity was used throughout the Tipton aquifer. A single value of transverse dispersivity was also treated as a calibration parameter.

Initial estimates of hydraulic conductivity were obtained from the flow-model calibration. The uncertainty in these estimates is related to the standard errors of estimated hydraulic conductivity given in table 4. Before calibration of a solute-transport model began, it was recognized that varying hydraulic conductivity, as well as porosity and dispersivity, would introduce more parameters to the calibration process than could be

identified successfully with the limited water-quality data. Therefore, hydraulic-conductivity estimates during the transport-model calibration were set equal to values given in table 3.

Field data are not available to determine porosity in the study area, but initial estimates can be established. Morris and Johnson (1967) indicated that sandstone and siltstone typically have a porosity of 35 percent. The presence of cementing materials and compaction tends to reduce porosity, whereas fractures and solution channels increase the amount of void space. Initial estimates of porosity were derived by considering the thickness of permeable to impermeable strata in each elemental layer. A porosity value of 35 percent was assigned to permeable strata, but the effective porosity of impermeable strata was 0 percent.

Calibration

The simulation of solute migration in the Tipton aquifer began with thiocyanate concentrations measured in October 1976 and continued until December 1981 when thiocyanate data were collected in wells hydraulically downgradient of site 9. No thiocyanate data were collected during the intervening years except those samples described by Stuber and others (1978) that were taken from wells within the retort chamber. Therefore, model calibration consisted of matching calculated thiocyanate concentrations to December 1981 data.

A trial-and-error calibration of the continuum model resulted in the calculated thiocyanate concentrations shown in figure 12. In general, the difference between calculated and measured thiocyanate concentrations is small (fig. 12). During the early time steps of the simulation, solute moved vertically upward from the retort chamber to the top sandstone bed of the aquifer. Horizontal Darcy velocity within the retort chamber was 5.5 ft/d, and vertical Darcy velocity was estimated to be 3.8 ft/d. In the undisturbed oil shale outside the retort chamber, the vertical velocity was estimated to be approximately four orders of magnitude less than the horizontal velocity. Because of the short vertical distance from the retort chamber to the permeable sandstone strata, virtually all solute migrated from the retort chamber into the sandstone within a horizontal distance of 400 ft. Solute migration within the sandstone was predominantly horizontal.

Calibration of the continuum model improved initial estimates of porosity and dispersivity in the retort chamber and the top sandstone unit of the aquifer but had no effect on estimates of these aquifer properties in other zones. This result was entirely expected because thiocyanate migration occurred primarily in the top sandstone unit of the Tipton aquifer. The optimal match between calculated and measured thiocyanate (fig. 12)

was obtained using a sandstone porosity of 12 percent and a retort-chamber porosity of 31 percent. The calibrated value of sandstone porosity is approximately three times smaller than initially estimated. This reduction probably reflects the large amount of cementing material present in the sandstone. The calibrated estimate of longitudinal dispersivity is 50 ft, and transverse dispersivity within the sandstone is estimated to be 30 ft.

It must be emphasized that the estimates of porosity and dispersivity are contingent upon the assumption that hydraulic-conductivity estimates given in table 3 are accurate. As indicated previously, uncertainty is associated with the hydraulic-conductivity estimates, but limited water-quality data have precluded any refinement of these estimates during transport-model calibration. Therefore, it must be recognized that any difference between hydraulic-conductivity estimates obtained while calibrating the flow model and actual hydraulic-conductivity values will cause corresponding errors in the porosity and dispersivity estimates given earlier.

Sensitivity Analysis

The fact that a good match of calculated thiocyanate concentrations to measured data was possible using the estimates of aquifer properties given previously does not ensure that these estimates are correct. It is possible that a second set of values for aquifer properties would give an equally acceptable match. This problem of uniqueness was investigated by arbitrarily varying porosity and dispersivity from calibrated values and observing the resulting lack of fit in thiocyanate concentrations calculated by the model. Although hydraulic conductivity was not varied during model calibration, a limited-sensitivity analysis was performed. The conclusions of this sensitivity analysis follow.

Varying the values of porosity for rocks within the retort chamber had a pronounced effect on calculated solute concentrations. Augmenting porosity within the retort chamber increased the thiocyanate present in the aquifer at the beginning of the simulation. Although it was possible to adjust sandstone porosity and dispersivity to successfully match the leading edge of the solute plume to observed concentrations, the change in thiocyanate mass caused a poor fit in the trailing section of the plume. Maintaining sandstone porosity and dispersivity at calibrated values and increasing retort-chamber porosity rapidly decreased the distance that the solute traveled during the course of the simulation.

The porosity of sandstone within the Tipton aquifer is also well defined by the calibrated value of 12 percent. Increasing sandstone porosity from the calibrated value decreased the distance the solute plume migrated during
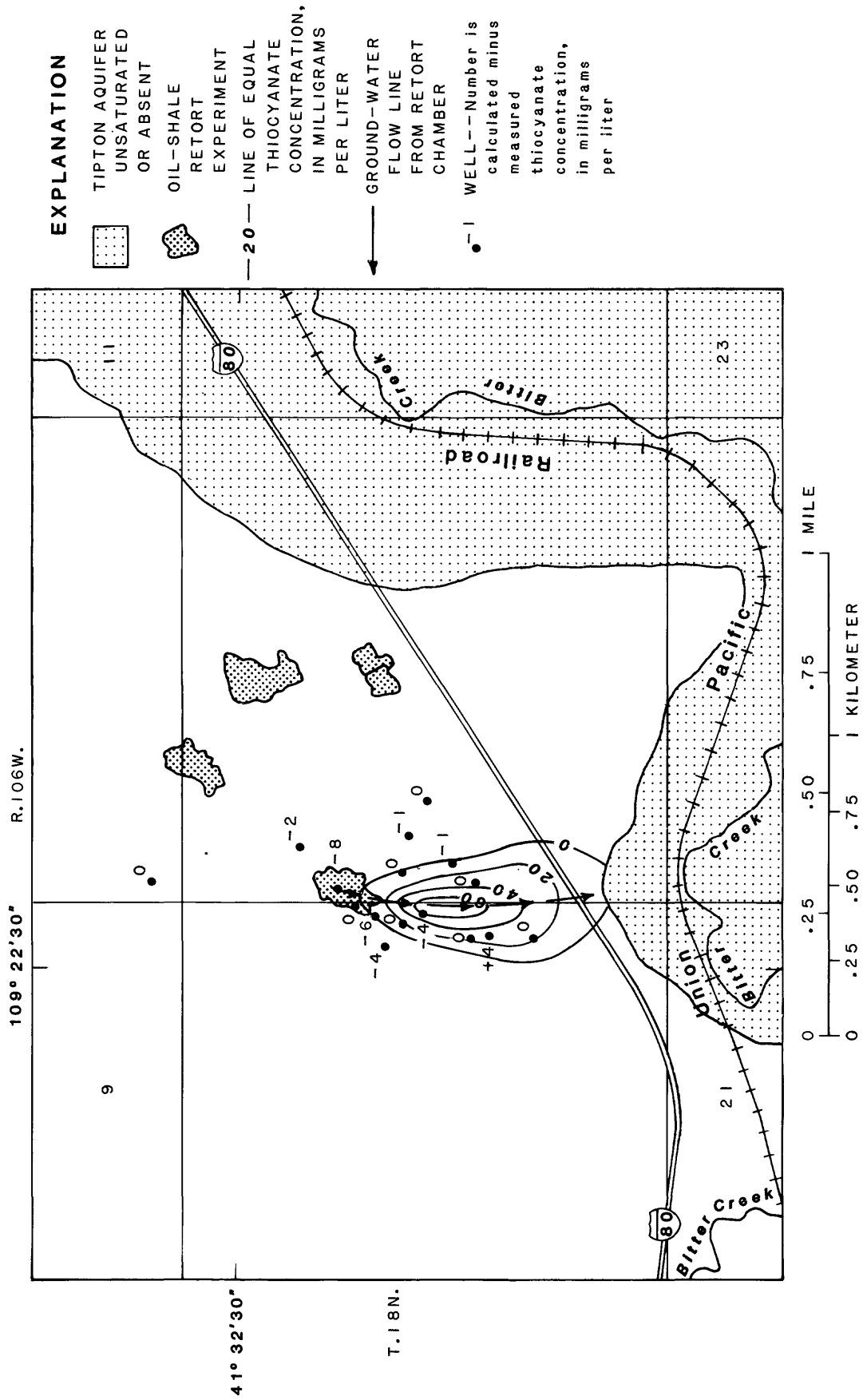
Figure 12. Thiocyanate concentration calculated by continuum model for top sandstone unit of the Tipton aquifer, December 1981.

the course of the simulation. The match between calculated and measured concentrations of thiocyanate became unacceptable for changes in sandstone porosity of 2 percent or more. Adjusting dispersivity and retort-chamber porosity did little to improve the match.

Longitudinal and transverse dispersivities of the Tipton aquifer are not as well defined as aquifer porosities. Of the two dispersivity parameters, longitudinal dispersivity is probably more precisely determined. Small decreases in longitudinal or transverse dispersivity were translated into a significant lack of fit between calculated and measured thiocyanate concentrations. However, a reasonable fit was possible by simultaneously increasing longitudinal dispersivity and decreasing transverse dispersivity. Increasing longitudinal dispersivity from the calibrated value of 50 ft to a value greater than 200 ft is probably unrealistic. Drilling and sampling additional wells located both along and perpendicular to the principal flow line of the solute plume would aid in precisely determining dispersivity.

The sensitivity analysis of hydraulic conductivity was of limited use in assessing uncertainty in the transport model. The lack of solute migration within the lower strata of the Tipton aquifer kept the model relatively insensitive to variations in hydraulic conductivity in these strata. Varying the hydraulic conductivity in zone 2 within a range of reasonable values, as indicated by table 4, also had little effect on calculated solute concentrations. Variations in hydraulic conductivity of the sandstone had pronounced effects on calculated solute concentration, similar to the effect of varying sandstone porosity.

The calibration of a solute-transport model showed two weaknesses in the continuum approach. First, although the match of calculated to measured thiocyanate concentrations obtained during calibration was generally good, the estimate of fracture porosity within the retort chamber appears to be large. Utilizing a dual-porosity model that explicitly accounts for porosity of fractures and porosity of the shale matrix might produce a reasonable calibration when using realistic porosity values. A discussion of the dual-porosity approach is given later in this report.

A second weakness in the continuum model resulted in consistently underestimating thiocyanate concentrations in the trailing part of the solute plume. The underestimates are probably the result of slightly underjudging the mass of solute present in the system. Increasing retort-chamber porosity cannot correct this problem without sacrificing accuracy in calculating the solute concentration of the leading part of the plume. One possible mechanism for introducing additional solute in the trailing part of the plume is mass transfer. This mechanism is discussed in the next section.

Mass-Transfer Mechanism

The continuum model of solute transport described in the previous sections consistently underestimated the thiocyanate concentration in the trailing part of the solute plume. This behavior was observed with the optimal set of aquifer-property estimates and indicates that the mass of solute in the continuum model was underestimated. An extension of the continuum model was needed that would contribute additional thiocyanate to the trailing part of the solute plume without adding mass to the leading part.

Hall (1982) performed leaching experiments with columns of retorted oil shale and observed a similar increase in mass in the trailing part of solute plumes. He explained the increase with the mass-transfer expression

$$Wc^* = K^*A\,(c_e - c) \tag{8}$$

where K^* is the mass-transfer coefficient, $L^{-2}T^{-1}$;
A is the area of water-shale interface, L^2;
c_e is the phase equilibrium concentration, ML^{-3}; and
c is the solute concentration, ML^{-3}.

This equation acts as a source term to the solute-transport equation (equation 6) and, according to Hall (1982), becomes the dominant mechanism for leaching of retorted oil shale after the passage of two to three pore volumes of water. Although Hall (1982) was unable to provide a good theoretical basis for equation 8, he did hypothesize that the mass-transfer mechanism involves the release of solute by slow dissolution of the mineral matrix from pore walls and the subsequent diffusion of solute within the nearly immobile water of the shale matrix toward fractures.

The use of this particular empirical equation to describe mass transfer essentially provides an infinite source of solute to the medium where in reality such a source is finite. Although it may be possible to estimate the coefficients in equation 8 through a calibration procedure, the resultant transport model may not be more reliable. An effort was made to calibrate the transport model using equation 8. Although it was possible throughout the study to minimize errors in calculated solute concentrations, there was no way to determine whether estimates of coefficients in equation 8 were reasonable. For this reason, no further discussion of the mass-transfer mechanism is included in this report. However, it is reasonable to conclude that the retort chamber will continue to act as a source of solute for some unknown time.

Dual-Porosity Approach

The solute-transport model described in this report is capable of simulating measured concentrations of

thiocyanate without the addition of sophisticated modeling techniques. This capability may be closely related to the scarcity of wells intercepting the solute plume. It may also be the result of solute migration occurring primarily in a sandstone bed, with movement in fractured media occurring only for a short time. However, the large value of retort-chamber porosity used in the simulation (31 percent) is probably unrealistic. A more reasonable approach is to partition the initial mass of solute between water in fractures and water in the shale matrix. Diffusion is used as a driving force to move solute from the relatively immobile water of the shale matrix to the fractures. The importance of such a dual-porosity approach increases if solute migration occurs in fractured strata. A number of dual-porosity models have been developed, including those described by Grisak and Pickens (1980), Bibby (1981), Noorishad and Mehran (1982), and Huyakorn and others (1983). Glover (1987) has synthesized features from several of these models into a computer program for simulating solute transport in oil shale.

A large number of coefficients must be known for even relatively simple fracture geometries if dual-porosity models are to be applied to field problems. Because in most studies these coefficients must be estimated during model development, the amount of water-quality data needed to calibrate a dual-porosity model is far greater than the amount needed to use a continuum model. Sufficient data are not available in the LETC study area to use a dual-porosity model. The short distance that the solute moved through fractured oil shale also minimizes the need to use the more complex model. However, in studies where solute migration does occur in fractured media, calibration of a continuum model can result in overestimating hydrodynamic dispersion and fracture porosity. Although the calibration of a continuum model in fractured media may successfully simulate measured water quality, the effects of incorrectly estimating aquifer properties can be severe in predictions of solute migration.

Predictive Capability

The extent to which any solute-transport model can be used to predict the future position and concentration of a solute plume is directly related to the accuracy of estimated aquifer properties and the amount of error introduced by any simplifying assumptions used in developing the model. A test of the predictive capability of a model is possible by comparing an independent set of water-quality data to simulated concentrations using calibrated estimates of aquifer properties. This test, often called model verification, can only be performed in the LETC study area to a limited degree. All reliable water-quality data were used to calibrate the model.

Nevertheless, predictions can be made with the solute-transport model. The results of the predictive analysis must be used with care because of the lack of model verification.

The principal concern of solute migration from oil-shale retorts is the possibility of contaminating water supplies. To this end, a simulation was made to determine the thiocyanate concentration of ground water discharging from the Tipton aquifer. The major discharge point is shown in figure 12 as the intersection of the mapped flow path with the outcrop area. Figure 13 shows the predicted concentration of thiocyanate at this discharge point as a function of time.

The peak concentration of thiocyanate in water discharging from the top sandstone unit of the Tipton aquifer was predicted to be about 45 mg/L. This reduction from the initial concentration of 78 mg/L was the result of hydrodynamic dispersion. The peak thiocyanate concentration occurred during 1985. No results are presented for the trailing part of the solute plume because of the poor match between calculated and measured solute concentrations that occurred during model calibration. Water discharging from the Tipton aquifer either evaporates or is used by plants. No direct runoff of ground water occurs, but salts left behind by evaporating water may be transported by surface water during periods of intense rainfall. The breakthrough curve for other chemicals may lag behind the curve shown for thiocyanate because of various geochemical reactions. Reactions such as adsorption or ion exchange may prevent some chemical species from ever discharging from the ground-water system.

Measurable concentrations of thiocyanate at discharge points during 1983 and 1984 are shown in figure 13. Unfortunately, attempts to collect samples of evaporative salts were unsuccessful because of the combined effects of small discharge rates, dilution by
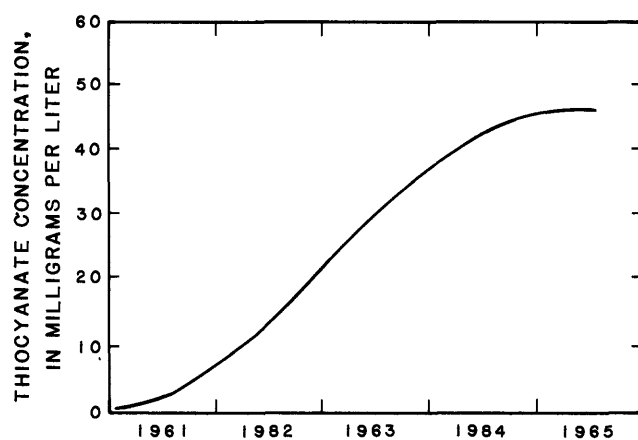
Figure 13. Predicted thiocyanate concentration in water discharging from sandstone unit of the Tipton aquifer, SW¼ SW¼ SW¼ sec. 15, T. 18 N., R. 106 W., Sweetwater County, Wyo.

surface water, and consumptive use by phreatophytes. Dark water, indicative of an oil-shale retort plume, was observed during May 1983 in the discharge area. However, this ponded water, having been diluted by extensive rainfall during April and May 1983, rendered chemical analysis of the water quantitatively meaningless. Nevertheless, the presence of black retort water in the discharge area provides some qualitative verification of the prediction. Attempts to collect salt samples in the discharge area during 1984 were unsuccessful because frequent rainfall prevented the accumulation of salt.

SUMMARY AND CONCLUSIONS

Hydrologic studies of the LETC oil-shale retorts near Rock Springs, Wyo., provided an opportunity to evaluate the importance of various investigative techniques before extensive oil-shale development occurs. This report describes the use of digital modeling techniques to predict the migration of solute from a retort chamber. The prediction is considered reasonable because water-quality data were available to calibrate the solute-transport model. However, a more common situation occurs during the planning stages of a retort facility when the hydrologist is forced to predict both the direction and rate of solute migration before development begins. Plans to minimize any hydrologic impacts can then be formed. Although water-quality models have been developed on a basinwide scale (Robson and Saulnier, 1981), solute migration on a site-specific scale can vary significantly from what might be predicted basinwide. This report provides information on the relative importance of many geohydrologic factors that influence solute transport in oil shale.

The most important conclusion to be drawn from the study is that detailed geologic information such as the location and thickness of thin, porous beds can be incorporated successfully in site-specific digital models. This conclusion is particularly useful if the sampled intervals of observation wells are accurately placed within this geologic framework. If geologic data are not considered in detail, models will be poorly calibrated or incorrectly used. Fortunately, such data can be obtained by test drilling and geophysical logging prior to retorting, and therefore can be used during the planning stages. Solute migration in the LETC study area occurs primarily in thin, permeable beds rather than the oil-shale strata. Because of this behavior, solute traveled far greater distances than might otherwise have been expected. Also, movement in permeable beds minimized the need to use dual-porosity models or consider shale-matrix diffusion.

With hydraulic conductivity calculated from a flow model and porosity obtained from a table of typical values, the estimated migration rate for thiocyanate is approximately three times slower than the observed migration rate. The calibration of a solute-transport model was possible only after sandstone porosity was reduced from 35 to 12 percent. This result points to the need for field determinations of porosity during the planning stages of an oil-shale retort facility. It also points to the need for water-quality monitoring after retorting stops.

It is worth noting that a small amount of dispersion is predicted to occur while solute migrates from the retort chamber. The concentration of thiocyanate is predicted to decrease only by a factor of two as far as ½ mile from the retort chamber. Robson and Saulnier (1981) also concluded that dispersivity coefficients for the Green River Formation in the Piceance basin of Colorado are small. Therefore, solute-transport models developed during the planning stages of future oil-shale retorts may be more accurate if dispersivity coefficients are assumed to be small or zero. One advantage of a site-specific model as described in this report is the ability to minimize undesirable numerical dispersion that can occur in regional models.

Fractures, solution channels, and other sources of secondary porosity were not a significant factor in the LETC study area. The importance of secondary porosity in other oil-shale areas must be assessed on a site-by-site basis. Nevertheless, the lithology of the Tipton Shale Member of the Green River Formation with oil shale having thin, interbedded tuff corresponds conceptually to a set of parallel, horizontal fractures. The flow model of the Tipton aquifer was calibrated by incorporating a hydraulic-conductivity structure that corresponds to anisotropic, fractured flow systems. This calibration resulted in hydraulic-conductivity estimates that were physically meaningful. The approach used in this study to calibrate a model of ground-water flow is widely applicable to other oil-shale areas.

Another useful observation is that solute migration did not occur after retorting until ground-water levels represented steady-state conditions. In the LETC study, this progression eliminated the need to consider mechanisms for transferring solute from rock to water as the abandoned retort chamber saturated. It also permitted the use of a steady-state model of ground-water flow to determine seepage velocities. The calibration of a site-specific flow model of the undisturbed ground-water system, therefore, is useful in predicting solute migration from planned retort facilities. The calibrated model can be used to determine the direction of solute movement by assuming various hydraulic-conductivity values for the planned retort chamber. If reasonable estimates of aquifer porosity and dispersivity are available, it also may be possible to predict rates of solute movement. Conservative estimates

of solute migration could be made by using large values of retort-chamber porosity and small values of undisturbed formation porosity and dispersivity.

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