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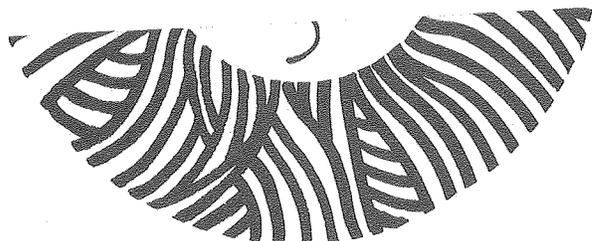
HYDRAULIC CALCULATIONS FOR A MODIFIED IN-SITU RETORT

W. G. Hall

March 1980

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W. G. Hall

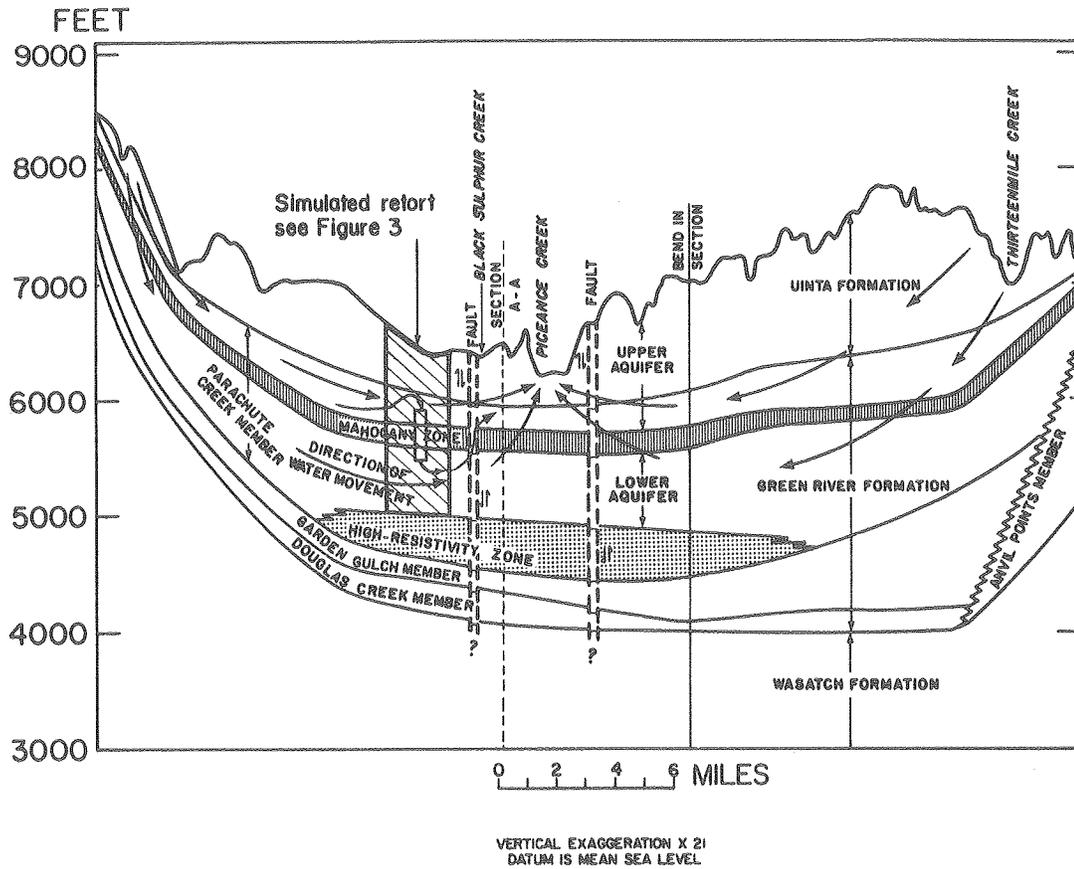
In many locations in the Piceance Creek Basin, the richest sources of oil shale are located below the groundwater table. Before and during retort rubblelization and burning the aquifer in the vicinity of the retort must be kept dewatered. After the retort is abandoned and the dewatering equipment shut down, the groundwater will return. Unless extensive impermeabilization measures are undertaken, the returning groundwater will enter the retort and leach substances from the spent shale. Groundwater carrying the leachate may then reenter the aquifer system and ultimately reach water supplies. The movement of the water during dewatering and subsequent return stages is difficult to define without the help of a model.

This report contains brief descriptions of a numerical model and the aquifer-retort system used to investigate hydraulics in the vicinity of a modified in-situ retort. The model is used to analyze several cases involving different physical and geohydrological parameters, and possible applications of the model to in-situ oil shale recovery are discussed.

PICEANCE CREEK BASIN HYDROGEOLOGY

The Piceance Creek Basin in Colorado was selected for investigation of the interrelation of groundwater aquifers and in-situ retorts. Data on the subsurface hydrogeology are available in reports by Weeks et al. of the U.S. Geological Survey and by Ashland Oil, Inc. and Shell Oil Company, the 1976 lessees of Colorado Oil Shale Tract C-b (Refs. 1,2).

A geologic cross section of the Basin is shown in Figure 1. There are three formations: the Uinta, the surface rock generally overlying the basin; the Green River, containing the oil shale; and the Wasatch foundation formation.



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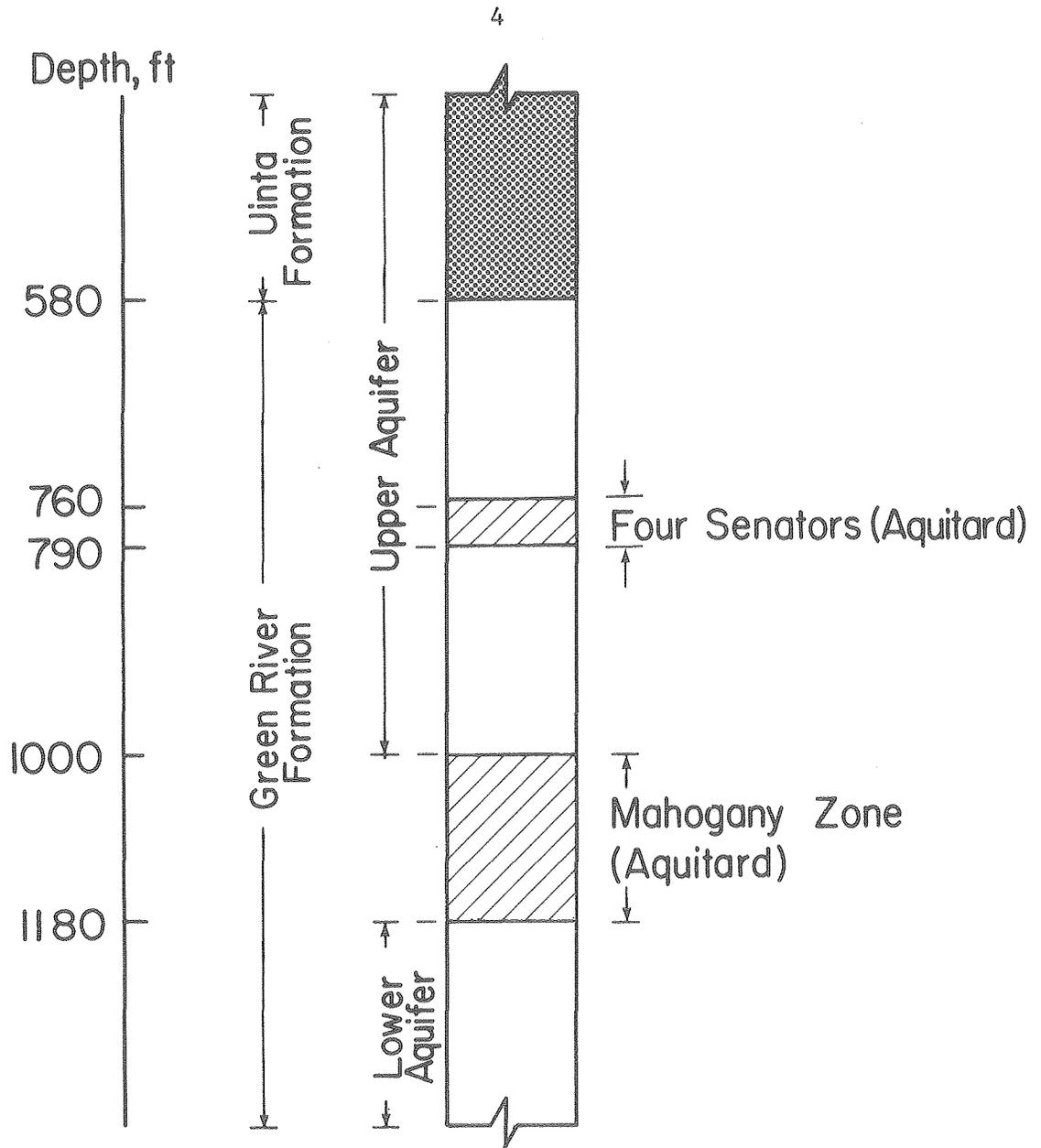
Figure 1. Geologic cross section of Piceance Creek Basin (modified from Ref. 1).

The Uinta Formation consists of intertonguing and gradational beds of sandstones, siltstones, and marlstones. The sandstone beds are predominately fine grained and have low permeability. Water moves primarily through fractures. There are substantial alluvium deposits in the major valleys of the basins. The Green River Formation contains four members, of which the most important to this study is the Parachute Creek member. This member is composed of dolomitic marlstone (oil shale) and soluble materials. Because of fracturing and solution of minerals, the Parachute Creek member is the principal bedrock aquifer in the study area. Particularly rich oil shale deposits are found in the Mahogany Zone, a unit that lies in the upper portion of the Parachute Creek member. The zone varies in thickness from about 100 feet at the edges of the basin to 200 feet near the center. The Mahogany Zone is significant with respect to aquifer-retort relationships for two reasons. First, since it contains the richest oil shale, in-situ retorts will be located in or near the zone; and second, the zone is considered relatively impermeable, and thereby acts as a barrier to flow between aquifers.

The deposits above and below the Mahogany Zone are porous and act as aquifers. The porosity was created both by fracturing of the rock and by leaching of salts from the marlstone. In the USGS study, two principal aquifers, the upper aquifer and the lower aquifer, were identified; they are shown in Figure 1. The upper aquifer includes both the Uinta Formation and the upper portion of the Parachute Creek member. The lower aquifer contains the leached zone lying beneath the Mahogany Zone and above the high-resistivity zone which is considered to be relatively impermeable.

Ashland/Shell found three aquifer systems under tract C-b. The upper aquifer is divided into two parts by an impermeable oil shale layer called the Four Senators. This aquitard is a rich layer of oil shale about 30 feet thick; it is shown schematically in Figure 2. Since the entire Parachute Creek member contains layers of oil shale in varying thicknesses, it is not unreasonable to expect that other aquitards exist, thus further subdividing the upper and lower aquifers.

Geohydrologic parameters including coefficients of transmissivity and storage are reported by the USGS (Ref. 1) and Ashland/Shell (Ref. 2). These are summarized as follows:



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Figure 2. Aquifers-aquitards in vicinity of oil shale tract C-b (from Ref. 2).

Upper Aquifer

Coefficients of transmissivity ranging from 8 to 1000 ft²/day were estimated by the USGS. Data from 26 wells, basin-wide, were used to derive these factors. Ashland/Shell estimated transmissivities ranging from 128 to 233 ft²/day, averaging 168 ft²/day. These values are based on pumping tests from 34 wells in and near Tract C-b. A storage coefficient of 10⁻³ was estimated by the USGS from an analysis of one well. The Tract C-b lessees found storage coefficients ranging from 1.68 x 10⁻³ to 6.92 x 10⁻⁵ with an average of 5 x 10⁻⁴. The Tract C-b lessee also determined a leakance factor ranging from 6.0 x 10⁻⁶ to 4.5 x 10⁻⁷ day⁻¹. Multiplying the leakance factor by the thickness of the aquifer gives vertical permeability.

Mahogany Zone

Based on indirect evidence, the USGS concluded that the Mahogany Zone is generally permeable. Although oil shale itself is relatively impermeable, some faulting and fractures in the zone permit passage of water. The Tract C-b investigators could find no vertical leakage in the zone.

Lower Aquifer

Based on an analysis of 20 wells, basin-wide, the USGS estimated transmissivities up to 1940 ft²/day; however, most transmissivities (75 percent) were less than 500 ft²/day. The Tract C-b lessees calculated transmissivities of about 15 to 92 ft²/day in their area, averaging about 40 ft²/day. The USGS estimated a storage coefficient of 10⁻⁴ in the lower aquifer. Estimates by the Tract C-b lessees ranged from 5.3 x 10⁻⁴ to 1.2 x 10⁻⁵ with an average of 1.7 x 10⁻⁴.

Leakance values were about the same as those for the Upper Aquifer, ranging from 3.9 x 10⁻⁷ to 1.9 x 10⁻⁵ day⁻¹.

Pressure Differences

Pressure differences of up to 100 feet between upper and lower aquifers were noted by the USGS with differences less than 50 ft being most common. Depending on location in the basin, the aquifer with the greater pressure--relative to the other--varies, as do pressures within the aquifer. Ashland/Shell found that pressures in the upper aquifer in the vicinity of Tract C-b were from five to six feet greater than in the lower aquifer.

MODELING GROUNDWATER SYSTEMS

Prior to about 1965 the major effort in mathematical modeling of groundwater systems was directed toward the solution of initial-boundary-value problems expressed as partial differential equations. The analytical techniques available for the solution of the equations severely limited the use of these classical methods. Recent application of numerical methods, together with fast computers, has permitted the solution of large real systems that have been unsolvable except through use of approximations that limit the application of the results.

An overview of recent developments in modeling groundwater systems is presented in a paper by Narasimhan and Witherspoon (Ref. 3). The following discussion is based on Ref. 3 and is directed specifically toward techniques used to investigate flow conditions in an in-situ retort and underground aquifer system. Detailed mathematical derivations are not presented. If more information is desired the reader should refer to Ref. 3 and to other references listed at the end of this appendix.

Application of the principle of conservation of mass to a finite element of a flow region results in the following integral flow equation:

$$\rho_w GV - \int_{\Gamma} \vec{q}_v \cdot \vec{n} d\Gamma = \frac{\partial M_w}{\partial t} \quad (1)$$

The first term expresses the change in fluid content in the element due to injection or removal of fluid of density ρ_w at a rate G to or from an element having a bulk volume V . Effects of injection and withdrawal wells can be so included. The second term represents the volume of fluid that crosses the boundaries of an element having a total surface area Γ ; $\vec{q}_v \cdot \vec{n}$ is the component of velocity along an outer normal of a surface of the element. For illustration, the total flow crossing the surfaces of a cube is the sum of the flows crossing each face which in turn is the sum of face areas times the respective normal velocities. The third term reflects the change in fluid storage, M_w , due to changes in pressure on the element; M_w is a function of the void space in the element, the degree of saturation, and the density of fluid. Each of these three factors varies with the pressure. Equation (1) is a general representation of a flow that is not tied to any coordinate system. It can be used to determine the following quantities in a flow system at any given time:

1. The amount of fluid stored in the system
2. The change in storage over a discrete time interval
3. The distribution of fluid potential over the system

4. The velocity of movement of the fluid in different parts of the system.

The introduction of two empirical relationships will permit the solution of the equation. These two relationships are:

The Darcy-Buckingham law:

$$q = K\Delta(z + \psi) \quad (2)$$

In Eq. (2), q is the flow velocity, K is a coefficient of permeability, and $\Delta(z + \psi)$ is the change in hydraulic head, the components of which are elevation z and pressure head ψ . The Darcy-Buckingham law is equally valid for flow in saturated and partially saturated media.

The relationship between storage and pressure:

$$M_w = V(h) \cdot S(h) \cdot \rho_w(h) \quad (4)$$

In Eq. (3), M_w is the volume of fluid contained in an element, V is the volume of voids, S is the percent of saturation, and ρ_w is the density of the fluid. Each of the three variables in turn is a function of hydraulic head h . When this relationship is differentiated with respect to head, the following equation results:

$$\frac{\partial M_w}{\partial h} = M_c = VS \frac{\partial \rho_w}{\partial h} + V \rho_w \frac{\partial S}{\partial h} + \rho_w S \frac{\partial V}{\partial h} \quad (4)$$

where M_c is defined as fluid mass capacity. The variations of void, volume, degree of saturation, and density, with respect to head, are available in the literature for many materials or may be determined in a laboratory for a specific material.

The integral equation can thus be written

$$\rho_w GV - \int_{\Gamma} \overrightarrow{K\Delta(z + \psi)} \cdot \vec{n} d\Gamma = M_c \frac{\partial h}{\partial t} \quad (5)$$

The real system can now be solved by dividing it into small elements and applying Eq. (5) to each element. Given an initial state of the system, geometry, boundary conditions, and material properties the governing equation can be applied over a discrete time step and then advanced step-by-step over time until some desired state is reached.

The method of mathematical analysis used to solve the integral equation depends on (1) how the system is divided into elements and (2) the means of evaluating the potential gradient h between adjacent elements. There are three methods of solving the integral equation: the finite difference method (FDM); the integrated finite difference method (IFDM); and the finite element method (FEM).

The finite difference method may be applied to rectangular-shaped elements whose faces are normal to the principal axes of symmetry of the system. If it is more convenient to use arbitrarily shaped elements, then the IFDM and FEM methods are applicable. FDM and IFDM evaluate the potential gradient h over collinear points. FEM, on the other hand, defines and evaluates spatial gradients over a set of non-collinear points.

Computer Solution of Integral Equation

The staffs of the Lawrence Livermore Laboratory (LLL) and the Lawrence Berkeley Laboratory (LBL) have developed a series of computer programs to solve Eq. (5). Edwards (Ref. 4) developed a computer code called TRUMP for determining transient and steady-state temperature distributions in multidimensional heterogeneous media with arbitrary geometry. TRUMP combines an IFDM approach with a mixed explicit-implicit scheme for advancing in the time domain. Since conductive heat transfer is analogous to flow of fluids in porous media, the basic computational model of TRUMP has been incorporated by LBL into several programs for studying transient groundwater movement by solving the integral flow equation.

A brief description of three of the LBL programs follows, together with citations of basic source material:

TRUST: This program deals with both saturated and unsaturated flow in porous media. It also includes the effect of consolidation of the mineral matrix due to fluid pressure reduction (Refs. 5,6).

FLUMP: Similar to TRUST but does not include consolidation effects. FLUMP is mnemonic for finite element TRUMP. It is a modification of TRUMP incorporating the finite element technique and handles two-dimensional transient heat-flow or fluid-flow problems under isothermal conditions (Refs. 7,8).

FREESURF 1: This program is applicable for steady-flow conditions with or without free surfaces; it permits the direct solution of the location of a free surface between saturated and unsaturated flow zones (Ref. 9).

The investigations reported in the following sections of this report are based on the FLUMP program. The program was made available to the author by T. N. Narasimhan of the LBL staff.

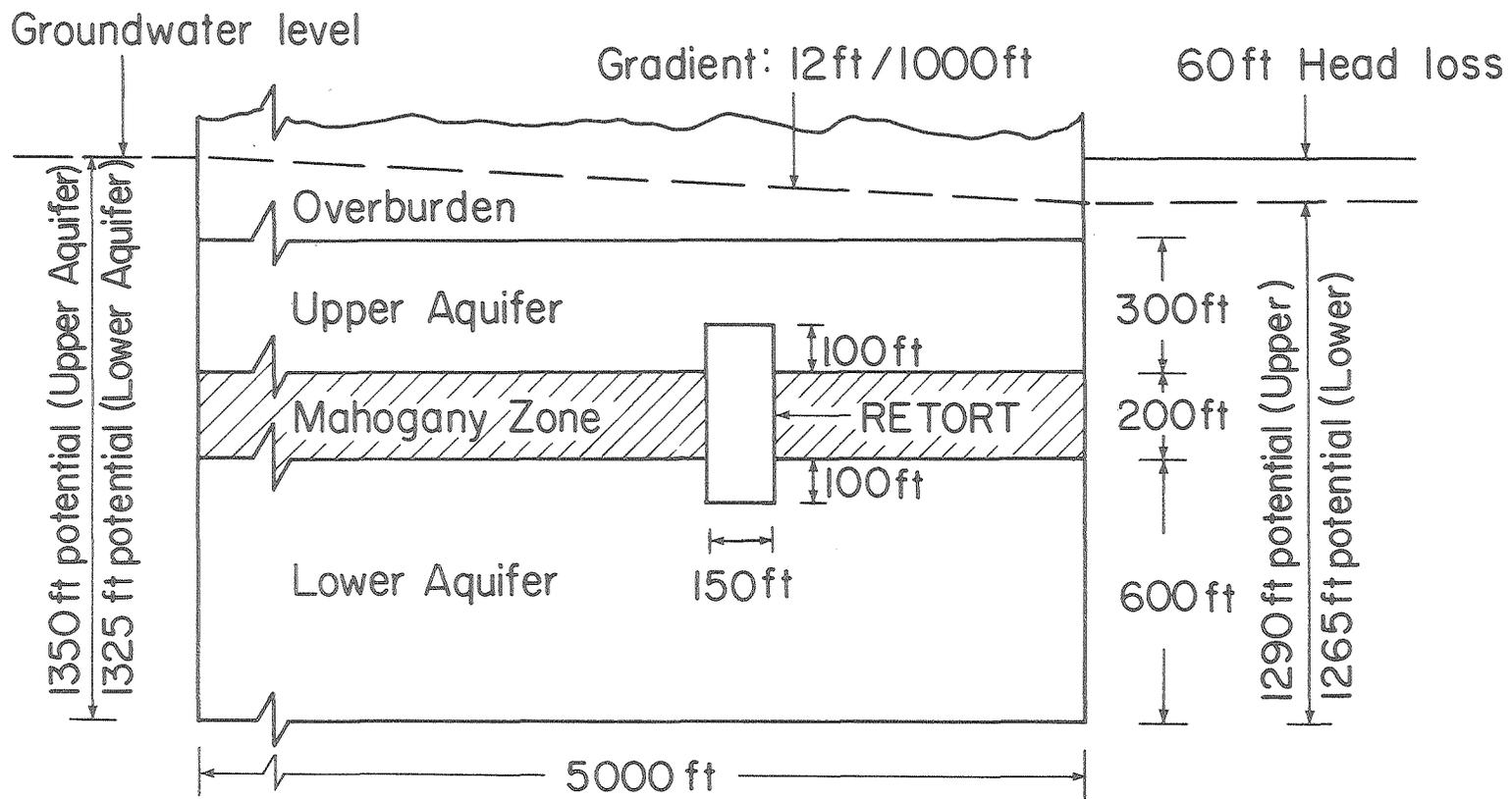
Analysis of Piceance Creek Basin Aquifer-Retort System

Assume that a single retort is located in the Mahogany Zone as indicated in Figure 1. A schematic of the retort together with the surrounding aquifers is shown in Figure 3. The retort is taken to be 150 feet wide, 400 feet in height, and one foot thick; the thickness of one foot was chosen to simplify calculations. Since the Mahogany Zone is only about 200 feet thick at this point, the retort is extended 100 feet into the material above and below the Mahogany Zone. The Mahogany Zone is assumed to be impervious. Porous aquifer materials 300 feet and 600 feet thick overlie and underlie the Mahogany Zone, respectively. A 5000-foot-long segment of the aquifer is included, with the retort centrally located. Zones immediately above the upper aquifer and below the lower aquifer are impervious.

Potentials are established at each end of the aquifers. The potentials reflect actual conditions observed in the Piceance Creek Basin by the USGS (Ref. 1). There is a 60-foot-drop in head over the length of the model and a head that is 25 feet greater in the Upper Aquifer than in the Lower Aquifer. With these boundary conditions, flow will be from left to right. With the retort included in the system, there will also be vertical flow downward through the retort because of the difference in head in the aquifers. The model is subdivided into 200 elements with 247 nodes. Each element and node is numbered and coordinates assigned to nodes. The smaller elements are located in and near the retort, where the greatest changes in flow direction occur. Larger elements are located at the extremities of the aquifers where flow is essentially horizontal. Element sizes vary from 50 feet high by 75 feet wide in the retort to 700 feet long by 200 feet high at the ends of the lower aquifer.

Some of the key assumed input parameters are described below.

Aquifer materials. A horizontal coefficient of permeability of 0.45 feet per day was derived from the USGS estimates of transmissivity reported in the Weeks report (Ref. 1). This was assumed to be applicable to both the lower and upper aquifer material. Available data did not justify calculating different permeabilities for two aquifers. The storage coefficients for both the upper and lower aquifers were assumed to be 2×10^{-5} . The aquifer material is highly anisotropic due primarily to the layering of oil shale. Horizontal permeabilities are several times higher than those in the vertical direction. In order to investigate the effect of the vertical permeability on the flow regime, the ratio of the vertical to horizontal permeabilities was varied from 1:1 to 1:10⁶.



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Figure 3. Retort-aquifer system basic model.

Retort material. The rubblized retort is assumed to have a porosity of 20 percent. The corresponding coefficient of permeability for the retort is assumed to be 4.5 feet per day, 10 times the horizontal permeability in the aquifer. Since the laminations in the retort are broken up during rubblization, the coefficients of permeability for the horizontal and vertical directions are taken to be the same. A storage coefficient of 2×10^{-5} is assumed for the retort.

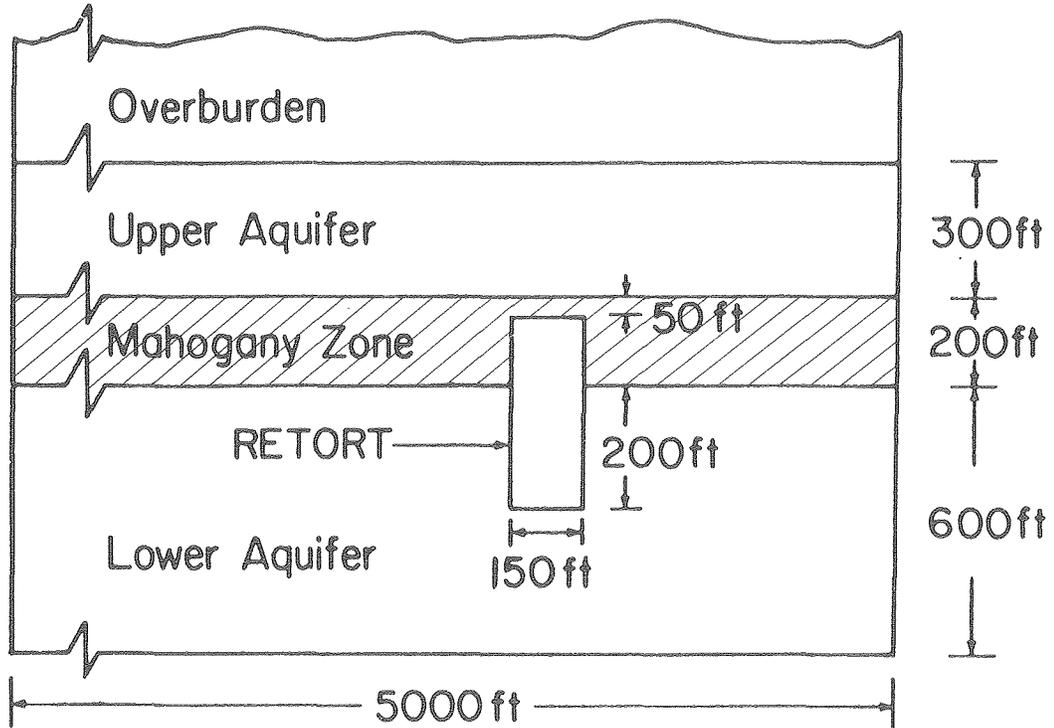
Retort cap. The position of the retort was modified for several runs. Occidental Oil, operator of Colorado Oil Shale Tract C-b, has proposed a retorting scheme somewhat different from the one shown in Figure 3. Occidental proposes to leave a cap over the retort in order to reduce or eliminate the infiltration and flow through the rubblized retort that would occur if the retort penetrated both aquifers. This cap would be composed of the impervious material of the Mahogany Zone. Two advantages of this scheme are claimed by Occidental. First, infiltration during retort rubblization would be greatly reduced; and, second, the chances of subsequent flow-through of groundwater carrying leachate would be reduced or eliminated. Correspondingly, the schematic shown in Figure 3 was modified to that shown in Figure 4. Permeabilities, ranging from 0.45 to 0.0045 feet per day, were then assigned to the cap rock to determine the effect if the material is not impervious.

Investigation of Flow Regimes

Investigations of groundwater flow regimes in the aquifer-retort system were conducted in three steps as follows:

Step 1: The main purpose of this step was to become familiar with the FLUMP program. System geometry, initial potentials, permeabilities, and storage coefficients were entered on punched cards for computer input. Program control parameters such as length of run, number of cycles, etc. were set and the time for the assumed system to reach steady-state flow was determined; isotropic flow conditions were used. The effects of pressure differences between the upper and lower aquifers were studied and results were verified by mass input-output balances.

Step 2: Anisotropic flow conditions were investigated. The horizontal (H) permeabilities of the upper and lower aquifers were held constant and the vertical (V) permeabilities allowed to vary from a V:H ratio of 1:1 to 1:1000. Flow conditions in the retort remained isotropic and permeability was held constant.



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Figure 4. Retort-aquifer system "capped" retort (see Fig. 3 for potentials).

Step 3: The effect of leaving a 50-foot-thick cap of undisturbed Mahogany Zone material over the retort was investigated. Cap permeabilities ranging from that of the horizontal permeability of the Lower and Upper aquifers to a permeability only one millionth that of the horizontal value were considered.

Eleven computer runs were made. A summary of key input variables and results for seven of these runs is given in Table 1. A discussion of the results for each of the three steps follows.

Observations

FLUMP gives complete flow distributions step-by-step over time for the period of investigation. Amount and direction of flows for the given inputs are calculated and are presented from node to node. Once the system geometry and other basic input variables have been placed on punched cards, it becomes very simple to investigate the effect of changing various inputs. Examples are illustrated in Table 1. Flow through the retort is determined as the sum of the individual flows occurring between nodes in the retort as measured on a horizontal cross section.

Runs A and B illustrate that the driving potential for flow between aquifers may be located in either aquifer. Runs B and C show the effect of changes in the ratio of the vertical-to-horizontal permeabilities. A reduction in vertical permeability from 0.45 to 0.0045 reduces the retort flow from 1.73 to 1.00 ft³/day/ft. Vertical flow in the aquifers is restrained and therefore less apt to contribute to flow through the retort. Run D shows the result of a further reduction in the V:H ratio. The retort flow is reduced to 0.68 ft³/day/ft. In other words, a reduction of the V-to-H permeability ratio to 1:1000 results in a retort flow reduction of 60 percent. Runs E, F, and G show the effect of a retort having a cap of relatively impervious rock as shown in Figure 4. These latter three runs can be compared with runs C and D on the basis of similar aquifer permeability coefficients. Since the basic configuration of the retort with respect to the aquifers is changed, the results are not directly compatible. As would be expected, however, a reduction in vertical permeability in the cap rock leads to a reduction in vertical flow in the retort.

Two additional investigations were made with lower vertical permeability values through the cap rock, but the results were inconclusive. Obvious inconsistencies in flow balances around nodes became apparent. It is presumed that the main reason is because lower permeabilities resulted in lower flows which, in turn, caused difficulties in solving the flow equations by the finite element method. Small differences tend to become lost in the solutions. Since this

Table 1. Summary of groundwater flow regime analyses: input variables and results for seven computer runs.

Run-step ^a	Length of run ^b (days)	Permeability, ft/day					Flow through retort ^d (ft ³ /day/ft)	Vertical flow velocity ^e (ft/yr)
		Aquifer		Retort		Cap ^c		
		vert.	horiz.	vert.	horiz.	vert.		
A-1	300	0.45	0.45	4.5	4.5	-	1.72	21
B-1	300	0.45	0.45	4.5	4.5	-	1.73	21
C-2	300	0.0045	0.45	4.5	4.5	-	1.00	12.2
D-2	400	0.00045	0.45	4.5	4.5	-	0.68	8.3
E-3	400	0.00045	0.45	4.5	4.5	0.45	0.39	4.8
F-3	400	0.00045	0.45	4.5	4.5	0.045	0.35	4.3
G-3	400	0.0045	0.45	4.5	4.5	0.0045	0.23	2.8

^aSee text for discussion of steps.

^bLength of runs was selected to ensure steady-state flow conditions.

^cRetort configured with cap as shown in Figure 4.

^dFlow direction in retort was upward in Run A, downward in all other runs. Flow driven by a 25 ft greater potential located in the Lower Aquifer for Run A and in the Upper Aquifer for all other runs.

^eFlow velocity based on retort porosity of 20 percent.

problem was obvious only during the investigations for the very low permeability rates, no modification was made to input variables or to the FLUMP program. Should it become necessary to make such modifications in the future, no difficulty is expected.

Flows and vertical flow velocities shown in Table 1 are valid only for the retort-aquifer model and geohydrologic parameters described herein and should not be applied to any other system unless further studies are made.

FUTURE APPLICATIONS OF GROUNDWATER MODEL

Apart from the determination of flow velocities through the retort and aquifers, the FLUMP and TRUST models have much wider applications to the problems of in-situ oil shale retorting. Narasimhan and Witherspoon (Ref. 3) have described recent developments in modeling groundwater systems in which case histories of actual applications are described.

Some potential applications of the fluid-flow models to in-situ oil shale recovery operations are listed below. These applications are not all inclusive and are intended to show only the range of problems that can be analyzed by using the FLUMP and TRUST fluid-flow models either alone or in conjunction with other models.

Migration of Pollutants

The nature of pollutant transport from spent in-situ chambers is controlled largely by the velocity of fluid flow. However, other phenomena also contribute. Dispersion occurs in the tortuous channels of the spent oil shale. There also may be reactions between the groundwater and the spent shale that change the chemical concentrations over space and time. The fluid flow equations can be modified to model the flow of chemical species by introducing terms to handle convection and chemical kinetic relationships.

Heat Transport

In the early stages of groundwater flow through the spent in-situ chambers, there will be simultaneous flow of heat and water. Two separate equation systems must be solved: fluid-flow equations based on mass conservation, and heat-flow equations based on energy conservation. These equations are similar and therefore FLUMP and TRUST can be used with minor modifications. There are, however, a few special features characteristic of heat transport. Fluid viscosity and density are dependent on temperature, and there may also be phase

changes from water to steam and vice versa. The heat transport problem may be further complicated by high-temperature reactions between the fluid and the rock and precipitation of solutes due to temperature changes.

Flow in Fractured Rocks

The stresses caused by the excavation and firing of the in-situ retorts may create systems of cracks in the rock mass. The general flow equations are still applicable although the fractures may be discontinuous to some degree. Permeability is strongly related to the aperture size which is a function of the stress-strain relations in the rock. The deformation of the solid matrix in a fracture system under stress is different from the deformation of a granular porous media as incorporated in the basic fluid flow programs. To handle deformation of a fracture system, we need to set up and solve independent stress-strain equations. The flow and stress-strain equations then have to be related through specified relationships using pore-water pressure and the stress tensor.

Deformation of Media Due to Overburden Loads

The stress changes in the aquifer and retort caused by dewatering operations and the subsequent reentry of water into the unsaturated aquifer and spent in-situ chamber may cause deformation of the solid media. Subsequent surface subsidence may then occur. The fluid-flow equation may be coupled to a soil mechanics stress-strain approach to determine the response and deformation of variably saturated soils.

SUMMARY AND CONCLUSIONS

FLUMP, an existing groundwater model developed by the staff of LBL, was applied to an aquifer in-situ retort system located in the Piceance Creek Basin. The purpose was to investigate the feasibility of using FLUMP or a similar model to simulate the underground flow regime in the aquifers in the vicinity of the retort. Actual physical and geohydrological factors were used in the model. Several runs were made to investigate the effects on flow patterns by varying the ratio of the vertical and horizontal permeabilities in the upper and lower aquifers.

An alternative aquifer-retort system was also investigated in which a cap of the impervious Mahogany Zone layer was left in place over the retort. The purpose of the cap was to isolate the retort from the upper aquifer. Several model runs were made with this later system to investigate the effects of varying the vertical permeability in the cap. A comparison of these runs based on flow through the retort is tabulated in the text.

The principal difficulty in applying a model such as FLUMP is that adequate geohydrological parameters, such as permeability, porosity, and storage coefficients, are not available. Even without these factors, however the models are useful to test system responses to variations in the several parameters.

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