LEACHATE MIGRATION FROM AN IN SITU OIL-SHALE RETORT NEAR ROCK SPRINGS, WYOMING

U.S. GEOLOGICAL SURVEY

OPEN-FILE REPORT 85-575

Fw aval.

ocli 11/19/86

U.S. DEPARTMENT OF THE INTERIOR
March 3, 1849

LEACHATE MIGRATION FROM AN IN SITU OIL-SHALE RETORT NEAR ROCK SPRINGS, WYOMING

By Kent C. Glover

U.S. GEOLOGICAL SURVEY

OPEN-FILE REPORT 85-575

Cheyenne, Wyoming
1986

DEPARTMENT OF THE INTERIOR

DONALD PAUL HODEL, SECRETARY

U.S. GEOLOGICAL SURVEY

Dallas L. Peck, Director

For additional information
write to:

District Chief
U.S. Geological Survey, WRD
2120 Capitol Avenue
P.O. Box 1125
Cheyenne, WY 82003

This report may be purchased
from:

U.S. Geological Survey
Books and Open-File Reports
Federal Center, Building 41
Box 25425
Denver, CO 80225
(Telephone: (303) 234-7476)

CONTENTS

FIGURES

TABLES

CONVERSION FACTORS

For those readers interested in using the International System of Units (SI), the following table may be used to convert 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

LEACHATE MIGRATION FROM AN IN SITU OIL-SHALE RETORT NEAR ROCK SPRINGS, WYOMING

By Kent C. Glover

ABSTRACT

Hydrogeologic factors influencing leachate movement from an in situ oil-shale retort near Rock Springs, Wyoming, were investigated by developing models of ground-water flow and solute transport. Leachate, indicated by the conservative ion thiocyanate, has been observed one-half 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 thiochanate--45 milligrams per liter or approximately one half the initial concentration of retort water--were 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 may introduce an unmanagable degree of complexity to basin-wide studies but can be incorporated readily in site-specific models. Solute migration in the study area primarily occurs 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 basin-wide 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 can not be determined prior to modeling, the hydraulic conductivity and ground-water velocity will be estimated poorly.

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 and could result in degradation of ground-water quality both within and adjacent to the retort sites. The in situ retorting process begins by fracturing 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 are also 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 may transfer from the burnt shale to the water. This 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 developed for use in rock such as oil shale in which permeability and porosity result from fracturing. To solve this shortcoming, a number of models have been developed in the last few years for use in fractured media. However, few in situ 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, in situ retorting facility operated by the Laramie Energy Technology Center (LETC) near Rock Springs, Wyoming (fig. 1) provides an opportunity to investigate changes in ground-water quality after the retorting of oil shale. This facility was active from 1969 through 1979, and adequate time has elapsed to permit significant migration of solute. 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 are 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 transferred to other oil-shale basins.

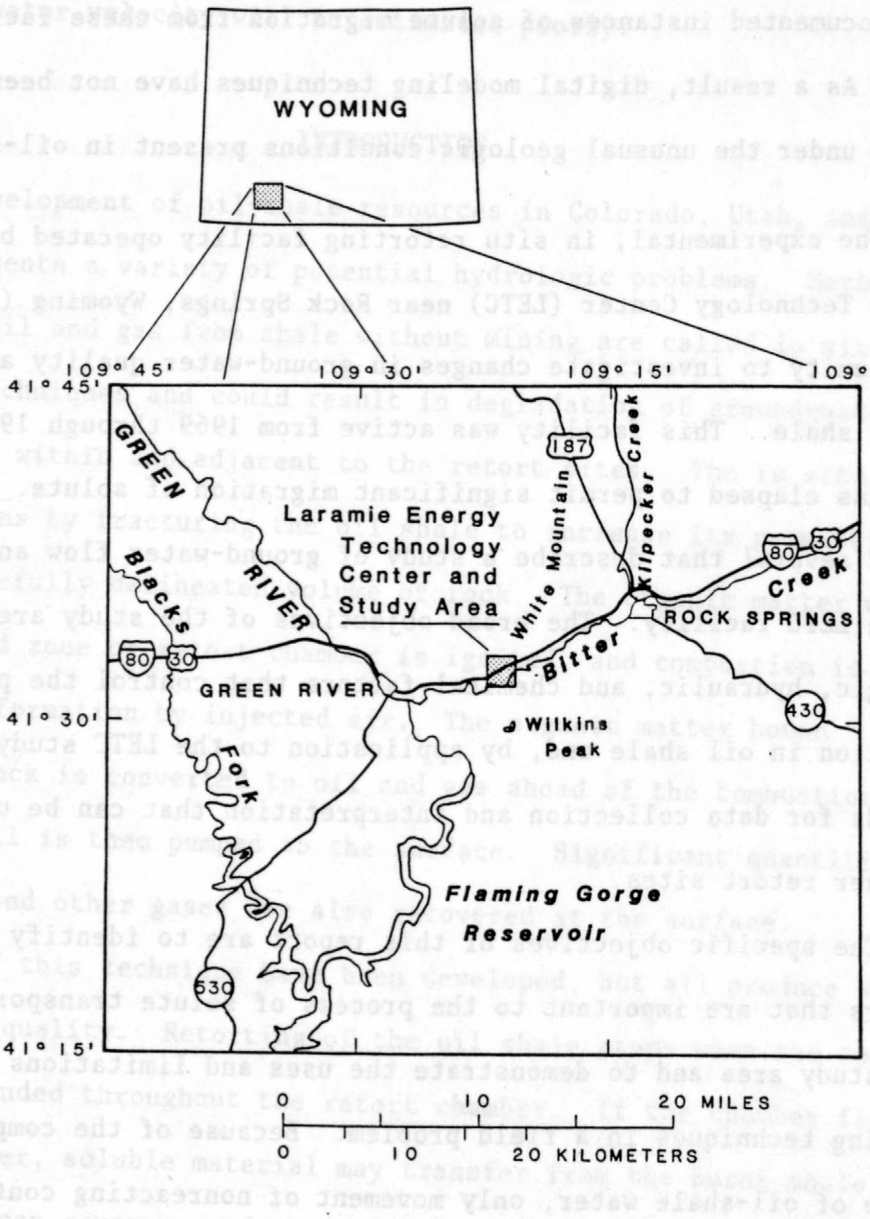

Figure 1.--Location of study area.

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 migration of solutes from this site; solute plumes from other experiments either have dispersed through the ground-water system or were of such limited areal extent as to be 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 may not be economical. Improvements on the LETC process have been made (Lekas, 1981), but the basic nature of the method has remained unchanged.

The site 9 retort experiment is 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 by 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 shock waves and limit the vertical extent of the rubblized zone. Problems with the system resulted in detonation of the explosive in the

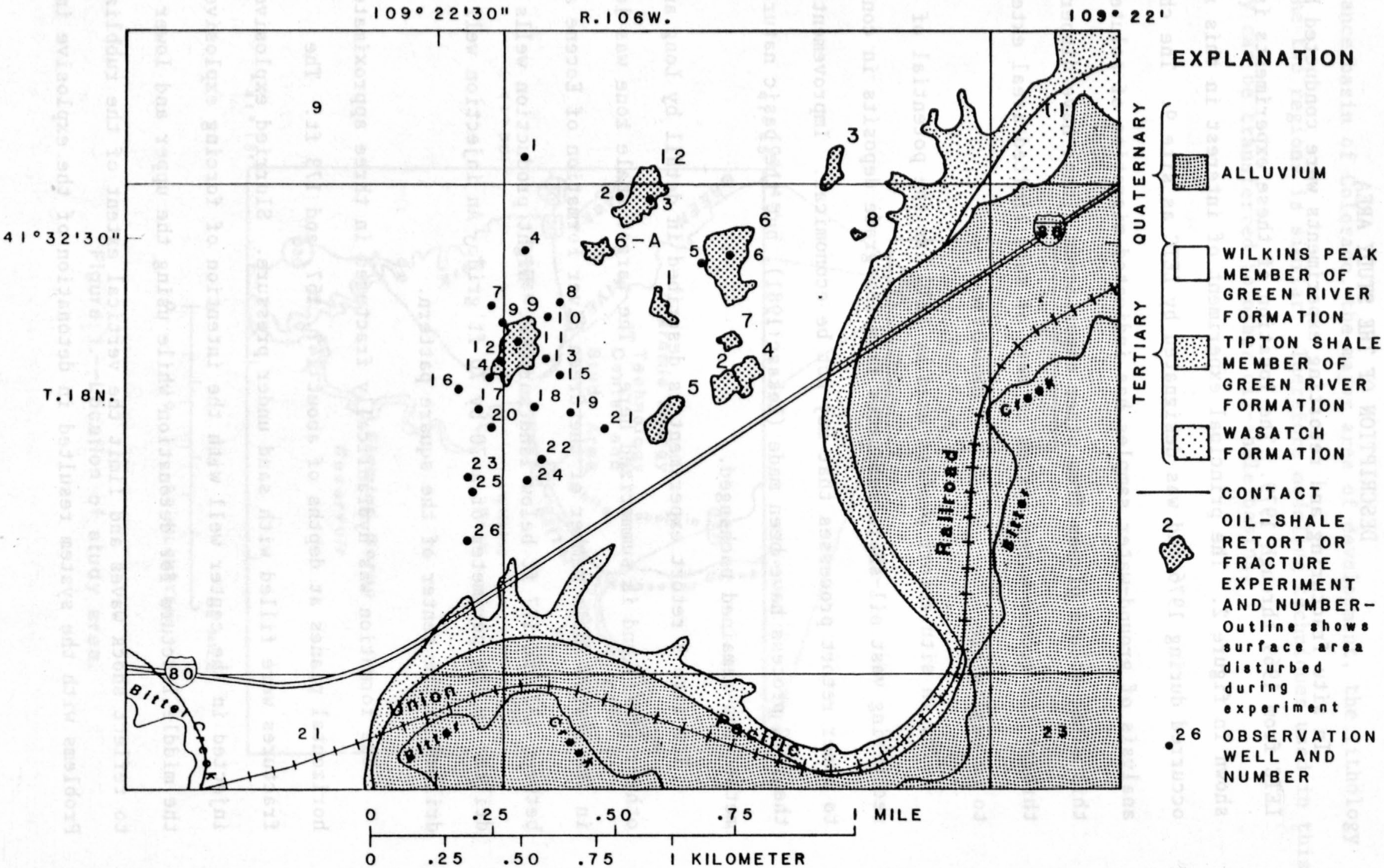

Figure 2.--Surface geology, well numbers, and location of in situ retort experiments.

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 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 by injecting propane in 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 indicate 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. A program to monitor ground-water levels and water quality in and adjacent to site 9 was begun by LETC shortly before the retorting experiment was started and continued through 1983.

STRATIGRAPHY

The oil-shale resource used by LETC near Rock Springs, Wyoming is contained in the Tipton Shale Member of the Green River Formation of Eocene age which conformably overlies ~~the~~ part of the Wasatch Formation of Eocene age throughout the study area. Geologic characteristics of these formations have been described basin-wide by Bradley (1964), and Culbertson and others (1980). Geologic investigations at the LETC facility are documented by Dana and Smith (1972). The Wasatch Formation consists of fluvial deposits while the Green River Formation is primarily lacustrine.

In general the Green River Formation overlies the Wasatch 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.

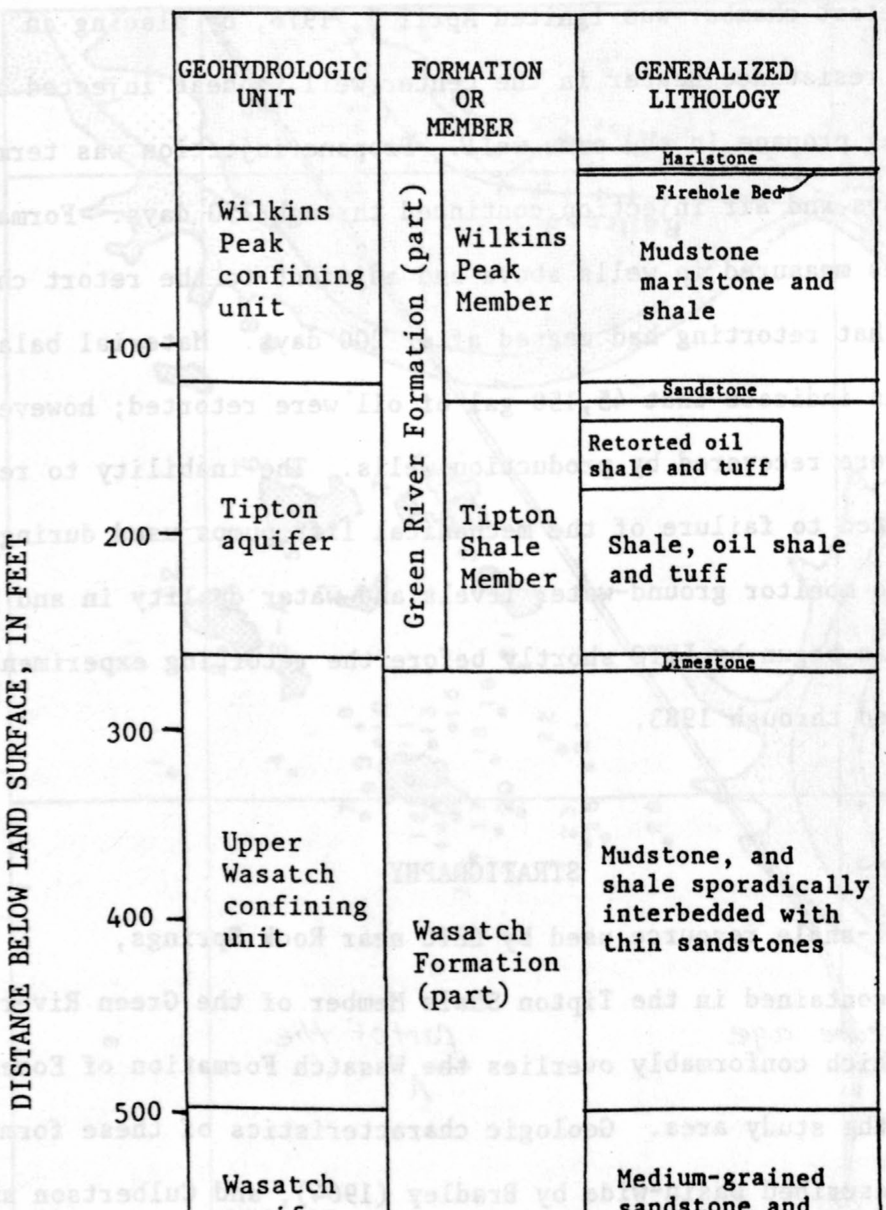

Figure 3.--Geohydrologic units, stratigraphic units, and generalized lithology of the Wasatch and Green River Formations at site 9

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 the basal unit will simply be called the Wasatch Formation in this report. The upper 225 ft of the Wasatch at the LETC facility consists of shale and mudstone sporadically interbedded with thin sandstones. Beneath this is 130 ft of sandstone and sandy mudstone, and approximately 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 and range in thickness from 1/2 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 horizonal variation in lithology has been noted within the Tipton 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.

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 (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- 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	0.9	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.

Core analyses by Pasini and others (1972) show that the direction of minimum tensile strength of oil shale in undisturbed areas of the Tipton 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. No reason for this difference is known. 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 base of the Wilkins Peak Member is marked by an 8-ft-thick limy sandstone that forms a cap rock 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 relationship 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 shaley, soft, erodable, and 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, approximately 30 miles southwest of the study area (E. A. Zimmerman, U.S. Geological Survey, written communication, 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 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) shows this trend clearly. Very limited

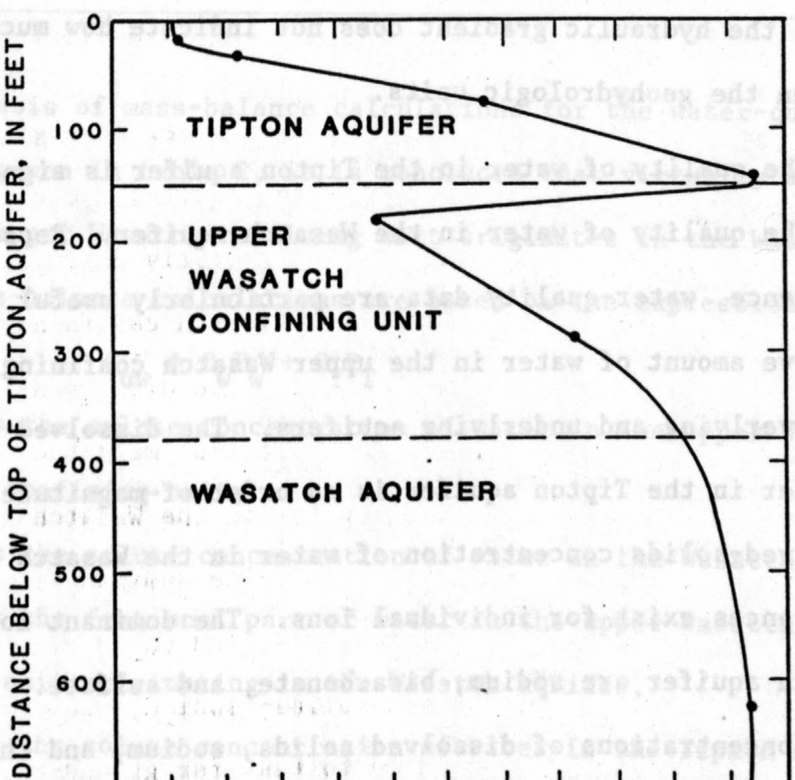

Figure 4.--Vertical variation in hydraulic head near well 16.

hydraulic-head data for wells open to the top part of the upper Wasatch confining unit indicate that horizontal-head gradients towards 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-solids concentration of water in the Tipton aquifer is an order-of-magnitude greater than the dissolved-solids 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 of ground-water samples (table 2) were used to test for ground-water movement between the Tipton aquifer and the upper Wasatch confining unit. Chloride is the most useful of these water-quality constituents because the ion normally is conservative in ground-water systems. Similar tables of water quality data can be constructed for other dates.

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

Geohydrologic unit	Number of samples	Dissolved-solids concentration (milligrams per liter) minimum	maximum	Sodium (milligrams per liter) minimum	maximum	Chloride (milligrams per liter) minimum	maximum
Lower part of Tipton aquifer	4	6040	11,100	2300	4600	2900	7500
Upper Wasatch confining unit	3	1040	1,330	400	520	66	170
Wasatch aquifer	2	1370	1,620	540	700	81	270

On the basis of mass-balance calculations for the water-quality constituents given in table 2, it is concluded that virtually all of 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 frational 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, it is possible to solve for P_T. For example, applying the equation to the range of chloride concentrations given in table 2 shows that less than one percent of water in the upper Wasatch confining units originates in the Tipton aquifer. One possible explanation for this conclusion is that the top 44 feet of the upper Wasatch confining unit, a particularly soft, shaley mudstone, is virtually impermeable.

A second possible explanation is that 7 feet of limestone at the contact between the Tipton aquifer and upper Wasatch confining unit is very permeable, permitting relatively rapid horizontal movement of water from the lower part of the Tipton aquifer towards 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 to support the hypothesis that the limestone at the Tipton-upper Wasatch contact is very permeable does not exist. Discharge from the limestone at outcrops adjacent to Bitter Creek has not been observed; and the limestone, in contrast to most permeable limestones, shows no signs of fractures or solution channels.

On the basis of existing lithologic and water-quality data it is 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 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 in the Green River Formation. The in situ 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 approximately 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 has been removed by erosion throughout most of the study area.

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 through unfractured shale and marlstone is very small by comparison. For purposes of solute transport, water in the shale and marlstone matrix may 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 complexly 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 the resistance to vertical movement of the retort chamber is less than that of 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.

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

Well	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

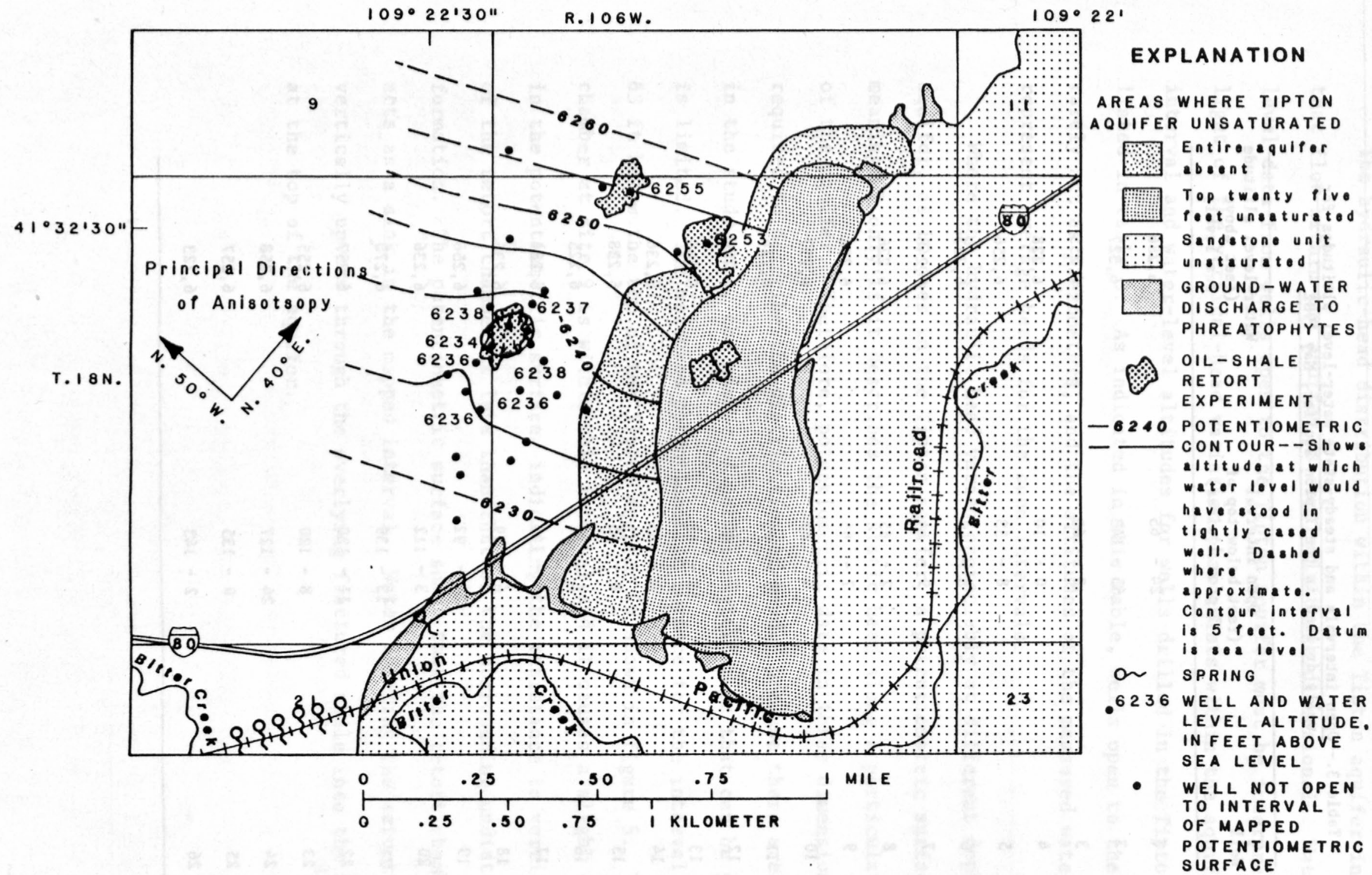

Figure 5.--Steady-state potentiometric surface for interval 13 to 63 feet below the top of the Tipton aquifer, May 1982.

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 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 by-product 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 obtaining water-quality samples from observation wells. Based on discussions with LETC personnel concerning sampling procedures, estimates of the quantity of water 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 hydraulic conductivity and storage coefficient from measured water-level changes were not successful. Attempts to analyze water-level recovery after retorting ceased also were 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.

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 north and is absent in the study area. Regardless of the source of water, the distance between recharge areas and the retort experiment 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) describes greasewood as very salt and alkali tolerant and as usually growing in a fine-textured, relatively impermeable soil with high salinity, exchangable 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 (1984), 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 matched 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 water from wells 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-solids concentration ranged from 12,000 to 19,000 mg/L, and virtually all of the cations were sodium. The water samples have a pH generally 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 predominately 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 may also result from the dissolution of trona and other evaporites.

A wide variety of chemicals have been observed in waters produced during the retorting experiment (Fox and others, 1978). Particularly noteworthy are the 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 anerobic 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 five years after the site 9 retort experiment. Two points are noteworthy in these data. From this figure it can be seen that the solute plume is moving within the top sandstone bed of the aquifer. The second point to note is that the solute plume has not completely flushed from the retort chamber. This incomplete flushing indicates 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 in figure 6.

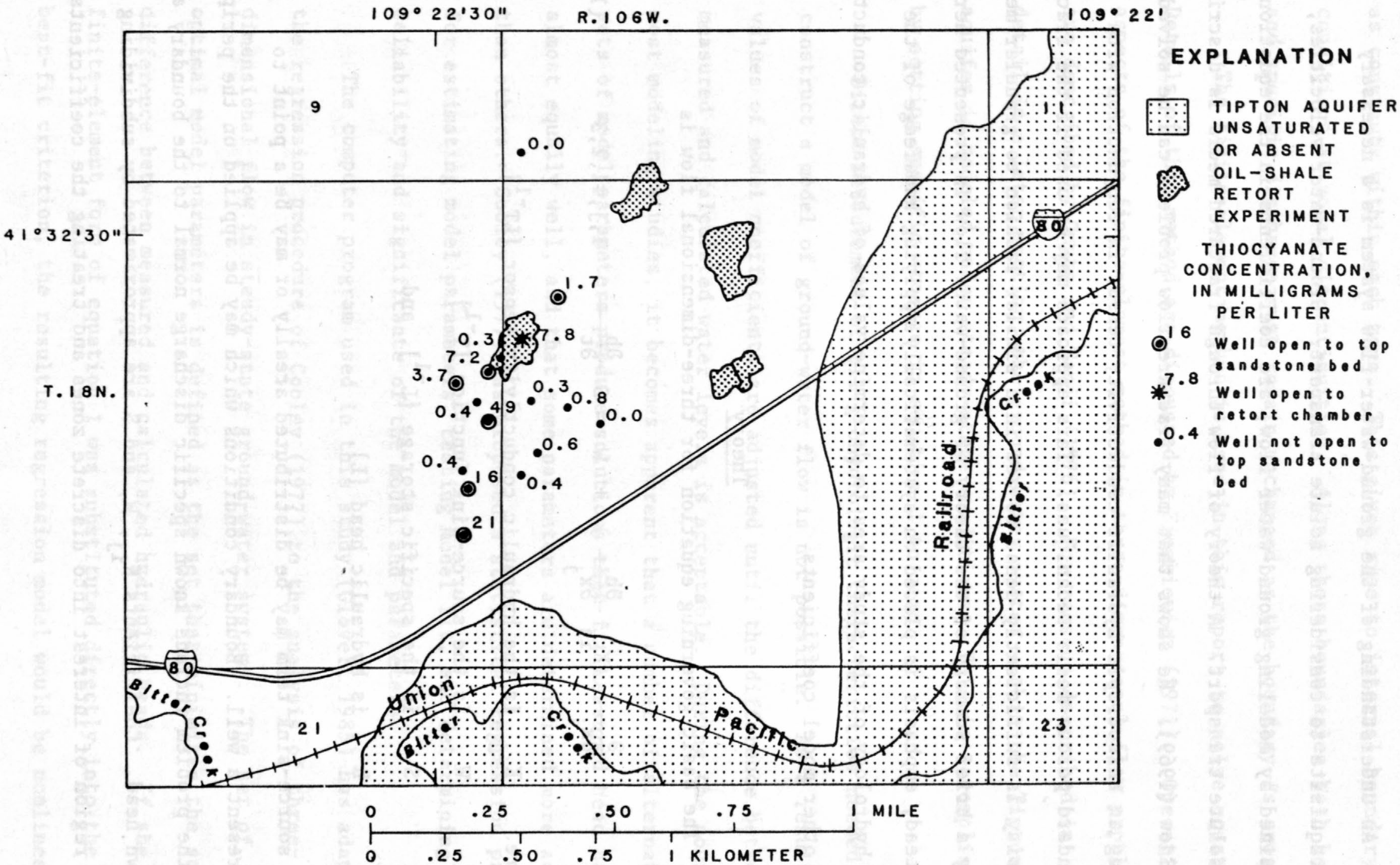

Figure 6.--Thiocyanate concentrations, December 1981.

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

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

where K_{ij} is the hydraulic conductivity tensor $[LT^{-1}]$,
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 which may be applied on the periphery of the problem include known specific discharge normal to the boundary and known head. 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 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 are discussed by Zienkiewiez (1971). Operational aspects of the finite-element method in three-dimensional flow problems are described by Gupta and Tanji (1976). For reasons described in detail in a later section, the ground-water system within the Tipton aquifer is modeled under steady-state conditions. This 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) has 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, 1985) has adapted 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 correlation coefficient of the model. Estimated standard errors of parameters are measures of the range over which the respective parameters may 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 a 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 is 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 analyse results of the regression model statistically, 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) presents methods for testing these assumptions including analysis of residuals and calculation of the degree of nonlinearlity of the regression model.

The relationship 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 relationship would require solving the three-dimensional equation of ground-water flow in the close vicinity of the well bore. This approach is not practical. Instead a relationship based on the steady-state conservation of water within the well bore and Darcy's law is used in this study. The result is a weighted average of hydraulic head over the open interval.

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

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 is given by Glover (1985). The depth-integrated head is directly comparable to measured water-level data. The regression technique of Cooley (1977) has been modified by Glover (1985) 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 have 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, there are similarities in data requirements. Reports by Konikow (1977) and Robson and Saulnier (1981), describing other flow and transport models, have discussed many of these requirements. Emphasis in this report will be 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 period of time. 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 then can be simulated. Unfortunately this approach requires the determination of numerous model coefficients related to mass transfer, conversion from water-table to confined conditions, and hydraulic-conductivity variation due to 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, more 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 below. 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 the chamber during the experiment, although water produced from the chamber contained large concentrations of numerous chemical constitutents. 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 water quality of water from wells outside the chamber continued to approximate preretorting conditions while 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 clearly 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.

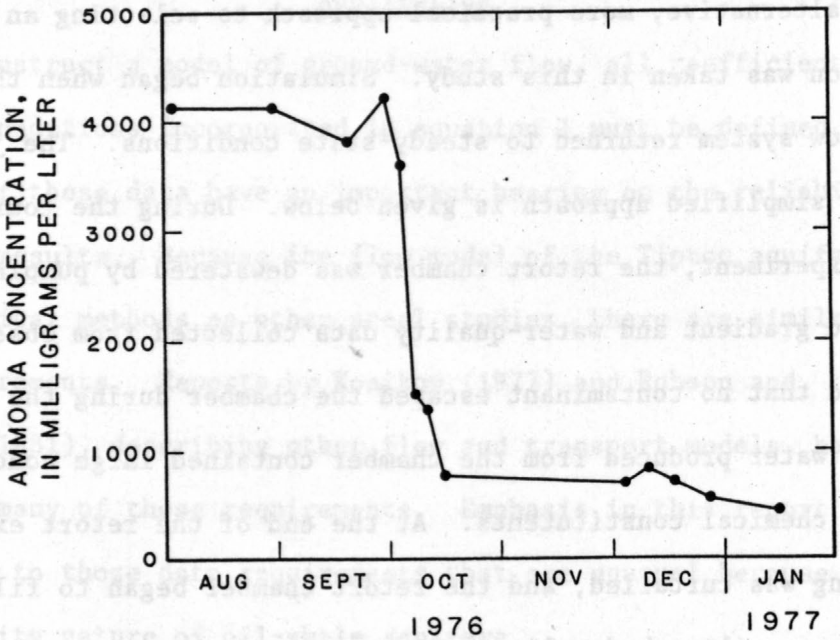

Figure 7.--Concentration of ammonia in water in well 11 completed in retort chamber, August 1976 to January 1977.

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 down-gradient of the retort operation where contaminant is likely to spread, and areas up-gradient 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.

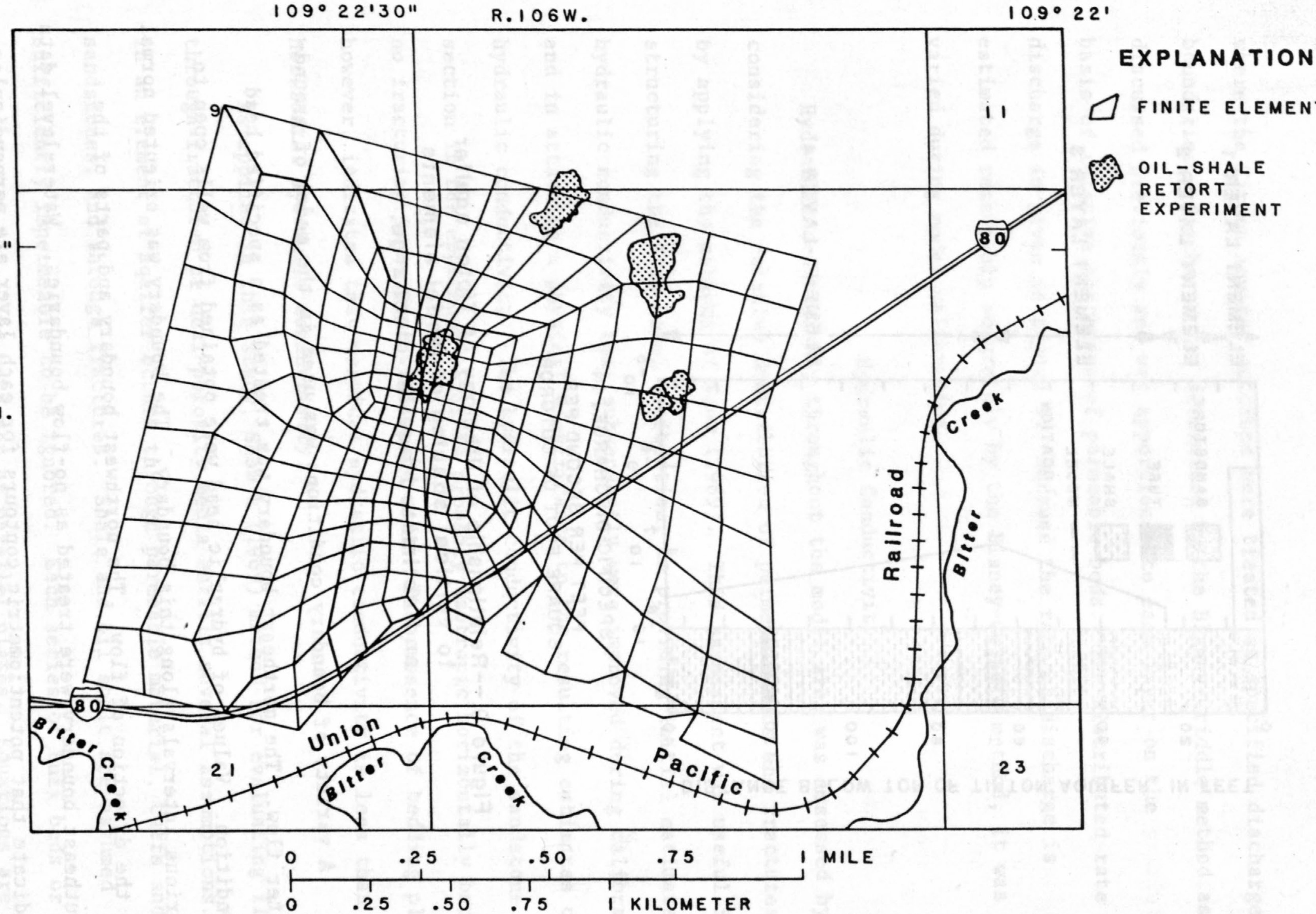

Figure 8.--Finite-element grid used to model the study area.

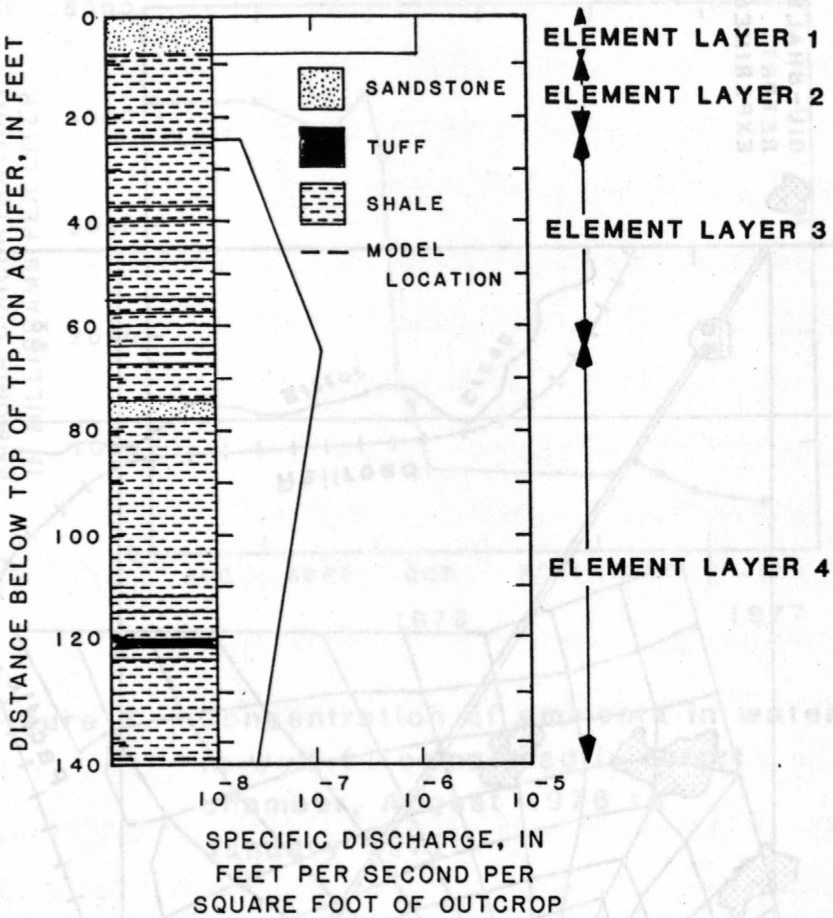

Figure 9.--Relationship of lithology of Tipton aquifer to vertical spacing of model elements and estimated aquifer discharge.

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 outcrops were treated as specified discharge boundaries. Discharge was determined by 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 estimated reasonably accurately by 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 by applying the methods of Snow (1969). This assessment was useful in structuring the flow-model calibration, in providing initial estimates of hydraulic conductivity that subsequently were improved during calibration, and in attaching a physical significance to the resulting estimates of hydraulic conductivity. The hydraulic conductivity of the sandstone section in the uppermost layer is probably isotropic horizontally 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 entails several assumptions. Flow in an element of aquifer occurs through permeable material, 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 as the y direction and treating the fracture system as a series of parallel conduits, (fig 10) the Navier-Stokes equation for flow through fractures can be written and equated to Darcy's law to give

$$\left.\begin{aligned} Q_{fx} &= 0 \\ Q_{fy} &= -\frac{2}{3}\frac{1}{\Delta}\frac{1}{n_f}\frac{g}{v}\, w_x\, w_z\, I_y \sum_{i=1}^{n_f} (b_i^*)^3 \\ Q_{fz} &= -\frac{2}{3}\frac{1}{\Delta}\frac{1}{n_f}\frac{g}{v}\, w_x\, w_y\, I_z \sum_{i=1}^{n_f} (b_i^*)^3 \end{aligned}\right\} \quad (3)$$

where Q_{fx}, Q_{fy}, and Q_{fz} are flow in the x, y, and z directions through fractures in each element $[L^3T^{-1}]$,

Δ is the average fracture spacing [L],

n_f is the number of fractures per element,

g is the constant of gravitational acceleration $[LT^{-2}]$,

v is the kinematic viscosity of the fluid $[L^2T^{-1}]$,

w_x, w_y, and w_z are element width in the x, y, and z directions [L],

I_y and I_z are hydraulic-head gradient in the y and z directions [dimensionless], and

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

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

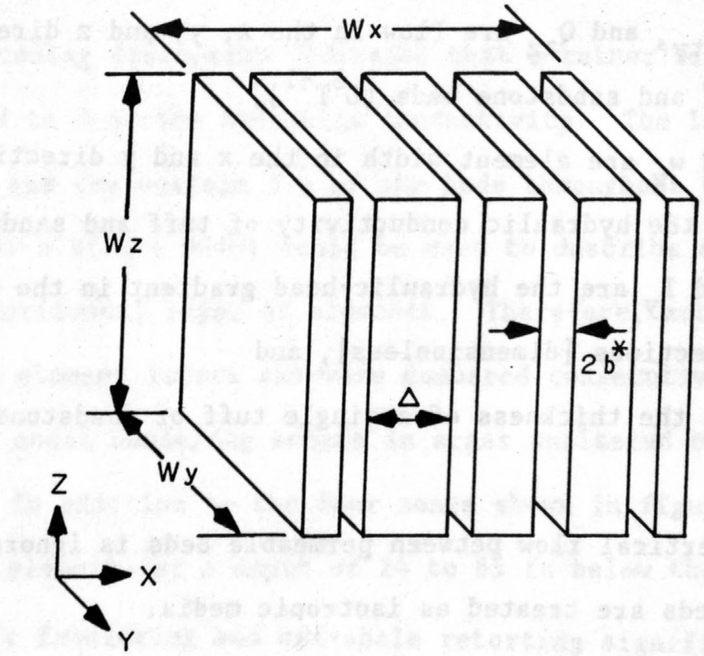

Figure 10.--A solid volume cut by parallel plane conduits.

The tuff and sandstone beds within the Tipton aquifer may 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

$$\left.\begin{aligned} Q_{tx} &= -w_y K_t I_x \sum_{i=1}^{n} b_i \\ Q_{ty} &= -w_x K_t I_y \sum_{i=1}^{n} b_i \\ Q_{tz} &= 0 \end{aligned}\right\} \qquad (4)$$

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

w_x and w_y are element width 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 gradient 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

$$\left.\begin{aligned}
\overline{K}_x &= K_t \frac{1}{w_z} \sum_{i=1}^{n} b_i \\
\overline{K}_y &= K_t \frac{1}{w_z} \sum_{i=1}^{n} b_i + \frac{2}{3} \frac{1}{\Delta} \frac{1}{n_f} \frac{g}{\nu} \sum_{i=1}^{n_f} (b_i^*)^3 \\
\overline{K}_z &= \frac{2}{3} \frac{1}{\Delta} \frac{1}{n_f} \frac{g}{\nu} \sum_{i=1}^{n_f} (b_i^*)^3
\end{aligned}\right\} \tag{5}$$

where $\overline{K}_x$, $\overline{K}_y$, and $\overline{K}_z$ 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 is probably small enough to be ignored. While accurate values of $\overline{K}_x$, $\overline{K}_y$, and $\overline{K}_z$ cannot be determined from field data, the preceding analysis does give an indication of the degree of anisotropy that occurs within the study area.

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 ~~3~~ 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

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

	Hydraulic conductivity, in feet per day		
	Horizontal		Vertical
Zone	N. 50° W.	N. 40° E.	
1	19.4	19.4	4.30×10^{-4}
2	0	4.30×10^{-5}	4.30×10^{-5}
3	.432	.432	4.30×10^{-7}
4	.670	.670	1.72×10^{-5}
retort	.436	.436	4.30×10^{-3}

	Standard error, in feet per day		
	Horizontal		Vertical
Zone	N. 50° W.	N. 40° E.	
1	1.62	1.62	2.02×10^{-3}
2	0	1.47×10^{-4}	1.47×10^{-4}
3	.881	.881	5.96×10^{-5}
4	0.475	0.475	1.21×10^{-4}
retort	.881	.881	5.62×10^{-3}

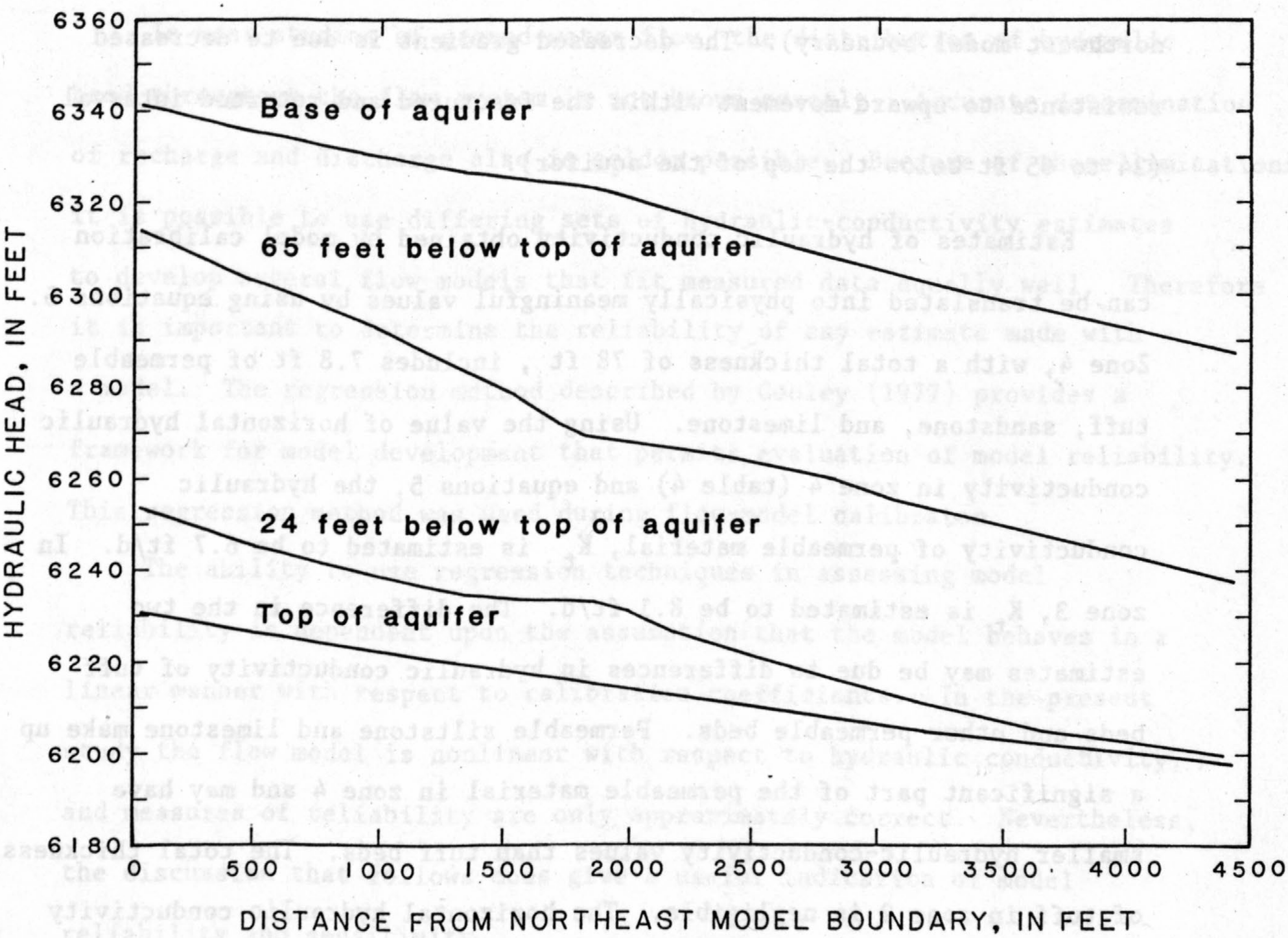

Figure 11.--Calculated distribution of hydraulic head within the Tipton aquifer along a line S. 15° W.

of the aquifer is decreased near the retort chamber (1800 ft from the northwest model boundary). The decreased gradient is due to decreased resistance to upward movement within the fractured and retorted interval (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, the hydraulic conductivity of permeable material, K_t is estimated to be 6.7 ft/d. In zone 3, K_t is estimated to be 8.1 ft/d. The difference in the two estimates may 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 may 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 calibraton.

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 hydraulic conductivity, and measures of reliability are only approximately correct. Nevertheless, the discussion that follows does give 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 precisely known. Therefore, measures of reliability, such as standard errors, probably are 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 precisely estimated. 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 preceeding 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 basin-wide studies. Data such as the distribution of thin permeable beds or fractures may introduce an unmanagable 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 in situ 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 more sophisticated fracture model, while 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) provide 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

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

where D_{ij} is the hydrodynamic-dispersion coefficient $[L^2T^{-1}]$,

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 $[ML^{-3}]$, and

c^* is solute concentration of a fluid source $[ML^{-3}]$.

When using 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

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

where a_{ijmn} is dispersivity of the aquifer [L], both

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]; $\qquad i = 1,2,3$

a_{iijj} is α_T, transverse dispersivity [L]; and $\qquad i,j = 1,2,3$

a_{ijij} is $\frac{1}{2}(\alpha_L - \alpha_T)$ $\qquad i,j = 1,2,3.$

All other components of dispersivity equal zero.

The form of the transport equation used in this study (equation 6) also is used by Pinder and Gray (1977), and Bibby (1981). Konikow (1977) and most studies of solute transport done by the U.S. Geological Survey use 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, it should be recognized 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 more easily calculated.

Galerkin's method of weighted residuals with isoparametric 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 is 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. By assuming steady-state conservation of solute and using Darcy's law, a simplified expression can be obtained:

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

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

c is solute concentration along the well bore $[ML^{-3}]$,

z_3 to z_4 is the segment of the well bore where water enters the well bore [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 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) present evidence that thiocyanate is non-reactive 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 (milligrams per liter) (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 note 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 0.0 mg/L is assumed.

A knowledge of initial solute concentration within the retort chamber is not sufficient information to insure 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 dispersivity and porosity of the top sandstone strata, and 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) indicate that sandstone and siltstone typically have a porosity of 35 percent. The presence of cementing materials and compaction tends to reduce porosity while 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 element layer. A porosity value of 35 percent was assigned to permeable strata while the effective porosity of impermeable strata was zero 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 down-gradient 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 difference between calculated and measured thiocyanate concentrations shown in figure 12. During the early time steps of the simulation, solute moved from the retort chamber vertically upward to the top sandstone bed of the aquifer. Horizontal Darcy velocity within the retort chamber was 5.5 ft/d while 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

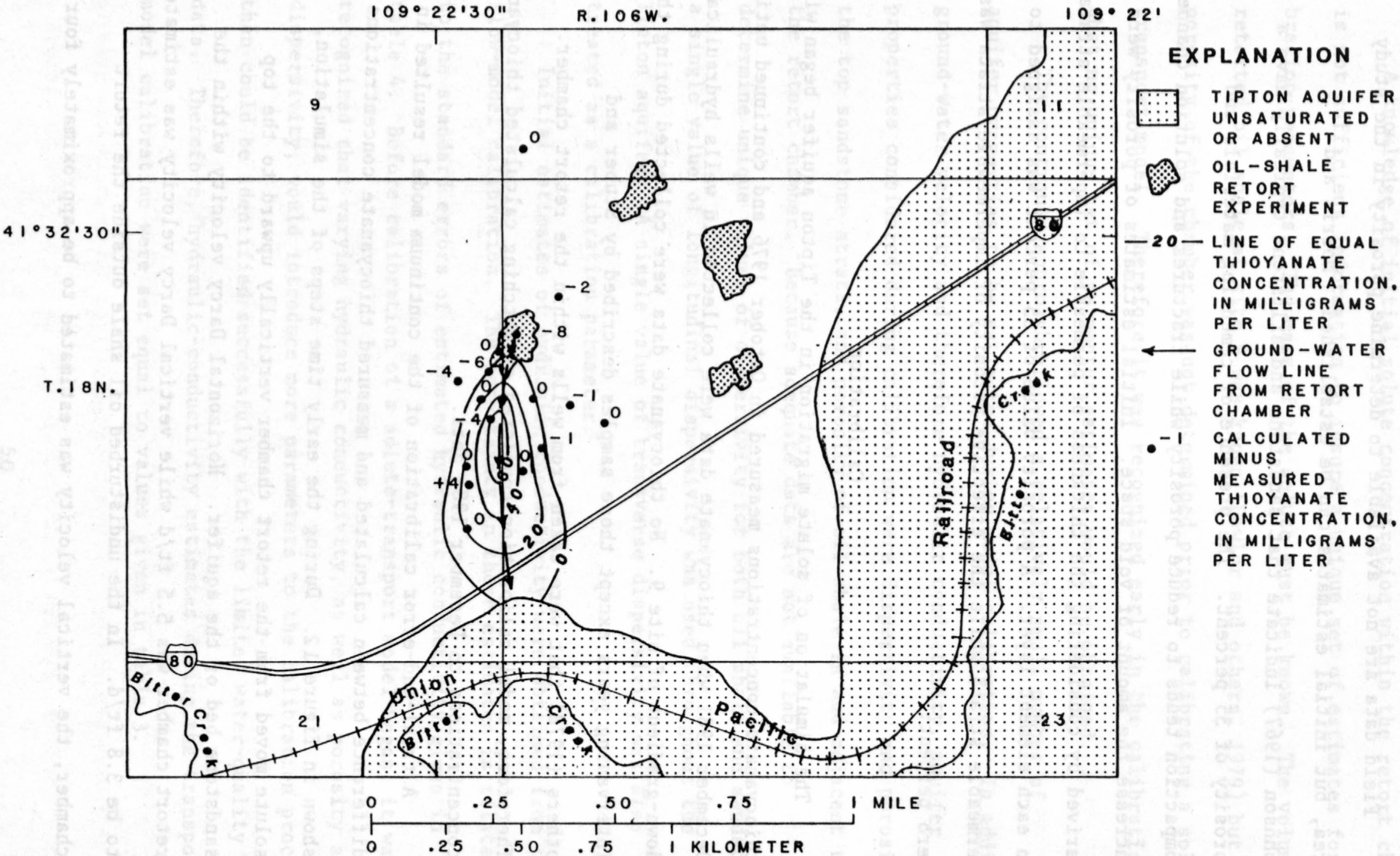

Figure 12.--Thiocyanate concentration calculated by the continuum model for the top sandstone unit of the Tipton aquifer, December 1981.

orders of magnitude less than horizontal velocity. Because of the short vertical distance from the retort chamber to the more 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 migration of thiocyanate occurred primarily in the top sandstone unit of the Tipton aquifer. The optimal match between calculated and measured thiocyanate (fig. 12) was obtained by using a sandstone porosity of 12 percent and porosity within the retort chamber 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, there is uncertainty 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 estimates of hydraulic conductivity obtained while calibrating the flow model and actual hydraulic-conductivity values will cause corresponding errors in porosity and dispersivity estimates given above.

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 insure that those estimates are correct. It is possible that a second set of values for aquifer properties would given 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 are given in the following discussion.

Varying the values of porosity for rocks within the retort chamber had a pronounced effect on calculated solute concentrations. Increasing 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 mass of thiocyanate caused a poor fit in the trailing section of the plume. By maintaining sandstone porosity and dispersivity at calibrated values and increasing retort-chamber porosity, the distance that the solute traveled during the course of the simulation was rapidly decreased.

The porosity of sandstone within the Tipton aquifer also is well defined by the calibrated value of 12 percent. Increasing sandstone porosity from the calibrated value decreased the distance the solute plume migrated during the course of the simulation. The match between calculated and measured concentrations of thiocyanate became unacceptable for changes in sandstone porosity of two percent or more. Adjusting dispersivity and retort-chamber porosity did little to improve the match.

Longitudinal and transverse dispersivity of the Tipton aquifer are less well defined than 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 determining dispersivity more precisely.

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 several weaknesses in the continuum approach. Although the match of calculated to measured thiocyanate concentrations obtained during calibration was generall good, the estimate of fracture porosity within the retort chamber appears to be large. Using a dual-porosity model that explicitly accounts for porosity of fractures and porosity of the shale matrix might produce a reasonable calibration while using realistic values of porosity. 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 portion of the solute plume. The underestimates are probably the result of slightly underestimating 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 portion of the plume. One possible mechanism for introducing additional solute in the trailing section of the plume is mass transfer. This mechanism is discussed in the next section of the report.

Mass-Transfer Mechanism

The continuum model of solute transport described in the previous sections consistently underestimated the concentration of thiocyanate in the trailing portion 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 portion of the solute plume without adding mass to the leading portion.

Hall (1982) performed leaching experiments with columns of retorted oil shale and observed a similar increase of mass in the trailing portion 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 towards 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. While it may be possible to estimate the coefficients in equation 8 through a calibration procedure, the resulting transport model may not be more reliable. An effort was made to calibrate the transport model with 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 more 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 (1985) 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. While 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 be performed in the LETC study area only 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 in situ 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 on 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 is predicted to be approximately 45 mg/L. This reduction from the initial concentration of 78 mg/L is the result of hydrodynamic dispersion. The peak thiocyanate concentration will occur 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 will either evaporate or be used by plants. No direct runoff of ground water will occur, 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.

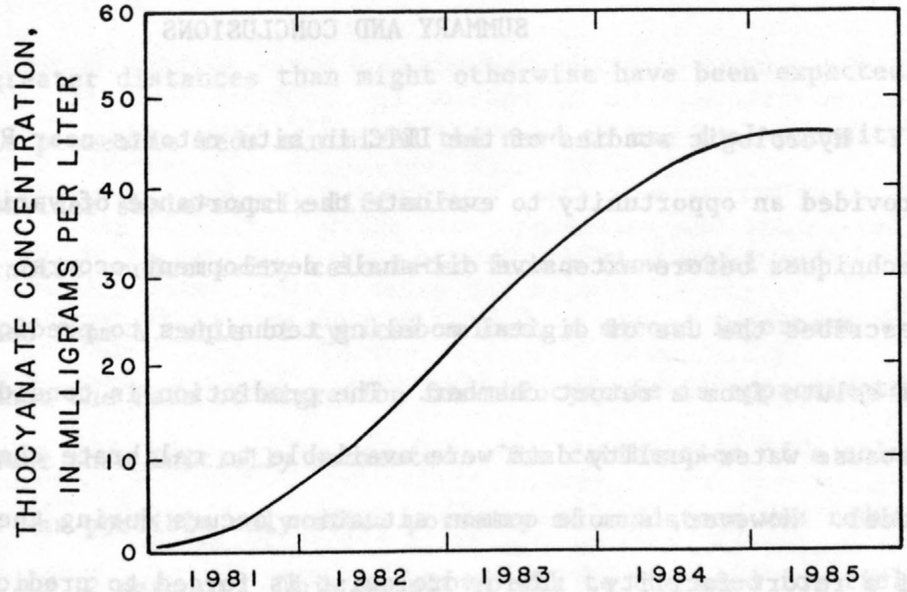

Figure 13.--Predicted thiocyanate concentration in water discharging from sandstone unit of the Tipton aquifer at SW 1/4 SW 1/4 SW 1/4 section 15, T.18N., R.106W.

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 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 accumulation of salts in the discharge area.

SUMMARY AND CONCLUSIONS

Hydrologic studies of the LETC in situ retorts near Rock Springs 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. 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 basin-wide scale (Robson and Saulnier, 1981), solute migration on a site-specific scale can vary significantly from what might be predicted basin-wide. This report provides information on the relative importance of many geohydrologic factors that influence solute transport in oil shale.

The most important conclusion that can be drawn from the study described in this report 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 is particularly true if the sampled intervals of observation wells are accurately placed within this geologic framework. Without considering geologic data in detail, models will be poorly calibrated or incorrectly used. Fortunately such information can be obtained by test drilling and geophysical logging prior to retorting and therefore be used during the planning stages of development. Solute migration in the LETC study area occurs primarily in thin permeable beds rather than the oil-shale strata. Because of this behavior, solute travelled far greater distances than might otherwise have been expected. Also movement in permeable beds minimized the need to use dual-porosity models or to consider shale-matrix diffusion.

Using hydraulic conductivity calculated from a flow model and porosity obtained from a table of typical values, a second important conclusion is that the rate of migration for thiocyanate is approximately three times faster than initially estimated. The calibration of a solute-transport model was possible only after porosity of sandstone was reduced from 35 percent to 12 percent. This result points to the need for field determinations of porosity during the planning stages of an in situ 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 one-half 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 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 eliminated the need to consider mechanisms for transferring solute from rocks to water as the abandoned retort chamber saturated. It also permitted the use of steady-state models 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.

REFERENCES

Bibby, Robert, 1981, Mass transport of solutes in dual-porosity media: Water Resources Research, v. 17, no. 4, p. 1075-1081.

Bradley, W. H., 1964, Geology of Green River Formation and associated Eocene rocks in southwestern Wyoming and adjacent parts of Colorado and Utah: U.S. Geological Survey Professional Paper 496-A, 86 p.

Cooley, R. L., 1977, A method of estimating parameters and assessing reliability for models of steady state groundwater flow, 1, theory and numerical properties: Water Resources Research, v. 13, no. 2, p. 318-324.

_____, 1979, A method of estimating parameters and assessing reliability for models of steady state groundwater flow, 2, application of statistical analysis: Water Resources Research, v. 15, no. 3, p. 603-617.

Cruff, R. W., and Thompson, T. H., 1967, A comparison of methods of estimating potential evapotranspiration from climatological data in arid and subhumid environments: U.S. Geological Survey Water-Supply Paper 1839-M, 28 p.

Culbertson, W. C., Smith, J. W., and Truedell, L. G., 1980, Oil shale resources and geology of the Green River Formation in the Green River Basin, Wyoming: U.S. Department of Energy, Laramie Energy Technology Center Report of Investigations 8016, 102 p.

Dana, F. G., and Smith, J. W., 1972, Oil yields and stratigraphy of the Green River formation's Tipton member at Bureau of Mines sites near Green River, Wyoming: U.S. Bureau of Mines Report of Investigations 7681, 46 p.

Fox, J. P., Farrier, D. S., and Poulson, R. E., 1978, Chemical characterization and analytical considerations for an in situ oil shale process water: U.S. Department of Energy, Laramie Energy Technology Center Report of Investigations 7817, 47 p.

Glover, K. C., in press, A dual-porosity model for simulating solute transport in oil shale: U.S. Geological Survey Water-Resources Investigations Report 86-4047,120 p.

Grisak, G. E., and Pickens, J. F., 1980, Solute transport through fractured media, 1, the effect of matrix diffusion: Water Resources Research, v. 16. no. 4, p. 719-730.

Gupta, S. K., and Tanji, K. K., 1976, A three-dimensional Galerkin finite element solution of flow through multiaquifers in Sutter Basin, California: Water Resources Research, v. 12, no. 2, p. 155-162.

Hall, W. G., 1982, The kinetics of leaching of organic carbon from in situ spent shale: Lawrence Berkley Laboratory Report LBL - 14231, 159 p.

Huyakorn, P. S., Lester, B. H., and Mercer, J. W. 1983, An efficient finite element technique for modeling transport in fractured porous media, 1, single species transport: Water Resources Research, v. 19, no. 3, p. 841-854.

Konikow, L. F., 1977, Modeling chloride movement in the alluvial aquifer at the Rocky Mountain Arsenal, Colorado: U.S. Geological Survey Water-Supply Paper 2044, 43 p.

Lawlor, D. L., Latham, D. R., Fausett, D. W., and Asplund, R. O., 1979, Post-burn study of the Rock Springs site 9 in situ retorting experiment: Oil Shale Symposium, 12th, Colorado School of Mines, Proceedings, p. 221-227.

Leenheer, J. G., Stuber, H. A., and Noyes, T. I., 1981, Chemical and physical interactions of an in situ oil shale process water with a surface soil: Oil Shale Symposium, 14th, Golden, Colorado, 1981, Proceedings, p. 357-375.

Lekas, M. A., 1981, The geokinetics horizontal in situ retorting process: Oil Shale Symposium, 14th, Colorado School of Mines, Proceedings, p. 146-153.

Lenfest, L. W., in press ~~1984~~, Evapotranspiration rates at selected sites in Alluvial valleys in the Powder River basin, Wyoming and Montana: U.S. Geological Survey Water-Resources Investigations Report 82-4105.

Long, A., Jr., Merriam, N. W., and Mones, C. G., 1977, Evaluation of Rock Springs site 9 in situ oil shale retorting experiment: Oil Shale Symposium, 10th, Colorado School of Mines, Proceedings, p. 146-153.

Morris, D. A., and Johnson, A. I., 1967, Summary of hydrologic and physical properties of rock and soil materials as analysed by the hydrologic laboratory of the U.S. Geological Survey 1948-60: U.S. Geological Survey Water-Supply Paper 1839-D, 42 p.

Noorishad, Jahan, and Mehran, Mohsen, 1982, An upstream finite element method for solution of transient transport equation in fractured porous media: Water Resources Research, v. 18, no. 3, p. 588-596.

Pasini, J., III., Komar, C. A., and Overbey, W. K., Jr., 1972, Directional properties of oil shale site 9: Morgantown Energy Research Center Technical Report, 13 p.

Pinder, G. F., and Gray, W. G., 1977, Finite element simulation in surface and subsurface hydrology: Academic Press, New York, 295 p.

Robson, S. G., and Saulnier, G. J., 1981, Hydrogeochemisty and simulated solute transport, Piceance Basin, northwestern Colorado: U.S. Geological Survey Professional Paper 1196, 65 p.

Roehler, H. W., 1981, Description of Eocene rocks in White Mountain at Rock Springs, Wyoming: U.S. Geological Survey Oil and Gas Investigations Chart OC-117, 1 sheet.

Slawson, G. C., Jr., editor, 1980, Monitoring ground water quality--the impact of in-situ oil shale retorting: U.S. Environmental Protection Agency GE 78MP-103, 280 p.

Snow, D. T., 1969, Anisotropic permeability of fractured media: Water Resources Research, v. 5, no. 6, p. 1273-1289.

Stuber, H. A., Leenheer, J. A., and Farrier, D. S., 1978, Inorganic sulfur species in waste water from in situ oil-shale processing: Journal of Environmental Science and Health, v. A13, p. 663-675.

U.S. Department of Agriculture, 1954, Diagnosis and improvement of saline and alkali soils: U.S. Department of Agriculture Handbook Number 60, p. 57.

Zienkiewicz, O. C., 1971, The finite element method in engineering science: McGraw-Hill, New York, 521 p.

Glover—LEACHATE MIGRATION FROM AN IN SITU OIL-SHALE RETORT, ROCK SPRINGS, WYOMING—U.S.G.S. WRIR 85-575