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REGIONAL FLOW AND SOLUTE TRANSPORT MODELING FOR SITE SUITABILITY - PART I

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SYNOPSIS

The nature of regional flow systems in large sedimentary basins will largely determine the effectiveness of regional flow as a barrier to radionuclide escape from deep geologic repositories. The purpose of the work reported herein and the proposed future work is to develop a methodology for evaluating regional flow barriers by using numerical models. The Williston Basin was chosen as an "archetype" case for the regional modeling study. However, due to the simplified nature of the study, the results are not meant to represent the behavior of a repository actually placed within the Williston Basin.

The major components of this phase I study are:

1. Assembly and reduction of available data
2. Formulation of a simplified geohydrologic model
3. Computer simulation of fluid flow
4. Computer simulation of solute transport.

As of this report, the first two items are essentially completed. Computer simulation of fluid flow will require some revision and further study, which will be done in the second phase of this study. Computer simulation of solute transport has been considered only on a very preliminary basis.

Important conclusions of this Phase I study are as follows.

- Assembly and reduction of data require an extensive work effort. Generally, the parameters describing fluid flow are poorly known on a regional basis and those describing solute transport are unknown.

- Significant uncertainties will always be associated with regional modeling (particularly of solute transport) because of the lack of data.
- Modeling of regional flow and solute transport using numerical computer programs appears feasible, at least on an approximate basis.
- In the Williston Basin, it was relatively difficult to locate suitable repository sites at which the vertical flow was downward from the repository to deep aquifers.
- The preliminary models presented in this report need refinement and could be substantially in error because they do not consider temperature and salinity effects.

INTRODUCTION

This report presents the first part of a study to investigate the nature of regional groundwater flow systems in sedimentary basins. The purpose of the study is to develop methodology to assess the effectiveness of a regional flow system as a barrier to radionuclide escape from deep geologic repositories. Primary considerations are:

- The nature of the flow systems
- The quantity and quality of available data
- The methodology of modeling the systems
- The degree of confidence/uncertainty in the models

Golder Associates' April 1979 report, "General Basin Modeling for Site Suitability - Baseline Data", discussed general characteristics of sedimentary basins such as geology, topography, geometry, climate, etc., which affect regional groundwater flow. It was determined that a single generic basin model was not an appropriate tool for studying regional flow systems within sedimentary basins because of the extreme complexity and variability of real systems. Instead, general types of basins were identified and archetype basins representing each general type were chosen. One of the archetype basins, the Williston Basin, is used in this study to investigate regional flow systems.

Four basic steps are involved in the study.

- Assembly and reduction of available data
- Formulation of a simplified geohydrologic model
- Computer simulation of fluid flow
- Computer simulation of solute transport

These four steps should constitute the major components of any investigation into regional groundwater flow and solute transport.

A high degree of simplification and idealization was necessary in this study because of the complexities of the natural flow system being investigated and the limited scope of the study. To achieve an acceptable level of confidence in the predictive models, an actual repository siting study would require substantially more effort in the assembly and reduction of data which in turn would result in a more complex geohydrologic model. Accordingly, it is important that the results presented in this report not be taken as indicative of the actual effect of a nuclear waste repository located in the Williston basin.

This report presents the first part of the project (the balance is planned to be done as part of FY80). The data assembly and reduction phase is essentially complete and preliminary numerical models have been run based upon the simplified geohydrologic model. The actual numerical results predicted by the preliminary solute transport model are not of particular significance except to indicate the general trend and relative concentration of the solute plume in the various layers. This is because the preliminary model (1) used a mesh too coarse to yield realistic results and (2) assumed continuous injection of solute for 1 million years whereas actual canister dissolution rates are probably in the range of 100 to 10,000 years.

Further modeling work is necessary for more realistic predictions of solute transport. Future work will involve the following:

1. More detailed models (i.e., finer mesh, consideration of geologic structure, salinity, temperature, etc.)
2. A comparison with simpler models (one-dimensional, or two dimensional) and possibly a complex three-dimensional model.
3. Incorporation of climatic and manmade changes (resource development)
4. Studies of other sedimentary basins.

2.0

DESCRIPTION OF WILLISTON BASIN

2.1 GENERAL

The following description of the Williston Basin is based primarily upon published information. Because of the limited scope of this study, it was not possible to review the vast quantity of unpublished data such as oil and gas well records, drillers' logs, etc., which exist in the Williston Basin. Also, many available published documents such as data reports put out by state and local government agencies were not reviewed in detail. Thus, the following description is very general in nature and is not the result of a detailed and exhaustive review of available information.

2.2 PHYSIOGRAPHY AND CLIMATE

The Williston Basin extends over an area of approximately 200,000 square miles in North Dakota, South Dakota, and parts of Montana, Wyoming, Manitoba, and Saskatchewan. Surface topography shown in Figure 2-1 ranges from about 3,000 feet in elevation along the western margin of the basin to about 1,000 feet along the eastern margin. The maximum elevation of over 7,000 feet is in the Black Hills in the southwest, and the minimum elevation of about 700 feet is near Lake Winnipeg in the northeast.

The Williston Basin receives approximately 15 inches of precipitation annually in the western half, increasing to 20 inches near the eastern boundary. The Black Hills in the southwest also receive about 20 inches annually. Average annual evaporation from an open-water surface ranges from 40 inches in the southwest to 26 inches in the northeast. Annual potential evapotranspiration is about 26 inches over the southern part of the basin and less than 24 inches over the remainder. Surface

LEGEND
— Land Surface Elevation (feet above M.S.L.)

runoff is less than 1 inch annually except in the Black Hills and in the northeastern portion of the basin, where it is slightly over 1 inch. More precise values of evapotranspiration and surface runoff are probably available but were not found for this study.

2.3 GEOLOGY

Sources of geologic information in the Williston Basin include information from water supply wells, deep oil and gas wells, and surface geologic mapping. Sandberg's (1962) relatively detailed summary of Williston Basin geology has been extensively used in this study. Information from state and federal geologic and groundwater studies was also extensively used and is referenced in this report.

2.3.1 Stratigraphy

The Williston Basin contains over 16,000 feet of sedimentary strata which comprise three distinct lithologic assemblages. A stratigraphic column and generalized geologic cross section are shown in figures 2-2 and 2-3, respectively.

Rocks of Middle Cambrian through Middle Ordovician age are about 1,200 feet thick in the central Williston Basin and consist of clastic rocks, largely shale and sandstone, with interbeds of limestone and limestone-pebble conglomerate.

Rocks of late Ordovician through Pennsylvanian age comprise a carbonate sequence about 7,500 feet thick. They consist largely of limestone and dolomite, but include one thick salt bed, seven thinner salt beds, and several thin beds of shale.

Figure 2-2

GENERALIZED GEOLOGIC CROSS SECTION
OF WILLISTON BASIN

Figure 2-3

Rocks of Permian through Tertiary age are about 8,000 feet thick. These beds consist predominantly of shale. Connecting interbeds and lenses of sandstone and siltstone exist in the lower and upper part of the sequence, and near the base are three thin salt beds.

Proportions of the various rock types which are of Tertiary age or older (Sandberg 1962) are sandstone 13 percent, shale 48 percent, limestone and dolomite 35 percent, and evaporites 4 percent. Shale layers range to over 2,000 feet thick, and salt layers from 100 to 400 feet thick are present at depths greater than 4,000 feet (Ekren et al. 1974).

2.3.2 Structure

The Williston Basin is a bowl-shaped structural basin, as illustrated by the structural contours on Precambrian basement rock shown in Figure 2-4. The deepest part of the basin, in northwest North Dakota, lies about 14,000 feet below sea level and is slightly west of the apparent center of the basin. Major structural features in the Williston Basin are shown in Figure 2-4. Regionally, beds dip at 1 degree or less from the margins toward the center. Basement lows around the perimeter of the basin are found to the south, to the west where the Williston Basin borders the Powder River Basin, and to the north where the Williston Basin extends into the Western Canada sedimentary basin. The Black Hills in the southwest form a basement high.

Most of the major folds are on the west side of the basin, with the east and south sides containing only minor folds. Major folds include the Cedar Creek anticline, extending from northwestern South Dakota to east-central Montana; the Nesson anticline, trending north-south and located near the deepest part of the basin; and the Poplar dome on the northwest margin of the

**STRUCTURAL CONTOURS ON PRECAMBRIAN
BASEMENT AND MAJOR STRUCTURAL FEATURES
IN THE WILLISTON BASIN**

Figure 2-4

basin. The major faults are associated with folds. The largest fault offsets the west limb of the Cedar Creek anticline (Sandberg 1962).

Recent studies have revealed a more complex structural nature in the Williston than was previously thought. For instance, Brown (1978) explains the variable thickness of the Madison Limestone (Mississippian age) and of Ordovician rocks in terms of topographic expression during deposition. Brown assumes that topography during deposition reflected the following.

...deep-seated structures that were propagated upward in response to compressional stress on basement plates. Such structural adjustment could be in the form of fracture sets with little or no displacement during time of deposition or could be major shear zones with significant vertical and horizontal movement.

Figure 2-5 illustrates this relatively complex structural pattern in the Madison Limestone.

Another recent study by Shurr (1978) indicates that deposition of Cretaceous strata was similarly controlled by paleotectonic activity along hingelines between structural blocks. The boundaries of the blocks are expressed by surface lineaments which were mapped using satellite images.

2.3.3 Relationship to Geohydrologic Model

Structural contours and isopachs of stratigraphic units are used to define aquifer and aquitard layers in the geohydrologic model described in Section 3.0. Structural contours were not always available on the bottom and top of the four aquifer layers used in the geohydrologic model. Thus, the contours that were available had to be modified in some cases. Table 2-1 describes how the available contours were used to produce the structural contours and isopachs of the model layers given in Section 3.0.

ISOPACH MAP SHOWING PALEO-STRUCTURAL LINEATIONS FOR THE MADISON LIMESTONE (MISSISSIPPIAN AGE)

Figure 2-5

From Brown, 1978

TABLE 2-1
DATA SOURCES USED TO PRODUCE STRUCTURAL CONTOUR MAPS
OF THE FOUR MODEL LAYERS

MODEL LAYER	BASIS FOR STRUCTURAL CONTOURS	REFERENCES
Layer A		
-Top	Isopach map of Layer A was made based on drill-hole logs and areal extent of formations. Thickness was added to structural contours on the bottom of Layer A to produce structural contours on the top.	Armstrong, 1969 Landis, 1973 Pettyjohn and Hutchinson, 1971 Randich, 1975 Randich and Hatchett, 1966 U.S. Geol. Survey et al., 1975
-Bottom	Structural contours on the bottom of Layer A based upon a published structural contour map of the Fuson Fm (in Dakota Group) and isopachs of overlying formations up to the bottom of Layer A.	Carlson and Anderson, 1970 Sandberg, 1962
Layer B		
-Thickness	Isopachs of Layer B (Newcastle and Dakota Sandstones) are available for South Dakota and North Dakota.	Schoon, 1971 Carlson and Anderson, 1970
-Bottom	Structural contours on the bottom of Layer B based on published contours of the Fuson Fm and isopachs of overlying formations up to the bottom of Layer B.	Carlson and Anderson, 1970 Sandberg, 1962
Layer C		
-Top	Structural contours on the top of Layer C were based on published contours of the Fuson Fm and thickness of the Fall River Sandstone.	Carlson and Anderson, 1970 Sandberg, 1962
-Bottom	Structural contours on the bottom of Layer C in North Dakota were taken from published contours of the middle of the Piper FM. Contours in South Dakota were based on deep well logs.	Sandberg, 1962 Rothrock, 1946

TABLE 2-1 continued

MODEL LAYER	BASIS FOR STRUCTURAL CONTOURS	REFERENCES
Layer D		
-Top	Structural contours on the top of Layer D were based on contours of the Pre-Mesozoic surface in North Dakota. In South Dakota and Montana they were based on well logs from deep holes.	Anderson and Mendoza, 1960 Rothrock, 1946 Hopkins, 1976
-Bottom	The bottom of Layer D was taken from published structural contours on Precambrian basement rock.	Bayley and Muehlberger, 1968 King, 1969

2.4 SURFACE WATER

The Williston Basin is transected by a principal surface drainage divide running approximately from the northwest to the southeast corner of North Dakota. Surface water to the west of this divide is drained by the Missouri River and eventually reaches the Gulf of Mexico. The area to the east of the divide is drained by the Red River which flows north into Lake Winnipeg and eventually to Hudson Bay.

Many areas within the basin do not contain integrated drainage systems due to the complex glacial terrain. Other areas contain well-defined drainages eroded in glacial or alluvial deposits.

The Missouri River drains the largest portion of the Williston Basin. Its major tributaries include the Yellowstone, Little Missouri, Knife, Heart, Cannonball, Grand, Jones, and Moreau rivers. Smaller tributaries, generally occupying large glacial runoff valleys, drain the area to the east and north of the Missouri River. Many of the tributaries, including some of the larger ones, may completely dry up during part of the year.

The Red River drains the northeast portion of the Williston Basin. Its tributaries include primarily the Sheyenne, Pembina, and Souris rivers. These tributaries can also completely dry up for some time during the year.

2.5 GROUNDWATER

Groundwater occurs in numerous aquifers above the Precambrian basement rock. Data from deep aquifers are primarily from oil and gas wells which are common in many parts of the Williston. Data from shallow aquifers are available from water

supply wells. The various aquifers in the Williston Basin are grouped into four aquifer layers (A to D) in the geohydrologic model described in Section 3.0. The relationship between actual aquifers existing in the Williston Basin and the four idealized aquifers used in the model is illustrated in Figure 2-2. The following aquifer descriptions also make reference to the idealized aquifers used in the geohydrologic model.

2.5.1 Aquifer Descriptions

Aquifers do not necessarily follow the same boundaries as stratigraphic units and thus are rather difficult to define based on geology alone. Many rock units within the basin are subject to facies changes over relatively short distances, which can significantly change hydraulic properties. The formations described below should not be considered uniform with characteristic hydraulic conductivities, porosities, heads, and gradients. Rather, the hydrologic properties will, in many instances, vary greatly in both vertical and horizontal directions, even within the same formation.

- Precambrian Aquifer (Lower Impermeable Boundary)

The Precambrian crystalline rocks underlie all of the Williston Basin and outcrop only outside the basin margins and in the Black Hills. They may yield small quantities of water from fractures near the southern and eastern perimeter of the basin. They are considered to be functionally impervious over the remainder of the basin.

- Paleozoic Aquifers (Layer E)

Groundwater occurs in confined Paleozoic aquifers throughout the Williston Basin to maximum depths of about 14,000 feet below sea level in northwestern North Dakota. Data on these aquifers are limited and thus

areal extent, thickness, and interconnection of these aquifers cannot be accurately determined in most areas. The Paleozoic aquifers are generally treated as one unit in the deeper areas of the Williston Basin. Water is found in fine sandstones, which generally yield small quantities, and porous cavernous limestones, which may yield very large quantities. Oil well exploration throughout the basin, and water wells (particularly near the basin edges) have yielded some information on the Paleozoic aquifers. Confined aquifers yielding or capable of yielding water in the South Dakota portion of the Williston include the Deadwood, Winnipeg, Red River, and Minneiusa formations along with the Madison Group (South Dakota State Geological Survey 1975). Brine is produced in conjunction with oil in many formations. Oil is currently being recovered from reservoirs in the Red River, Interlake, Winnipegosis, Duperow, Bakken, Madison, Tyler, and Spearfish formations (Borchert 1977).

Water quality within the Paleozoic aquifers is generally low. Brines produced with oil may contain over 300,000 mg/l total dissolved solids. Quality generally deteriorates toward the center of the basin, with the highest quality found near the basin margins where the aquifers are recharged with fresh meteoric waters. Typical water quality in the Paleozoic aquifers ranges from 14,000 to 54,000 mg/l in eastern North Dakota; from 58,000 to 140,000 mg/l in north-central North Dakota; and from 200,000 to 330,000 in western North Dakota.

- Upper Jurassic-Lower Cretaceous Aquifers (Layer C)

The major aquifer in this interval is the Dakota Group aquifer comprised of the Lakota and Fall River

sandstones. It consists of interbedded quartzose sand and shale, with sand predominating in the east and shale predominating in the west. The aquifer underlies most of the Williston Basin and ranges in depth from 100 feet along the eastern margin to over 5,600 feet in the center of the basin.

The Dakota Group is under artesian pressures high enough to cause outflow at the surface along the eastern margin of the Williston Basin. Aquifer development has resulted in an uneven piezometric surface. Withdrawal for stock, irrigation, and domestic use has caused a pressure decline in the eastern side of the basin. In the north-central and western regions of North Dakota, water has been pumped from the Dakota into deeper formations to maintain oil field pressures. Brine produced in conjunction with oil has also been reinjected into the aquifer. This over-pressurized the aquifer at some locations, particularly north of Minot, North Dakota.

Water quality within the Dakota, although variable, is usually higher near the basin margins with meteoric (recharge areas) and lower near the basin center. Quality near the margins ranges from 1,000 to 10,000 mg/l. The lowest quality found in the basin center is about 11,000 mg/l.

● Newcastle-Dakota Aquifer (Layer B)

This aquifer consists of the Newcastle Sandstone in the western part of the basin and the prolific Dakota Sandstone in the southeast. It is a major source of water for South Dakota and has been extensively used since the early 1900's. Current use is estimated at 36.5 million gallons per year (Schoon 1971).

Water quality within the aquifer is generally 1,800 to 2,300 mg/l total dissolved solids in wells drilled east of the Missouri River. West of the Missouri River, water in wells ranges from less than 1,000 mg/l to over 6,000 mg/l. Schoon (1971) defines three types of water in the Newcastle-Dakota aquifer: (1) a sodium chloride water which occurs in the northwestern two-thirds of South Dakota and is described as mostly connate, (2) a sodium sulfate water which extends in a belt from south-central to northeastern South Dakota and originates from the underlying Dakota Group aquifer, and (3) a calcium sulfate water which occurs in southeastern South Dakota and originates from underlying Paleozoic aquifers.

- Pierre Shale (Aquitard-Repository Layer)

The Pierre Shale is an aquitard with low hydraulic conductivity. For the purpose of this study, it is assumed to be the location of a hypothetical nuclear-waste repository. In some localities where it outcrops, the Pierre Shale is an aquifer. The only source of water is from fractures which extend down several hundred feet. These fractures generally do not yield significant water much below 100 feet.

The hydrologic characteristics of the Pierre Shale are not well known where it occurs buried at depth. Values of permeability and porosity have not been adequately evaluated. The degree of fracturing at depth and whether open fractures exist at all is not known.

The water quality of the Pierre near outcrops is extremely variable (ranging from 700 to 12,500 mg/l). The water quality in the Pierre near the central portions of the basin has not been measured.

- Fox Hills-Hell Creek Aquifer (Layer A)

The Fox Hills-Hell Creek aquifer consists of interbedded sand, clay, silt, and lignite. It contains many individual sand lenses, generally medium- to fine-grained, which extend only a few miles areally. These individual permeable layers are found in both the Fox Hills and Hell Creek formations. However, since they appear to be hydraulically connected, they are treated as one aquifer. The depth to the top of the aquifer increases from several feet near outcrop areas to more than 1,400 feet at the center of the basin.

- Fort Union Aquifer (Layer A)

The Fort Union aquifer overlies the Fox Hills-Hell Creek aquifer. It is formed by interbedded sand, silty clay, clay, and lignite beds, with most beds traceable over distances less than 1 mile. The aquifer is confined except at outcrops and may be over 1,100 feet deep near the basin center. Several local aquifers probably exist within the Fort Union at any point, but they are considered as one unit in this study.

Water quality within the Fort Union ranges from 200 to 6,700 mg/l total dissolved solids. The high dissolved solids concentrations are found in areas covered with glacial drift, usually at depths of 300 feet or less.

- Glacial and Alluvial Aquifer

Glacial drift aquifers are scattered throughout the glaciated parts of the Williston Basin. They form the most important source of groundwater in many areas and are generally unconfined, but may be locally confined by silt and clay layers. Water level elevations are dependent upon local variations in topography and follow no regional pattern. Water quality varies widely.

Surficial outwash deposits generally contain less than 1,000 mg/l in areas with sufficient discharge for adequate flushing. In small enclosed glacial-fluvial deposits or areas of low topography, water quality is lower, sometimes exceeding 5,000 mg/l. Along the eastern margin of the basin, water in glacial drift may contain as much as 26,000 mg/l total dissolved solids, although it is usually less than 10,000 mg/l. This is thought to indicate contamination from the underlying Paleozoic and Dakota aquifers along the eastern edge of North Dakota.

Alluvial aquifers are also present along modern and ancient buried stream channels. These may constitute an important local source of water, but the aquifers are of limited depth and areal extent. Water levels are generally closely related to the level of the river or stream in the valley. Quality is generally good, due to constant flushing by the river. Buried stream valley aquifers range from 400 to 2,500 mg/l in dissolved solids.

2.5.2 Hydrologic Properties

Few data relating to hydrologic properties of the aquifers and aquitards in the Williston Basin were found. Those available were generally measured at shallow depths and are probably applicable only to very local areas. Table 2-2 lists the miscellaneous data that were found. Both field and laboratory test results are represented.

A substantial volume of data is available from petroleum well drill stem tests and, to a lesser extent, core tests. These data were not readily available from published sources and therefore were beyond the scope of this particular study. A

TABLE 2-2
MISCELLANEOUS VALUES OF HYDROLOGIC PARAMETERS IN THE WILLISTON BASIN
AND POWDER RIVER BASIN

FORMATION	MODEL LAYER	TEST	HYDRAULIC CONDUCTIVITY (cm/sec)	POROSITY	SPECIFIC STORAGE (m ⁻¹)	REFERENCE
1. Fort Union Sandstone	A	Field	3.7×10^{-4} and 1.2×10^{-4}			Lowry, 1966
2. Fox Hills Sandstone	A	Lab	2.5×10^{-3} to 5.6×10^{-3}			Randich, 1977
3. Lakota & Fall River Sandstone	C	Field	7.4×10^{-5} to 5.4×10^{-4}			Armstrong, 1971
4. Lakota & Fall River Sandstone	C	Field	1.2×10^{-2} 3.6×10^{-2}		2.0×10^{-6} 9.8×10^{-7}	Jensen and Klausing, 1971
5. Madison Group (except Charles Fm)	D	Field	3.5×10^{-4} to 5.1×10^{-4}			Konikow, 1976
6. Charles Formation	D	Lab	9.7×10^{-8}	0.084		Murray, 1960
7. Red River Formation	D	Lab	1.6×10^{-5} 9.7×10^{-7}	0.119 0.063		Murray, 1960
8. Madison Limestone (Powder River Basin)	D					Wyoming State Engineer, 1976
- near Bighorn Mtns.		Field	5.4×10^{-4} to 6.0×10^{-3}		1.4×10^{-7} to 1.9×10^{-7}	
- near Laramie Range		Field	1.9×10^{-4} to 3.8×10^{-4}		2.4×10^{-7}	
- near Hartville Uplift		Field	1.6×10^{-4} to 4.7×10^{-4}		5.2×10^{-8} to 1.0×10^{-7}	
- near Newcastle, Wyo.		Field	5.9×10^{-4} to 1.8×10^{-3}		7.6×10^{-8}	

detailed basin study (like those currently being conducted by the U.S. Geological Survey of the Powder River and Williston basins) may have thousands of drill-stem tests available for data. Generally, these tests are limited to particular formations and outproducing zones and to particular regions within a basin. Supplementary deep hydrologic data will be necessary in any detailed basin study.

Test results from two deep wells drilled by the U.S. Geological Survey for the purpose of obtaining hydrologic data are given in Table 2-3. Location of the two wells is given in Figure 2-8. Heads are estimated from down-hole pressure measurements and are in terms of freshwater head. Hydraulic conductivities are also in terms of freshwater at 20°C. Actual water temperatures were substantially higher, ranging up to 75°C.

2.5.3 Piezometric Head

Contours of piezometric head in terms of freshwater are given for each of the four layers used in the model in figures 2-6 to 2-9. They have been estimated from published head contour maps and isolated head or pressure measurements in individual wells. Freshwater head is defined by the height to which a column of water with density equal to 1.00 g/cm³ would rise in a standpipe piezometer located within the aquifer. This will be greater than the actual height of water measured in a piezometer if the aquifer contains saline water with density greater than 1.00 g/cm³.

Vertical head variations between different formations within one aquifer layer are common. Where possible, the head within a single formation was used for consistency in developing the contour maps. Even so, each head map is to some degree a

TABLE 2-3
MEASURED PERMEABILITIES AND HEADS FROM USGS TEST WELL NO. 1 (CROOK CO., WYOMING)
AND TEST WELL NO. 2 (CUSTER CO., MONTANA)

FORMATION	INTERVAL TESTED (ft below LS)	INTRINSIC PERMEABILITY (md)	HYDRAULIC ^(a) CONDUCTIVITY (cm/sec)	ESTIMATED HEAD ^(a) (ft above LS)
<u>Test Well No. 1^(b)</u>				
Minnekahta	1,486 - 1,561	242.1	2.3×10^{-4}	108
Minnelusa & Amsden	2,204 - 2,284	23.6	2.3×10^{-5}	84
Red River	3,286 - 3,466	1,952.2	1.9×10^{-3}	92
Madison (Mission Canyon)	2,516 - 2,556	29,016.8	2.8×10^{-2}	72
Madison (Charles & Mission Canyon)	2,420 - 2,516	1,596.8	1.5×10^{-3}	90
			Avg 3.4×10^{-3} (d)	
<u>Test Well No. 2^(c)</u>				
Minnelusa	6,118 - 6,228	3.1	3.0×10^{-6}	699
Red River	8,099 - 8,339	9.6	9.3×10^{-6}	763
Devonian (undifferentiated) and Interlake	7,759 - 7,999	2.6	2.5×10^{-6}	889
Madison (Lower Mission Canyon and Upper Lodgepole)	6,798 - 7,038	3.4	3.3×10^{-6}	814
Madison (Mission Canyon)	7,048 - 7,288	2.8	2.7×10^{-6}	836
Winnipeg Sandstone and Deadwood	8,504 - 9,378	342.9	3.3×10^{-4}	799
			Avg 1.5×10^{-4} (d)	

(a) Based on freshwater at 20°C

(b) Land surface (LS) is 3,604 feet above sea level

(c) Land surface (LS) is 2,793 feet above sea level

(d) Average hydraulic conductivity =
$$\frac{\text{combined length of intervals tested}}{(\text{length of interval})(\text{hydraulic conductivity of interval})}$$

References: Blankennagel, 1977; Brown, 1977

HEAD CONTOURS IN LAYER A

Figure 2-6

LEGEND

- Published Head Contour (in feet)
- - - Estimated Head Contour (in feet)
- Measured Value

Note: Refer to Table 2-4 for sources of data

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Project No. _____ Date _____
Reviewed _____

HEAD CONTOURS IN LAYER B

Figure 2-7

LEGEND

- Published Head Contour (in feet)
- - - Estimated Head Contour (in feet)
- Measured Value

Note: Refer to Table 2-4 for sources of data

Project No. _____ Date _____ Reviewed _____

END

- Published Head Contour (in feet)
- Estimated Head Contour (in feet)
- Measured Value

Notes: Refer to Table 2-4 for sources of data

HEAD CONTOURS IN LAYER D

Figure 2-9

LEGEND

- Published Head Contour (in feet)
- - - Estimated Head Contour (in feet)
- Measured Value

Note: Refer to Table 2-4 for sources of data

composite of piezometric potentials in the different formations represented by the model layer and as such may not agree very closely with other head contour maps or individual measured values for a particular formation.

Table 2-4 indicates the various data sources used to develop the head maps. Lack of knowledge about factors such as land surface elevation (many water levels are given only in terms of the depth below land surface), pumping history of the measured wells or nearby wells, water quality, and well completion details (many wells are open to several aquifers, shallow aquifers included) make the estimated head contours very uncertain.

TABLE 2-4
DATA SOURCES USED TO PRODUCE HEAD CONTOUR MAPS OF THE FOUR MODEL LAYERS

MODEL LAYER	BASIS FOR HEAD CONTOURS	REFERENCES
Layer A	Contours are based upon single hole measurements primarily from the Fox Hills Sandstone. No regional head contours for formations in Layer A were found.	Armstrong, 1975 Brown, 1977 North Dakota Geological Survey, 1973 Randich, 1975 U.S. Geological Survey, 1972
Layer B	Regional contours in South Dakota are based on water levels measured prior to 1909 by Darton. They should reflect minimal influence from water well withdrawal since water use was relatively small.	Darton, 1909 Schoon, 1971
Layer C	Contours in Canada are from a hydraulic head map by Hitchon of the Lower Cretaceous Mannville Group which is equivalent to the Dakota Group in the U.S. Single hole measurements are from wells in the Dakota Group.	Armstrong, 1969, 1975 Blankennagel, 1977 Brown, 1977 Hitchon, 1969 Jensen and Klausning, 1971 North Dakota Geological Survey, 1973 Randich, 1977 Swenson, 1968 U.S. Geological Survey, 1969
Layer D	Contours in Canada are from a hydraulic head map by Hitchon of the Upper Devonian Woodbend Group (equivalent to Jefferson Group in U.S.). Contours in U.S. along western side of the basin are from a hydraulic head map of the Madison Group by Konikow. Single hole measurements are from the Madison Group.	Blankennagel, 1977 Brown, 1977 Hitchon, 1969 Konikow, 1976 U.S. Geological Survey, 1972

3.0

GEOHYDROLOGIC MODEL

3.1 GENERAL

Based upon the geology and geohydrology of the Williston Basin presented in Section 2.0, a simplified geohydrologic model was formulated that could be readily used in the fluid flow and mass transport computer programs. The basic components of the geohydrologic model include the following:

- Aquifer layers (confined aquifers)
- Reservoir layer (shallow water table aquifers, lakes)
- Separator layers (confining layers between aquifers or between an aquifer and a reservoir)
- Hydrologic parameters
- Boundary and initial conditions.

The basic data used to develop the geohydrologic model are given in Section 2.0. To illustrate the various components of the geohydrologic model, computer plots of structural contours and isopachs for each layer in the model are used. The elevation, thickness, areal extent, etc., of the various layers in the geohydrologic model may differ somewhat from that of the actual formations as a result of simplification from a complex, real basin to a less complex model of a basin which can be simulated by computer.

A schematic drawing of a portion of the geohydrologic model and the finite element mesh is shown in Figure 3-1. It clearly illustrates the layer-cake approach used to simulate the three-dimensional flow system. The components of the geohydrologic model are discussed below. The formulation of the computer model using the finite element mesh is described in Section 4.0.

SCHEMATIC ILLUSTRATION OF THE QUASI-THREE-DIMENSIONAL MODEL

Figure 3-1

Not to Scale

① Schematic Cross Section Through a Portion of the Williston Basin

② Finite Element Mesh

The layers in the geohydrologic model are subdivided areally into zones with each zone defined by a particular material type. The hydrologic properties within a material type are assumed to be homogeneous. Changes in aquifer properties are reflected by changes in material type within a particular layer.

3.2 Aquifer Layers

The sedimentary strata in the Williston Basin contain numerous aquifers primarily in sandstone and limestone. These aquifers were grouped into four model layers for the purpose of modeling. Each model layer contains from several hundred to several thousand feet of strata which are made up of individual aquifer and aquitard layers. The relationship between the formations in the Williston Basin and the layers used in the geohydrologic model was shown in Figure 2-2.

3.2.1 Layer A

The Layer A aquifer consists of the Fort Union, Hell Creek, and Fox Hills formations. Structural contours on the bottom of Layer A are given in Figure 3-2 and thickness of the layer is given in Figure 3-3. The aquifer layer extends over the central portion of the basin and west into Wyoming and Montana. It is hydraulically connected with the Missouri River along its southern margin where the river has eroded through overlying rocks. The entire aquifer layer is represented by one material type (Mat 1), as shown in Figure 3-4.

Layer A is confined on top by either a siltstone and shale sequence or glacial drift. It is confined below by the Pierre Shale, which for the purpose of this study is assumed to be the repository layer.

STRUCTURAL CONTOURS ON THE BOTTOM OF LAYER A

Figure 3-2

LEGEND

—500—Elevation in feet

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

ISOPACH MAP OF LAYER A

Figure 3-3

LEGEND

Thickness in feet

LEGEND

Material Type	Description
①	All Layer A

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

3.2.2 Layer B

The Layer B aquifer extends over the southern portion of the basin but is largely absent in the north. Structural contours of the bottom of layer B and isopachs of thickness are shown in figures 3-5 and 3-6, respectively.

Layer B is comprised of the Newcastle Sandstone (Mat 3) in the west, which grades into the Dakota Sandstone (Mat 2) toward the east. The two material zones are shown in Figure 3-7.

Layer B is overlain by the Mowry and Belle Fourche shales and is underlain by the Skull Creek Shale. Towards the eastern side of the basin the Skull Creek is absent and Layer B is directly underlain by Layer C. Layer B outcrops in the Black Hills, which is a recharge area for freshwater.

3.2.3 Layer C

The Layer C aquifer is comprised of the Lower Cretaceous Dakota Group and Upper to Middle Jurassic rocks. It extends over almost the entire basin from an outcrop in the Black Hills in the southwest to an outcrop in the northeast near Lake Winnipeg. Structural contours on the bottom of Layer C and isopachs of thickness are given in figures 3-8 and 3-9, respectively.

Layer C is represented by three material types, as shown in Figure 3-10. Material 5 is in the outcrop area, Material 6 is a zone of relatively high hydraulic conductivity, and Material 9 includes two zones of lower hydraulic conductivity.

Layer C is overlain by the Skull Creek Shale, except in the southeast where it is overlain by Layer B. It is underlain

STRUCTURAL CONTOURS ON THE BOTTOM OF LAYER B

Figure 3-5

LEGEND

—1000— Elevation in feet

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

ISOPACH MAP OF LAYER B

Figure 3-6

LEGEND

-100- Thickness in feet

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

LEGEND

Material Type	Description
②	Dakota S.S. and Newcastle outcrop
③	Newcastle S.S.

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

STRUCTURAL CONTOURS ON THE BOTTOM OF LAYER C

Figure 3-8

LEGEND

— 1000 — Elevation in feet

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

ISOPACH MAP OF LAYER C

Figure - 3-9

LEGEND

-400- Thickness in feet

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

LEGEND

Material Description:

Type

5

Outcrop in Black Hills and NE basin

6

High Hydraulic Conductivity Zone

9

Low Hydraulic Conductivity Zone

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

primarily by Middle Jurassic and Triassic sediments, including shale and evaporites. In some areas in the eastern portion of the basin it is underlain directly by Layer D.

3.2.4 Layer D

The Layer D aquifer includes a thick sequence of rocks of Permian age and older. These include porous limestone and sandstone along with some shale and evaporite. Layer D extends over most of the basin and outcrops in the Black Hills in the southwest and near Lake Winnipeg in the northeast. Structural contours on the bottom of Aquifer D and isopachs of thickness are given in figures 3-11 and 3-12, respectively.

Aquifer D is comprised of three material types, as shown in Figure 3-13. Material 7 is in the outcrop areas, Material 8 includes the major portion of Layer D, and Material 10 is a region of lower hydraulic conductivity.

Layer D is overlain either by Triassic shale and evaporite or directly by Layer C. It is underlain by Precambrian basement rocks which form the lower impermeable boundary of the geohydrologic model.

Layer D is actually composed of many individual aquifers which are to various degrees isolated from each other by confining layers. Whereas it is possible to further subdivide Layer D into component aquifers, it is not possible to accurately define all of these aquifers and confining layers within Layer D, nor is it critical for the geohydrologic model, since Layer D is far removed from the repository layer.

STRUCTURAL CONTOURS ON THE BOTTOM OF LAYER D Figure 3-11

LEGEND

~2000~ Elevation in feet

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

ISOPACH MAP OF LAYER D

Figure 3-12

LEGEND

1000 Thickness in feet

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

MATERIALS IN LAYER D

Figure 3-13

LEGEND

Material Type	Description
7	Outcrop in Black Hills and NE basin
8	High Hydraulic Conductivity Zone
10	Low Hydraulic Conductivity Zone

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

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3.3 Reservoir Layer

The Williston Basin is overlain by shallow water table and confined aquifers which are located primarily in glacial drift and alluvium and are generally of localized areal extent. The shallow aquifers are recharged primarily by local precipitation and discharge to surface streams and rivers. Water levels in these shallow aquifers are controlled mainly by local topography; thus, topographical elevation generally provides a fair approximation of water table elevation.

The geohydrologic model considers the shallow aquifers as reservoirs with constant head and an infinite water supply. This is a valid approximation for modeling as long as the shallow aquifers are not hydraulically connected to any large degree with the deeper, confined aquifers. This appears to be the case over most of the Williston Basin. Reservoirs are also a valid approximation where aquifers are directly connected to large quantities of water such as lakes, rivers, or shallow aquifers with high recharge rates. Such conditions exist over the discharge area of the deep aquifers in the northeast portion of the basin near Lake Winnipeg.

Reservoirs are specified in the geohydrologic model for all aquifers that can leak directly to or from the ground surface (outcrop, shallow aquifer, or lake). In the computer program, reservoir heads are specified on an element-by-element basis. Reservoir head in an element is set equal to the average land surface elevation for that particular element. This introduces some error, since the water levels in shallow aquifers are not always coincident with the land surface but instead can be up to several hundred feet below. Generally, however, the elevation of major stream and river channels is a good approximation to the water table.

The major advantage in using reservoirs to model shallow aquifers is that it significantly reduces the number of elements in the computer model by eliminating the need for defining a separate aquifer layer for the shallow aquifers. This saves substantial computation time and expense.

3.4 SEPARATOR LAYERS

The four aquifer layers are generally separated vertically from each other and from the reservoirs by low permeability aquitards which are referred to in the model as separator layers. The formations comprising the separator layers are shown in the geologic column in Figure 2-2 and are composed mainly of shale or evaporite.

Flow in the separator layers is assumed to be strictly vertical in the model. This is a good approximation when separator hydraulic conductivity is several orders of magnitude lower than aquifer hydraulic conductivity.

The thickness of the separators has not been contoured specifically; however, it can be determined by taking the difference in elevation between the top of the aquifer layer underlying the separator and the bottom of the aquifer layer overlying it. In areas where two aquifer layers are in contact (i.e., no aquitard exists), a minimal separator thickness, generally 10 feet, has been assumed in order to simulate the effects of low vertical hydraulic conductivity, which is usually characteristic of layered sedimentary strata. Experience has shown that the ratio of vertical to horizontal hydraulic conductivity within a layer usually ranges between 1:1 to 100:1, although ratios outside of this range are also possible.

Assuming a 100:1 ratio of vertical-to-horizontal hydraulic conductivity within an aquifer, a typical aquifer thickness of 500 feet, and a typical aquifer horizontal hydraulic conductivity of 5.170×10^3 ft/yr (5×10^{-3} cm/sec), the vertical resistance to flow in the aquifer is defined by:

$$\frac{K_v}{L} = \frac{5.170 \times 10^1 \text{ ft/yr}}{500 \text{ ft}} = 1.035 \times 10^{-2} / \text{yr}$$

For an equivalent resistance to flow in a 10-foot separator layer, it must have a vertical hydraulic conductivity of 1.035×10^{-1} ft/yr (10^{-7} cm/sec), as shown below:

$$K_v = 10 \text{ ft} \times 1.035 \times 10^{-2} / \text{yr} = 1.035 \times 10^{-2} \text{ ft/yr}$$

This is the value of separator hydraulic conductivity used in the model at contact areas. The actual value of hydraulic conductivity is not critical, since experience has shown that heads in the two aquifers in contact will equilibrate over relatively short distances even at values of separator conductivity less than 1.035×10^{-1} ft/yr (10^{-7} cm/sec).

A nominal separator thickness was also used to simulate lower vertical hydraulic conductivities in areas where aquifer layers outcrop, as described in Section 4.4.1.

Material types are assigned to the various separators in a manner similar to that used for the aquifer layers. Figures 3-14 to 3-17 show the separator material types overlying each aquifer layer. Also indicated is the type of leakage connection which can connect two aquifer layers or connect an aquifer layer and a reservoir.

SEPARATOR MATERIALS ABOVE LAYER A

Figure 3-14

LEGEND

Material Type

Leakage Connection

(23)

Layer A and Reservoir

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

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Project No. _____ Date _____
Reviewed _____

LEGENDMaterial
TypeLeakage
Connection

⑬

Layer B and Layer A

⑭

Layer B and Reservoir
(outcrop area)

⑮

Layer B and Reservoir

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

Layer C and Layer B

Layer C and Layer A

Layer C and Layer B

(contact area)

Layer C and Reservoirs

(outcrop area)

Layer C and Reservoir

SEPARATOR MATERIALS ABOVE LAYER D

Figure 3-17

LEGEND

Material Type

Leakage Connection

(17)

Layer D and Layer C

(18)

Layer D and Layer C (contact area)

(28)

Layer D and Reservoir (outcrop area)

(29)

Layer D and Reservoir

Scale in Miles
0 40
Scale in Kilomet
0 40 80 1

3.5 HYDROLOGIC PARAMETERS

Because of the long times involved in the studies, only simulations of the average steady-state flow in the basin were performed. Hydraulic conductivity was thus the major hydrologic parameter required, and specific storage and specific yield were not needed. Other parameters such as distributed inflow/outflow, evapotranspiration, etc., were also not used in the model which used fixed-head "reservoirs" as the boundary condition at the ground surface.

Hydraulic conductivity was assumed to be horizontally isotropic in all layers. Since the program assumes no vertical head gradients in the aquifer layers, no values of vertical hydraulic conductivity were specified. Similarly, no horizontal hydraulic conductivity was specified for the separator layers, since flow was assumed to be strictly vertical.

The initial hydraulic conductivities assigned to the aquifer layers and separators were estimates based upon rock type and a few measured values such as given in Section 2.0. These initial estimates were later modified according to the results of the computer simulations until the final values gave a reasonably good fit between computed and observed piezometric conditions, as discussed in Section 4.4.2. Actual measured values of hydraulic conductivity are few and generally pertain to only a small vertical section of an aquifer layer at a specific location. Thus, the available hydraulic conductivity data discussed in Section 2.0 was only of limited use.

3.6 BOUNDARY AND INITIAL CONDITIONS

3.6.1 Western and Eastern Boundaries

The geohydrologic model does not include the complete flow paths from recharge to discharge of all aquifers in the Williston Basin. Layers C and D receive some recharge at outcrops in the Black Hills, but the primary source is to the west at outcrops in Wyoming and Montana. This recharge enters the Williston Basin as subsurface flow along the western edge of the area considered in the geohydrologic model. Since the amount of recharge to the Williston occurring as underflow from Wyoming and Montana was not known, the boundary along the west side of the basin was set at a constant head rather than a specified inflow. The discharge zone for layers C and D occurs where the layers outcrop in the northeast portion of the basin and is included within the geohydrologic model. Most of the eastern boundary of the geohydrologic model is formed by outcrop of Precambrian basement which is modeled by a no-flow boundary condition.

3.6.2 Southern and Northern Boundaries

The southern boundary of the geohydrologic model is approximately parallel to streamlines in layers B, C, and D and thus can be considered as a no-flow boundary. The northern boundary of Layer B is impermeable, since the aquifer layer thins to zero thickness in the north. The northern boundary of layers C and D is set at a constant head determined from the observed piezometric head plots.

Layer A is almost entirely contained within the model area. The western edge of the layer which extends beyond the model area into Montana is set as a constant head. The remainder of the aquifer layer is delimited by a no-flow boundary.

Constant head boundary conditions assigned to the geohydrologic model and used in the computer simulation are in most cases based upon relatively poorly defined piezometric head contours (figures 2-6 to 2-9). This is the result of the general lack of available data relating to head, particularly in the deeper aquifers.

No initial conditions are needed for the steady-state simulation. Should transient cases be considered in the future, initial conditions can be set to those calculated in the steady-state case. Possible scenarios requiring transient analysis include pumping, mining, and climatic change.

3.8 UNCERTAINTY

Major uncertainties are associated with the geohydrologic model. These uncertainties are discussed in Section 4.5.2.

4.0 DESCRIPTION AND RESULTS OF FLUID FLOW COMPUTER PROGRAM

4.1 GENERAL

The geohydrological model of the Williston Basin was formulated so it could be readily incorporated into Golder Associates' Groundwater Computer Package. The Groundwater Computer Package is an integrated suite of computer programs which mathematically simulate the hydraulic and solute transport characteristics of groundwater flow in regional aquifer systems. Additional computer programs are included in the package to provide auxiliary services such as input data preparation, presentation of model results, and calibration of field data with model results. A technical summary of the Groundwater Package is provided in Appendix A, along with references to the theory and user manuals.

The Groundwater Computer Package incorporates the finite element method for the solution of the fundamental equations governing flow and solute transport in various groundwater flow systems. The package can be used to model both steady-state and transient flow conditions in three-dimensional, layered aquifer systems; however, only the steady-state option was used for this study.

The package uses a quasi-three-dimensional approach for the hydraulic solution. It consists of a number of aquifer layers in which only horizontal gradients are considered (that is, heads at the top and bottom of an aquifer layer are assumed to be equivalent). The aquifers are connected vertically by separator layers in which flow is assumed to be strictly vertical. Horizontal anisotropy can be considered within the aquifer layers by the model.

The package includes four basic components which were used in this study:

- Mesh Generation and Data Input (MLTMSH, AFPOL)
- Hydraulic Solution (AFPM)
- Output Presentation (FLOCON)
- Mass Transport Solution (SOLTR).

The first three components of the package are discussed in this section, while the fourth (SOLTR) is discussed in Section 5.0. A second hydraulic solution program called FPM, which is used for two-dimensional planar or radially axisymmetric flow in a vertical section, is available in the package but was not used in the Williston Basin study.

4.2 MESH GENERATION AND DATA INPUT

The AFPM finite element computer program must be provided with information relating to the nodes, elements, and materials within the mesh. In a complicated, multi-layered aquifer system such as the Williston Basin, where the mesh contains hundreds of nodes and elements, this is most efficiently done by using a mesh generation and data preparation program called MLTMSH. The steps involved in its use are as follows.

1. Define Basic Mesh

The basic mesh defined for the Williston Basin is shown in Figure 4-1. The elements are irregular in shape because they incorporate the areal extent and outcrop areas of each of the four aquifer layers. Each node and element within the basic mesh is assigned a number.

LEGEND

- Element Boundaries
- - - Geographic Boundaries

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

2. Define Aquifer Layers

For each node in the basic mesh, the aquifer layers existing vertically at the node are defined by identifiers A to D and the elevation at the top and bottom of each layer is taken from the structural contour and isopach maps.

3. Define Layer Materials

The various material types (in the range 1 to 30) in each layer are specified as shown in figures 3-3, 3-6, 3-9, and 3-12. Each material type is later assigned hydrologic properties in the AFPOL or AFPM programs.

4. Define Aquifer Layer Separator Materials

For each aquifer layer underlain by another aquifer, the material type of the separator immediately below it is defined. The various separator materials are shown in figures 3-13 to 3-16. Separator thickness is automatically calculated from aquifer elevations. In areas where two aquifer layers are in contact (i.e., no confining layer exists), a nominal separator thickness of 10 feet is specified for resistance to flow between the layers. This resistance is due to the relatively low vertical permeability which is common in layered sedimentary aquifers.

5. Define Reservoir Separator Materials

For each aquifer connected to a reservoir, the material type and thickness of the reservoir separator are defined. The reservoir separator material types are included in figures 3-13 to 3-16.

The MLTMSH program includes extensive data checking facilities as well as various plotting capabilities. It produces an output data file containing the complete topology and geometry of the multi-layered finite element mesh. This file is then modified by AFPOL for input to AFPM.

The AFPOL program is used to assemble the remaining input data, including problem units, material properties (in this case, just hydraulic conductivity), and nodal boundary conditions required by the AFPM solution. Many of the material properties and boundary conditions defined by AFPOL were later changed during the calibration of the AFPM model.

4.3 OUTPUT PRESENTATION

The FLOCON computer program prepares finite element mesh, contour and vector plots of two- and three-dimensional groundwater flow hydraulic analysis results produced by the AFPM (and FPM) computer programs. It also prepares similar plots of groundwater contaminant transport results produced by the SOLTR computer program. The FLOCON program is the output plotting and display component for the Groundwater Computer Package.

4.4. HYDRAULIC SOLUTION USING AFPM FLOW MODEL

4.4.1 Description

The AFPM computer program uses the finite element method to model fluid flow within a multi-layered aquifer system such as the Williston Basin. The program determines fluid potentials and fluid pressures as well as flow rates, quantities, and directions in both steady-state and transient three-dimensional multi-aquifer flow regimes. Only a steady-state analysis was performed in this study.

The geohydrologic model described in Section 3.0 was simulated using the AFPM computer program. The four aquifer layers were represented by triangular and quadrilateral elements which varied in thickness and were inclined from the horizontal. The potential (head) in a layer element was presumed to be constant in the vertical direction. Aquifer layers (A-D) were separated by aquitards (separators) through which leakage could occur. Leakage was calculated by assuming a linear gradient across the separator based upon the aquifer heads and then using Darcy's law to compute flow based upon the separator thickness and vertical hydraulic conductivity. All leakage through separators is assumed to be strictly vertical between aquifer elements in the computer model. Where two aquifer layers came in contact vertically, a nominal aquitard thickness was specified to simulate the residual resistance to vertical flow between the layers. Leakage also occurred, through aquitards, between aquifer layers and reservoirs. Reservoirs were used to simulate shallow water table aquifers and bodies of surface water without treating them as separate aquifer layers.

A nominal aquitard thickness was used to separate an aquifer layer from a reservoir in areas where the aquifer layer outcropped. This artifice had the effect of setting outcrop areas to constant head boundaries while allowing easy output of groundwater discharge. In reality, the aquifers rarely outcrop at the surface but instead are overlain by glacial drift and alluvium. The nominal separator was assigned a relatively high vertical hydraulic conductivity (10,000 times greater than normal separators between aquifers) which provided a minimal resistance to vertical flow between the aquifer and the reservoir.

Input data for AFPM were prepared by the MLTMSH and AFPOL programs. Many of the parameter values were subsequently changed during calibration of the AFPM model. The calibration was accomplished by comparing computer heads against measured heads.

All parameter values used in this report are final calibrated values unless otherwise specified.

A technical summary of the Groundwater Computer Package is given in Appendix A. References are also given in Appendix A to the various user and theory manuals available which completely describe the computer package.

4.4.2 Calibration and Results

The computer model of the Williston Basin was calibrated primarily by adjusting hydraulic conductivities of the various aquifer and separator materials until computer head contours approximately matched the measured head contours for the four aquifer layers. The computed heads plotted in figures 4-2 to 4-5 for layers A to D, respectively, were compared to the measured heads shown in figures 2-6 to 2-9. The match between computed and measured heads is very approximate but is considered adequate for the purpose of this study. Table 4-1 lists for each material type the values of hydraulic conductivity used to compute the above head potentials. Hydraulic conductivities given for layers A to D are horizontal, while those given for the aquifer and reservoir separators are vertical. It became obvious during the calibration process that vertical hydraulic conductivity was a major factor in the regional flow model and that values as low as 1.035×10^{-4} ft/yr (10^{-10} cm/sec) were not sufficient to maintain large vertical head differences between aquifer layers over a regional scale.

The computed hydraulic head contours are generally much more regular in shape than the measured head contours. This is probably because irregularities in head caused by local structural and stratigraphic features are not incorporated into the finite element model. Also, measured head contours may

COMPUTED PIEZOMETRIC HEAD ELEVATIONS IN LAYER A

Figure 4-2

LEGEND

~2000~ Computed Piezometric Elevation in feet

Refer to Figure 2-6 for Measured Contours

Golder Associates

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

Project No. _____ Date _____
Reviewed _____

COMPUTED PIEZOMETRIC HEAD ELEVATIONS IN LAYER B

Figure 4-3

LEGEND

—2000— Computed Piezometric Elevation in feet

Refer to Figure 2-7 for Measured Contours

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

Golden Associates

COMPUTED PIEZOMETRIC HEAD ELEVATIONS IN LAYER C

Figure 4-4

LEGEND

Computed Piezometric Elevation in feet

Refer to Figure 2-8 for Measured Contours

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

Golder Associates

Project No. _____ Date _____
Reviewed _____

COMPUTED PIEZOMETRIC HEAD ELEVATIONS IN LAYER D

Figure 4-5

LEGEND

—2000— Computed Piezometric Elevation in feet

Refer to Figure 2-9 for Measured Contours

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

TABLE 4-1

Final Values of Hydraulic Conductivity Determined
By Model Calibration

<u>MODEL LAYER</u>	<u>MATERIAL TYPE</u>	<u>HYDRAULIC</u>	
		<u>CONDUCTIVITY-FT/YR</u>	<u>(CM/SEC)</u>
A	1	1.035×10^2	(1×10^{-4})
B	2	2.070×10^3	(2×10^{-3})
	3	1.035×10^2	(1×10^{-4})
C	5	5.170×10^1	(5×10^{-5})
	6	2.070×10^2	(2×10^{-3})
	9	5.170×10^1	(5×10^{-5})
D	7	2.070×10^2	(2×10^{-3})
	8	1.035×10^2	(1×10^{-4})
	10	1.035×10^1	(1×10^{-4})
Aquifer			
Separators	13	1.035×10^{-4}	(1×10^{-10})
	14	1.035×10^{-4}	(1×10^{-10})
	15	1.035×10^{-4}	(1×10^{-10})
	16	1.035×10^{-1}	(1×10^{-7})
	17	1.035×10^{-4}	(1×10^{-10})
	18	1.035×10^{-1}	(1×10^{-7})
Reservoir			
Separators	23	1.035×10^{-1}	(1×10^{-7})
	24	1.035	(1×10^{-6})
	25	1.035×10^{-4}	(1×10^{-10})
	26	1.035	(1×10^{-6})
	27	1.035×10^{-4}	(1×10^{-10})
	28	1.035	(1×10^{-6})
	29	1.035×10^{-2}	(1×10^{-8})

reflect irregularities caused by pumpage or injection in wells, a process which was not considered in the model. Factors causing uncertainty in both the measured and computed heads are discussed in the next section.

In order to eliminate negative pressures, model calibration also involved some minor adjustments in aquifer elevation and thickness and in reservoir elevations in the Black Hills area. Negative pressures occurred where the computed head elevation fell below the bottom of the aquifer. They were due to using a coarse mesh in areas of rapidly changing aquifer elevation and head.

The direction of flow to reservoirs from the first aquifer layer underlying them is shown in Figure 4-6. Downward flow represents areas of recharge to the aquifer layers, whereas upward flow represents areas of aquifer discharge.

The areal rate of groundwater discharge from the layers C and D outcrop area near Lake Winnipeg was calculated by the model to be approximately 3.1 inches per year. No measured values or estimates of actual groundwater discharge were found for comparison purposes. Surface runoff, which is comprised of both direct surface runoff from precipitation and groundwater base flow, is about 1 to 2 inches per year in the Lake Winnipeg area. Thus, at least some of the calculated groundwater discharge must be lost as evapotranspiration. Assuming such a loss, the calculated discharge rate from layers C and D appears reasonable. Should measured groundwater discharge (or recharge) values become available, it would constitute an important basis for additional model calibration.

DIRECTION OF LEAKAGE BETWEEN AQUIFERS AND RESERVOIRS

Figure 4-6

Recharge to layers C and D comes from overlying aquifers and from the fixed head boundary along the western edge of the mesh. Water entering the Williston Basin from the west originates in Montana and Wyoming along outcrops of these two aquifer layers beyond the area considered by the model. Much of the recharging water must flow through the Powder River Basin located in northeast Wyoming and southeast Montana before entering the Williston Basin as underflow. The volume of underflow is not known, although one estimate puts the recharge to the Madison aquifer in northeast Wyoming (a major component of Layer D) at about 3.3×10^9 ft³/yr (Wyoming State Engineers Office 1976). A look at the fixed head boundary nodes along the west side of the mesh in Layer D shows that some nodes have outflows while some have inflows, but that the net flow across the western boundary into the Williston is 5.9×10^9 ft³/yr, which compares reasonably well to the published estimate for the Madison aquifer.

There are many other types of data which can be used to help in calibrating basin flow models. In particular, hydrogeochemical studies and radioisotope studies can be extremely valuable aids to understanding both directions and rates of flow. Comprehensive data of this type were not available for the Williston Basin at the time of this study.

The purpose of this study was not to develop an accurate geohydrologic model of the Williston Basin. It was recognized that such a task would involve an enormous effort, as evidenced by the current U.S. Geological Survey study of the Madison aquifer which has been underway for several years. Rather, the purpose of this study was to develop a realistic geohydrologic model of a large sedimentary basin and to use the model to study solute transport on a regional scale. On this basis, the lack of a one-to-one correspondence between measured heads, recharge

rates, etc., in the Williston Basin and those calculated using the geohydrologic model and AFPM computer program should not invalidate the general conclusions made about solute transport on a regional scale.

4.5 UNCERTAINTY

The four-layer geohydrologic model of the Williston Basin is very simplified from the actual geohydrology within the basin. Accordingly, there is significant uncertainty in the predicted flow system. A substantially more complex (and thus more realistic) geohydrologic model would have required an effort in data acquisition and modeling which was beyond the scope of this study. Even an extremely complex geohydrologic model would probably still have major uncertainties associated with it.

The uncertainty in the predicted flow model of the Williston Basin results from three primary sources:

1. Basic geologic and hydrologic data
2. Geohydrologic model
3. Comput programs.

These sources of uncertainty will always exist to some degree when dealing with regional modeling of fluid flow and mass transport. In the present study, the uncertainty due to the first two sources is large, while that from the third source is considered to be smaller.

4.5.1 Basic Geologic and Hydrologic Data

Uncertainty is associated with the following basic data as used in the geohydrologic and computer model of fluid flow.

1. Stratigraphy. Stratigraphic elevations determined from structural contour and isopach maps are used to define aquifer thickness. Ideally, aquifers should be defined in terms of hydrologic rather than geologic boundaries. For example, a single geologic unit may have both aquifer and aquitard zones. Defining hydrologic units in terms of geologic boundaries introduces uncertainty into their actual thickness and extent. Other stratigraphic features such as facies changes, sedimentary features, depositional environment, etc., can affect the hydrologic properties of a rock unit. Such features are difficult to adequately explore and describe and introduce uncertainty into the geohydrologic model.

2. Structure. Structural features were not investigated and included as part of the geohydrologic model. Thus, a large uncertainty exists for this reason alone. Structure is often difficult to describe, and the effect of structure on the geohydrology is even more difficult. For instance, several recent articles (Shurr 1978; Brown 1978) have indicated that faulting in basement rock could have controlled the thickness and type of sediment accumulation in the Williston Basin during its geologic history. Fractures are also often associated with regional tectonic activity that is poorly understood. Such structural features can significantly affect or even control groundwater flow. Large uncertainties exist in the geohydrologic model due to structure, and significant uncertainties will probably exist in any geohydrologic model of a large sedimentary basin.

3. Hydrologic Parameters. Field measurements of hydrologic parameters are sparse, particularly in deep sedimentary basin environments. Generally, the major source of data in these areas is from oil and gas well tests and core samples. These data are useful as point measurements of permeability, temperature, quality, porosity, pressure, etc., but a large uncertainty is introduced when these point values are extended to give regional estimates. Large-scale anisotropy and heterogeneity which may control groundwater flow on a regional scale are difficult to describe using limited point measurements, and thus a significant uncertainty exists in the values of hydrologic parameters determined from field measurements. In this study, only a few measured values of hydraulic conductivity were found, and the values actually used in the model were determined by calibration of computed head potentials.
4. Head (Potential). Head, based on water levels in wells or on downhole fluid pressures, is generally one of the most easily measured and reliable hydrologic parameters. Large uncertainties in head measurements do exist in deep saline aquifers such as those in the Williston Basin. In such environments, where downhole pressures may be in terms of thousands of pounds per square inch, relatively small inaccuracies in pressure measurement (on the order of several percent or less) can result in substantial errors in estimated heads (up to 100 feet or more). In sedimentary basins where horizontal gradients are commonly several feet per mile, such errors in estimated heads can cause significant uncertainty in using measured values to predict flow gradients. Measured heads can also be influenced by temperature, salinity and nearby pumping. All of these factors

introduce uncertainty in measured heads. What effect all these factors have on measured heads in the Williston which are used to calibrate the computer model is not known.

4.5.2 Geohydrologic Model

The geohydrologic model formulated from the basic data is a much simplified model of the Williston Basin. Because it is greatly simplified from the real basin (so that it can be simulated using a computer model), there is a substantial uncertainty associated with the geohydrologic model.

1. Aquifer layers. As previously mentioned under basic data uncertainty, it is difficult to define aquifers over large areas where data are scarce. Using geologic boundaries alone without hydrologic data can often be misleading. An additional and substantial uncertainty is introduced when two or more different aquifer layers are combined into one layer in the geohydrologic model. In particular, Layer D of the present model, which can contain several thousand feet of sedimentary rock, cannot be expected to behave as a single aquifer unit as assumed in the geohydrologic model. The lack of basic data and the limited scope of this study do not allow formulation of a more complicated geohydrologic model.
2. Reservoir layer. Treatment of surface water bodies and shallow groundwater aquifers as constant head reservoirs introduces uncertainty. Although reservoirs are probably not a bad approximation for these features, a more detailed and correct geohydrologic model would treat shallow water-table aquifers as separate aquifer layers with phreatic surfaces. Such a model would

require a finer mesh, better topographic expression, and substantially more data relating to shallow aquifer characteristics, recharge/discharge, climate, aquifer extent, and past and present groundwater use.

3. Separator layers. Aquitards between aquifer layers are called separator layers in the geohydrologic model. The separators considered in the geohydrologic model are shale layers between actual aquifers within the basin. The major uncertainty associated with the separators is the degree to which they isolate one aquifer from another (i.e., their vertical hydraulic conductivity). This critical parameter is extremely difficult to measure in the field and, hence, is normally deduced during the model-calibration process. Another source of uncertainty is in areas where two aquifer layers come into contact. The geohydrologic model assumes that a nominal separator thickness of 10 feet exists between the two aquifers. In reality, vertical hydraulic conductivity within the two aquifers is probably quite low, so that the assumption of a thin separator may be a fair approximation.
4. Hydrologic parameters. Large uncertainties are associated with the values of hydraulic conductivity derived through model calibration against measured heads. These uncertainties result from anisotropy, heterogeneity, density variations, and viscosity variations (the latter two caused by temperature and salinity) which are very difficult to define and include in a geohydrologic model. Large uncertainties will probably always be associated with regional values of hydraulic conductivity and other hydrologic parameters (porosity, specific storage, distributed inflows, etc.)

because of their variable nature and the difficulties involved in their measurement on a regional scale. Calibration of computer models is probably one of the most effective methods of estimating hydrologic parameters on a regional scale, although spot measurements from well tests should be used as checks.

5. Boundary and initial conditions. Boundary conditions used in the geohydrologic model were either no-flow or specified head. Both conditions have some uncertainty because of uncertainty in the basic data, as described in Section 4.5.1. More appropriate boundary conditions for the geohydrologic model would be specified recharge and discharge rates; however, these conditions were not possible to use because of lack of data. Uncertainty also results because not all of the real aquifers constituting a single aquifer layer in the geohydrologic model are subject to the same boundary conditions. Thus, typical or average conditions must be used. No initial conditions were specified because the analysis was of steady-state conditions only.
6. Other factors. There are major uncertainties resulting from factors not considered in the geohydrologic model. Temperature, which generally increases with depth, causes corresponding increases in hydraulic conductivity due to decreased fluid viscosity. Salinity variations within an aquifer and between aquifers can cause flow in directions quite different from those caused by the apparent head gradients. Salinity variations in the Williston Basin are the rule rather than the exception. For example, it is thought that a highly saline zone in the central portion of the Williston Basin acts as a barrier to flow, causing deflection of flow to the east (personal communication with U.S. Geological Survey).

Flow deflection can result because dense saline water tends to collect and settle in the deeper aquifers near the center of the basin. The less dense freshwater coming from recharge cannot displace the dense saline water but instead flows around it. Head potentials alone can be misleading unless density differences are recognized and compensated for. For instance, the direction of flow based upon both observed and simulated head potentials in the Williston Basin is to the northeast, directly through the saline zone.

Consideration of density variations was not possible using the current computer model. This may have led to substantial errors in the predicted flow paths. Factors such as horizontal anisotropy, heterogeneity, and preferred pathways along structural features are not addressed in the geohydrologic model and are the source of major uncertainties.

4.5.3 Computer Program

Uncertainty is associated with the finite element program used to exercise the geohydrologic model. The uncertainty arises from the numerical scheme and certain simplifications used in the program. Specific uncertainties include the following.

1. Size of mesh. Because the Williston Basin is very large, a moderately coarse mesh was used in order to keep the number of nodes and elements to reasonable levels. Since element properties are either constant within an element (hydraulic conductivity, reservoir elevation, etc.) or vary linearly between nodes (head, velocity, etc.), the use of large elements on the order of 40 mile across results in some uncertainty, since real propertie can vary significantly and in a non-linear manner within elements of this size.

2. Aquifer flow. Flow within aquifers is assumed to be strictly parallel to the layer. Thus, gradients across an aquifer layer are not considered, though this would be the case in a true three-dimensional model. Vertical gradients within aquifers are probably important to consider when the aquifers are on the order of thousands of feet thick (i.e., Layer D), and some uncertainty results when they are not considered. Vertical flow within aquifers is particularly important with respect to mass transport analysis.
3. Separator flow. Flow between aquifer layers or between an aquifer and a reservoir is assumed to be strictly vertical and instantaneous. In most situations, the assumption on strictly vertical flow within separators is nearly correct if the hydraulic conductivity of the separator is several orders of magnitude lower than that of the aquifer, as is the case in this model. Instantaneous flow does not cause any uncertainty in the hydraulic solution, since time is not a factor in steady-state flow. However, uncertainty is introduced by the assumption of instantaneous flow with respect to mass transport, since solute residence time within separators cannot be considered by the computer program as it is currently coded. Instantaneous flow would also cause uncertainties if phenomenon requiring transient hydraulic solutions (i.e., wells, mines, climate change, etc.) were considered.
4. Temperature effects. The program does not consider the effects of temperature upon viscosity and density.

5. Salinity effects. The program does not consider the effects of salinity. This is considered a major uncertainty, since entire regional flow systems may be substantially affected by fluid density.
6. Mass balance. No checks are made in the computer program to verify that mass balance is maintained. The algorithm for the steady-state solution forces continuity of mass, and the only possible errors are due to round-off. Theoretically, there could be errors in the mass balance during a transient hydraulic solution if time steps in the analysis are too large. To date, no mass-balance errors have been detected when program results are checked against analytical results or against field data. However, it is very difficult to detect small-mass balance errors by checking against other results. Since no transient hydraulic analyses were run at the Williston Basin, there is no uncertainty due to mass balance in the hydraulic solution.

5.0 COMPUTER SIMULATION OF SOLUTE TRANSPORT

5.1 GENERAL

The results of the AFPM hydraulic solution were used in the SOLTR computer program to predict solute transport from a constant point source (i.e., the repository) located in Layer B. The purpose of the simulation was to study regional mass transport and the methodology involved in modeling it. Also it provided an opportunity to assess the performance of the SOLTR computer program using a model of regional scale. It was not expected that the results would be a realistic prediction of solute transport in the Williston Basin because of the enormous uncertainties in the hydraulic flow system and in the values of solute transport material properties. However, the results produced by SOLTR do indicate the general growth pattern of a solute plume within a large sedimentary basin over a time period of 1 million years.

In addition, the results presented in this chapter represent a preliminary analysis using an extremely coarse mesh and non-realistic rates of nuclide dissolution.

5.2 SOLUTE TRANSPORT PROGRAM - SOLTR

The SOLTR finite element computer program predicts solute transport histories throughout a specified region in a multi-layered aquifer system modeled by the AFPM program (or a planar or axisymmetric system modeled by FPM). Output from AFPM (or FPM) in the form of a checkpoint file is directly input into SOLTR to define the steady-state or transient hydraulic conditions existing within the mesh. Additional input data to

SOLTR provided by the user includes solute transport material properties plus nodal boundary and initial conditions. SOLTR output concentrations are presented in tabulations and in optional computer plots.

5.2.1 Input Data

The major portion of input data to SOLTR is a description of the groundwater flow velocities within the mesh. Velocities are supplied by a checkpoint file created by the AFPM (or FPM) computer program which is read directly by SOLTR.

Data which must be input to SOLTR by the user include nodal boundary conditions and solute transport material properties. Available nodal boundary conditions include:

1. Variable concentration
2. Fixed concentration
3. Fixed rate of solute addition
4. Fixed rate of water removal at ambient solute concentration.

For the Williston Basin study all nodes were variable-concentration nodes, except for a single node representing the repository which was given a fixed rate of solute addition. All of the variable concentration nodes were given zero initial concentrations.

Four parameters describing solute transport material properties were also input. They included longitudinal dispersivity, transverse dispersivity, retardation factor, and effective porosity. Values of these parameters were assigned by material type.

Several other options are available in the SOLTR program but were not used in this study. One option allows definition of a window over a region of interest in the AFPM mesh which reduces the size of the mesh analyzed by SOLTR. Another option allows elimination of one or more elements from the AFPM mesh again to reduce the size of the SOLTR mesh. In the Williston Basin study the entire AFPM mesh was analyzed by SOLTR.

5.2.2 Location of Repository

The site-selection criteria were:

- The site should be in an area of downward groundwater flow (a recharge area) in order to ensure that any escaping radionuclides would be drawn into the regional flow system rather than flowing upward into shallow aquifers and possibly to surface water bodies (and thus escape the regional groundwater system altogether).
- The site should have a thick salt or shale layer to contain the repository.
- The repository should be between 1,000 to 3,000 feet deep for reasons of mine design.

Given these criteria, it proved surprisingly difficult to locate an acceptable site in the basin. Due to the depth constraint, the most likely repository location was in the Pierre Shale, between layers A and B of the model. Areas within the Williston Basin where flow was directed downward from Layer B to Layer C are shown in Figure 5-1. They are few and occur primarily near the Black Hills, which is a recharge area for the deeper aquifers. Other recharge areas where downward flow occurs are outside of the model area to the west.

DIRECTION OF VERTICAL FLOW (LEAKAGE) FROM LAYER B

Figure 5-1

LEGEND

- Flow from Layer B to overlying Layers
- Flow from Layer B to underlying Layers

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

Although an actual repository might be located within the Pierre Shale between layers A and B, the computer model cannot realistically consider solute transport within separators (because it assumes instantaneous transport). Therefore, for the purpose of this model the repository was assumed to be a constant point source located in Layer B. This ignores the time needed for nuclides to flow vertically downward in the Pierre Shale to Layer B and also any dispersion and retardation within the Pierre Shale.

The time for nuclides to travel from a repository in the Pierre Shale to the Layer B aquifer can be estimated. It would take about 3,600 years for nuclides to reach Layer B from the repository based on the following parameters.

Vertical hydraulic conductivity of Pierre Shale = 10^{-4} ft/yr

Distance from repository to Layer B = 1800 ft

Vertical gradient between Layers A and B = 0.05

Effective porosity (fracture porosity) = 10^{-5}

This length of time is very important because of significant nuclide decay soon after burial (i.e., within 1,000 years) and should be considered in an actual repository performance model. However, it is relatively short compared to the time span of 1 million years being considered in this study and will have a minimal effect upon the overall shape and development of the solute plume.

5.2.3 Output Presentation

The SOLTR program produces tabulations of nodal concentration (mass per volume), nodal discharge (mass/time), and solute flux rates in elements (mass/area/time). It also produces line-printer plots of concentration contours specified by material

types. SOLTR writes a checkpoint file of results which can be input to FLOCON to produce various mechanical plots.

5.3 RESULTS

5.3.1 Parameter Values

The following values for solute transport material properties were used for all materials in the SOLTR computer program.

Longitudinal Dispersivity = 50,000 feet

Transverse Dispersivity = 20,000 feet

Retardation Factor = 1.0

Effective Porosity = 0.05

None of the above properties have been measured on a regional scale in the Williston Basin, and in fact very little field data relating to their values exist in any area. Because of this, values were chosen which allowed use of the AFPM output without modifications (i.e., without mesh refinement) so that some idea of solute transport on a regional scale could be gained.

The above longitudinal and transverse dispersivities were chosen so that the relatively coarse finite element mesh used in AFPM could be used in SOLTR. For solute transport analysis a coarse mesh will not produce meaningful results unless accompanied by large dispersivities. Smaller dispersivities would require a correspondingly finer mesh. Normally the fineness of the mesh is governed by the amount of dispersion the solute is expected to undergo. Since dispersion (both longitudinal and transverse) about the mean flow path is assumed by current theory to be defined by a normal distribution, the amount of dispersion

can be estimated by calculating the standard deviation of the distribution. One standard deviation is defined by:

$$\sigma = \left(2\alpha_{L,T} L \right)^{\frac{1}{2}}$$

where: σ = standard deviation

$\alpha_{L,T}$ = longitudinal or transverse dispersivity

L = length along mean flow path from source.

In general, the distance defined by one standard deviation should contain at least several elements in the mesh. Thus, for a distance of 50 miles and a dispersivity of 500 feet the standard deviation is 16,248 feet. This would probably require nodes spaced at about 4,000 feet for good results.

Nodal spacing in the AFPM mesh is on the order of 40 miles over much of the area; therefore, to utilize the AFPM mesh, dispersivities were calculated using the above equation. Examples of the required spacing for the assumed values of dispersivity are given in Table 5-1.

For the assumed dispersivities, Table 5-1 indicates that the AFPM mesh may be somewhat too coarse at distances close to the solute source but should give reasonable results for relatively large distances.

Field values for dispersivity have not been measured over distances as great as those considered in this study. Available data (Holdsworth, et al. 1977) indicates dispersivities on the order of a few feet up to about 600 feet. These values were obtained from tests of up to several miles in distance and generally much less. On a regional scale, heterogeneities would probably result in dispersivities much larger than the measured values above.

TABLE 5-1
CALCULATED STANDARD DEVIATIONS FOR
VARIOUS DISTANCES ALONG MEAN FLOW PATH

Length (L)	Standard Deviation (σ_L)	Standard Deviation (σ_T)
<u>in miles</u>	<u>in miles for $\alpha_L = 50,000$ ft.</u>	<u>in miles for $\alpha_T = 20,000$ ft.</u>
50	30.8	19.5
100	43.5	27.5
200	61.5	38.9
300	75.4	47.7
400	87.0	55.0

Dispersion is known to be scale dependent. On the microscopic scale, dispersion is caused by diffusion and microscopic differences in flow velocity. On the larger macroscopic or megascopic scale, dispersion is caused primarily by geologic heterogeneities. At the scale of the Williston Basin model, these heterogeneities could result from faults, fractures, buried channels, facies changes, and a number of other-large scale geologic features that were not defined in the model. Whether these large-scale heterogeneities result in dispersivities as large as those used in the model is unknown.

Retardation factor is an extremely variable parameter. Depending upon the solute, the water chemistry, and the rock chemistry, it can range from 1 up to about 10,000. The value of 1 chosen for this study represents the worst case.

Effective porosity along with hydraulic conductivity and gradient determines the flow velocity of water within a porous medium. It can range from about 0.30 in porous media with intergranular porosity down to 10^{-4} and less in very tight media with only fracture porosity. The value of 0.05 was chosen as representative of aquifers with moderate interstitial or secondary (solution vugs) porosity.

The repository was treated as a point source in Layer B. A constant solute addition rate of 10^{10} mass units/yr was specified. This was an arbitrarily high value used to produce contours of solute concentration and does not represent the quantity of nuclides in the repository available for dissolution. Based upon data provided by Lawrence Livermore Laboratory (letter from Dana Isherwood, July 1978) the total mass of nuclides in a repository containing 10^6 MWe-yr of waste is about 1.22×10^8 g; which, if dissolved over a period of 10^6 years, yields a dissolution rate of 122 g/yr. Thus, one mass unit per

year is approximately equivalent to 1.22×10^{-8} g/yr based upon the above data. The actual rate of solute addition will depend upon the time it takes for the canister to deteriorate. Estimates place this time between 100 and 10,000 years, depending upon the type of canister and the surrounding geochemical environment. No attempt has been made in the preliminary solute transport model to include the effects of canister dissolution.

5.3.2 Computed Solute Concentrations

Solute transport prediction was carried out to a total time of 1 million years. The solute concentrations in the four model layers at times of 200,000, 600,000, and 1,000,000 years are shown in the contours plotted in figures 5-2 to 5-13. The contours are often irregular in shape primarily as a result of the relatively coarse mesh. The coarse mesh also caused minor negative concentrations and spurious positive concentrations primarily outside the area of the main solute plume. The negative concentrations were ignored by the computer plotting program used to produce the concentration contours. Another effect of the coarse mesh was that the solute plume at distances close to the solute source (repository) was much larger than expected and extended "upstream" of the source. Although some of the upstream solute flow is legitimately caused by localized flow to the west (because of addition and loss of water to the mesh along the boundary nodes; see Section 4.4.2), much of it would probably disappear with a finer mesh.

The development of solute plumes in the various aquifer layers is outlined below.

Layer A. Concentrations in Layer A shown in figures 5-2, 5-6, and 5-10 were low with a maximum of only 0.3 mass units/ft³ at 1 million years. This is probably the result of

COMPUTED CONCENTRATIONS IN LAYER A AT 200,000 YEARS

Figure 5-2

LEGEND

—(00)— Contaminant Concentration in mass units/ft³ (refer to text)
(Contour Interval varies)

Scale 1:
0
0 25
Scale in

Project No. _____ Reviewed _____ Date _____

Golder Associates

LEGEND

Contaminant Concentration in mass units/ft³ (refer to text)
(Contour Interval varies)

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

COMPUTED CONCENTRATIONS IN LAYER C AT 200,000 YEARS

Figure 5-4

LEGEND

—100— Contaminant Concentration in mass units/ft³ (refer to text)
(Contour Interval varies)

Scale in Miles
0 40
Scale in Miles
0 40

Project No. _____ Date _____
Revised _____

Golder Associates

COMPUTED CONCENTRATIONS IN LAYER D
AT 200,000 YEARS

Figure 5-5

LEGEND

—100— Contaminant Concentration in mass units/ft³ (refer to text)
(Contour Interval varies)

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

COMPUTED CONCENTRATIONS IN LAYER A AT 600,000 YEARS

Figure 5-6

LEGEND

—100— Contaminant Concentration in mass units/ ft^3 (refer to text)
(Contour Interval varies)

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80

Figure 5-7

LEGEND

—100— Contaminant Concentration in mass units/ft³ (refer to text)
(Contour Interval varies)

COMPUTED CONCENTRATIONS IN LAYER C AT 600,000 YEARS

Figure 5-8

LEGEND

—100— Contaminant Concentration in mass units/ f_1^3 (refer to text)
(Contour Interval varies)

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

COMPUTED CONCENTRATIONS IN LAYER D AT 600,000 YEARS

Figure 5-9

LEGEND

—0.05— Contaminant Concentration in mass units/ft³ (refer to text)
(Contour Interval varies)

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

Goldor Associates

COMPUTED CONCENTRATIONS IN LAYER A AT 1,000,000 YEARS

Figure 5-10

LEGEND

— 100 — Contaminant Concentration in mass units/ft³ (refer to text)
(Contour interval varies)

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

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COMPUTED CONCENTRATIONS IN LAYER B AT 1,000,000 YEARS

Figure 5-11

LEGEND

- 100— Contaminant Concentration in mass units/ ft^3 (refer to text)
(Contour interval varies)

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

COMPUTED CONCENTRATIONS IN LAYER C AT 1,000,000 YEARS

Figure 5-12

LEGEND

—100— Contaminant Concentration in mass units/ft³ (refer to text)
(Contour Interval varies)

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

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Goldier Associates

COMPUTED CONCENTRATIONS IN LAYER D AT 1,000,000 YEARS

Figure 5-13

LEGEND

— 100 — Contaminant Concentration in mass units/ft³ (refer to text)
(Contour interval varies)

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

the thick Pierre Shale aquitard (the repository layer) separating Layer A from Layer B. Two of the plumes apparently developing at 200,000 years were not present at 600,000 and 1 million years, which indicates that they were probably spurious.

Layer B. Concentrations near the solute source in Layer B reached about 40,000 mass units/ft³. The plume shown in figures 5-3, 5-7, and 5-11 spreads generally northeast from the source. Contours of the leading edge of the plume are irregular due to the coarse mesh used. A finer mesh would produce a much more regular plume.

Layer C. Solute concentrations in Layer C shown in figures 5-4, 5-8, and 5-12 reached a maximum of about 500 mass units/ft³ directly below the solute source. The main solute plume extended northeastward, with some extension to the west. The westward extension is probably due to loss of water from a boundary node and can be considered a numerical error. The leading edge of the plume in Layer C at 600,000 years is irregular due to the coarse mesh.

Layer D. Concentrations in Layer D are shown in figures 5-5, 5-9, and 5-13. At 200,000 years no measurable solute concentration was in Layer D. By 600,000 years a mound began forming in the central portion of the aquifer caused by leakage from Layer C. At 1 million years the solute concentration in the plume had reached 3 mass units/ft³ and the plume itself had dispersed. It appears that relatively low concentrations of solute (0.1 mass units/ft³) are leaking upward into C and eventually to the land surface.

Due to the lack of solute in Layer A, it appears that very little solute escapes the system into the reservoir layer except near the outcrop of Layer C where some limited solute outflow is indicated.

5.4 UNCERTAINTY

Uncertainty in solute transport calculations derives from three major sources.

1. Hydraulic model. This includes all of the uncertainty discussed in section 4.5. Since solute transport is controlled by the direction and velocity of groundwater flow, an accurate prediction of solute transport cannot be made without first fully understanding the fluid flow system.
2. Solute transport parameters. This includes longitudinal and transverse dispersivity, retardation, and effective porosity. All of these parameters are extremely difficult to measure on a regional scale. We are not aware of any studies in which even one of these parameters has been adequately defined on the scale of this study. Limited field testing can and has been done (in other areas), but extending the results of point measurements to the entire region of interest will introduce large uncertainties.
3. Solute transport model. The theory of solute transport is relatively new and has not yet been well proven by field observation. Any model of solute transport is very difficult to validate and calibrate because of the very long times involved. For instance, calibration of a model of a regional flow system could require field

observations over thousands of years. A possible alternative to long-term field experiments is to calibrate the model against natural solute transport processes which have been occurring over long times. Such an approach would require an accurate knowledge of the fluid flow plus substantial geochemical testing.

4. Mass balance. In general, the comments in Section 4.5.3 also apply to the solute transport solution. (That is, continuity of mass is forced by the algorithm for the steady-state solution but not for the transient solution.) Because a transient analysis of solute transport was made of the Williston Basin, there is some uncertainty in the mass balance.

6.0

CONCLUSIONS

This is a preliminary report on the first part of the project (the balance is to be done as part of FY80 work). The data assembly and reduction phase is essentially complete and a simple geohydrologic model has been formulated. The numerical models that have been run to date are preliminary, and more detailed modeling is necessary before specific conclusions about solute transport in the Williston Basin can be made. Some general conclusions regarding the data and modeling can be made based upon this study.

6.1 DATA

- Data assembly and reduction requires a substantial man effort based upon a current U.S. Geological Survey study of the Powder River and Williston basins (on the order of 10 to 20 man-years) in order to obtain a relatively complete model of a large sedimentary basin. The major sources of data in most sedimentary basins are deep oil and gas wells and, less important, shallow water wells. In the Williston Basin many thousands of petroleum exploration holes exist with even greater number of shallow water wells.
- Parameters defining fluid flow are poorly known in the Williston Basin, but a large amount of useful data does currently exist. Existing data on deep aquifers are generally concentrated near petroleum-producing areas. New boreholes are probably needed in other areas to supplement existing data.

- Parameters defining solute transport are currently not known. Some rough estimates of effective porosity can be made based on drill core data, but no measurements of dispersivity or retardation exist.
- Significant uncertainties will always be associated with regional modeling. These uncertainties will be greatest for solute transport models because of the lack of measured data.

6.2 MODELING - PRELIMINARY CONCLUSIONS

- Modeling of regional flow and solute transport is essential if the regional flow system is to be relied upon as a barrier. The degree of complexity required of such models to adequately predict regional flow and solute transport is not known because it has not been determined just what constitutes an adequate prediction. Models more complex in terms of processes (i.e., salinity and temperature-induced flow) than the one used in this study are available or can theoretically be developed. However, the limitations associated with models will probably not be because they do not consider processes but because they lack data or are too big and expensive to run on the current generation of computer.
- The inclusion of temperature and salinity effects into the regional models is essential.
- It is desirable but may be relatively difficult to locate suitable repository sites in areas of downward hydraulic gradients, except near regions where deep aquifers are recharged by surface water (i.e., at

outcrops). Such areas are often mountainous and may not be suitable for a repository for various other reasons (access, faulting, etc.).

- Regional flow system modeling will involve two steps. First, a regional flow model should be formulated and calibrated. A preliminary solute transport model can be run using the regional model, but results cannot be expected to be very realistic. Second, a much more detailed model of a particular region of interest within the basin should be formulated and used for solute transport analysis. The detailed model (i.e., finer mesh) is necessary because of numerical errors resulting from the coarse mesh generally necessary with regional models.
- The preliminary flow model presented in this report may be substantially in error because it does not consider temperature and salinity effects. The amount of error involved cannot be quantified until these effects are considered. Additional errors in the flow model can result from the treatment of a true three-dimensional layer-cake system, from treating variable hydrologic parameters as discrete values within a given region, from combining thick stratigraphic units into a single aquifer layer, and from other simplifications and idealizations necessary for any numerical modeling of natural systems. Evaluation of these additional errors is not possible with the current level of data and model results.
- The preliminary solute transport model is unrealistic because of the large dispersivities (used as a result of the coarse mesh), the lack of any retardation, and

the treatment of the repository as a constant point source for 1 million years. The preliminary transport model was run in order to illustrate the methodology involved and the general form of the results rather than to actually predict solute transport in the Williston Basin.

6.3 SUMMARY OF COMPUTING TIME AND COST

All computing for this study was run on a CDC Cyber 75 computer operated by Boeing Computer Services

The time and cost to run the MLTMSH and AFPOL data preparation programs is very minimal. The time and cost of the AFPM fluid flow program and the SOLTR solute transport program are as indicated below.

A. Steady-State AFPM Solution

Mesh Size: 447 nodes, 392 elements

Core Space: 52,740 decimal

Time: 7.8 CPU seconds

Approximate Cost (based on medium priority): \$10.

Costs for the steady-state solution are low. Costs for transient solutions (not run in this study) will increase as the number of time-steps increase.

B. Transient SOLTR Solution

Mesh Size: as above

Core Space: 63,680 decimal

Time: 52.3 CPU seconds

Approximate cost (based on medium priority): \$130.

The transient solution utilized 10 primary time-steps (at 100,000-year intervals) with each primary step broken into 12 substeps. Thus, a total of 120 time-steps were required for the entire solution.

G.4 MAXIMUM PROBLEM SIZE

The current version of the AFPM and SOLTR programs can accommodate a maximum of 4,096 nodes and 30 different material types. The largest AFPM problem for which data are available contained 1,340 nodes and 1,480 elements. A steady-state solution of the problem required core space of 124,800 decimal, took 40 CPU seconds to execute and cost approximately \$70. A transient solution using the same mesh was run for a total of 17 time-steps. It used 124,800 decimal core storage, took 217 CPU seconds to run, and cost approximately \$430.

No time or cost data are available at this time for SOLTR solutions of problems with more nodes than the Williston Basin study.

7.0

RECOMMENDATIONS FOR FUTURE STUDY

This study provides a basis from which to pursue further studies. Future studies would lead to important conclusions regarding regional modeling of flow and solute transport in the Williston Basin and other sedimentary basins. The following work should be performed in the future.

- Refine the finite element mesh in the area around the repository site. This would reduce numerical errors and allow smaller values of dispersivity to be used. The procedure for mesh refinement is described in Section 7.1.
- Use a realistic rate of solute leaching from the repository and shut it off after a given time (i.e., after all the canisters have dissolved). Solute leaching rates would be easy to incorporate into the existing model.
- Include transient effects caused by climatic change or resource use. In particular, the effects of large-scale fluid withdrawals should be investigated. These effects could be included with only minor changes to the existing fluid-flow model.
- Compare the results of the quasi-three-dimensional model used in this study with simple one- and two-dimensional models to see if the simpler models are sufficient for fluid flow and/or solute transport prediction. Also compare with a true three-dimensional model to determine validity of quasi-three-dimensional approach.

- Include the effects of temperature and salinity to determine their significance. This would require a basic programming change in the fluid-flow model. However, it is believed necessary to realistically predict flow on a regional scale because both temperature and salinity can drastically affect fluid flow and solute transport.
- Look at models required for other types of sedimentary basins and compare them with the Williston Basin model.

7.1 METHODOLOGY FOR MESH REFINEMENT

As mentioned above, the mesh used in this study is too coarse for realistic modeling of solute transport. Several alternatives are available to overcome this problem. The first would be to refine the existing mesh by adding more nodes and elements. The current number of 447 nodes could be increased by about nine times and still be within the limits of the computer program. This degree of refinement would probably still not allow detailed solute transport modeling.

Another method of mesh refinement involves reducing the areal extent of the problem to the region actually being affected by the solute plume. This could be accomplished by defining a window in the existing mesh and constructing a new, more detailed mesh within the window. By applying the hydraulic conditions previously derived using the coarse mesh to the boundaries of the detailed mesh, the area outside of the window could be eliminated from consideration.

Figure 7-1 shows a refined mesh in the area of the Williston Basin affected by the solute plume predicted by the coarse mesh. Actual dispersivities are probably smaller than the values used

REFINED FINITE ELEMENT MESH FOR SOLUTE TRANSPORT STUDIES

Figure 7-1

LEGEND

- Element Boundaries
- - - Geographic Boundaries

Scale in Miles
0 40 80
Scale in Kilometers
0 40 80 120

in this study; thus, the extent of the solute plume should be less when realistic dispersivities are used. This assures that the window shown in Figure 7-1 will be adequate to include the entire plume in the refined mesh.

The refined second-generation mesh would contain about 1,350 nodes and 1,280 elements. Elements adjacent to the repository would have dimensions of about 2 miles (these dimensions increase up to about 20 miles at large distances from the repository). The mesh is finer along the primary flow path determined from the first-generation model. This allows more accurate prediction of rapidly changing solute concentrations which occur along and laterally away from the hydraulic streamline. The refined mesh should allow use of dispersivities on the order of 5,000 feet. No measured regional dispersivity values are available with which to evaluate whether this is a realistic dispersivity to use.

Measured values of dispersivity derived from single- and two-well tracer tests are generally 500 feet or less. The usefulness of these measured values is questionable because of the small scale of the tests used to derive them. Should these measured values be used in the computer model, a third-generation mesh based upon the extent of the plume modeled by the second-generation mesh would be required. Such a third-generation mesh may be too complex (i.e., require too many nodes) for the current model.

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APPENDIX
GROUNDWATER COMPUTER PACKAGE
TECHNICAL SUMMARY

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1.0 INTRODUCTION

Numerical modelling and simulation of flow in groundwater basins are essential analytical elements in water resource planning and management. Recent developments in numerical methods for groundwater hydrology, when coupled with the results of field observations and investigations, provide powerful, as well as reliable, tools for prediction of groundwater regime behaviour. Computer modelling of groundwater flow quantity and quality permits efficient and cost-effective evaluation of alternative water resource management plans.

The Groundwater Computer Package has been prepared by Golder Associates to a practical capability for numerical modelling of flow quantity and quality in regional groundwater regimes. The Groundwater Computer Package is an integrated suite of computer programs which mathematically simulate the hydraulic and solute transport characteristics of groundwater flow in regional aquifer systems. Additional computer programs are incorporated in the package to provide auxiliary services such as input data preparation, presentation of model results and calibration of field data with model results.

The Groundwater Computer Package incorporates the finite element method for the solution of the fundamental equations governing flow and solute transport in various groundwater regime geometries. The package can be used to model both steady-state and transient flow conditions in three-dimensional regional aquifer layer systems and in simpler two-dimensional analogues. This document contains basic descriptions of the finite element methods incorporated in the package along with an outline of their groundwater modelling and simulation capabilities.

2.0 GROUNDWATER MODELLING BY FINITE ELEMENTS

The finite element method has been and remains the subject of a diverse but immense research and development effort in many engineering fields. It has been accepted and used as a general analysis tool in only a few esoteric engineering areas - aerospace structures and nuclear reactor design being prime examples. The finite element method has, however, achieved quite wide acceptance in the groundwater engineering field, where the situations encountered in practice are often too complex for hand analysis or physical model simulation.

The approach to groundwater modelling offered by the finite element method is the use of two- and three-dimensional elements in synthesizing general three-dimensional flow regimes. The essential geometry of most three-dimensional regimes can be adequately and accurately represented as an assemblage of appropriately shaped elements. This feature is the distinguishing point between the finite element method and other analytical or numerical methods as applied to general groundwater modelling and simulation problems.

The formulation and application of the finite element method for groundwater modelling are multi-step processes. The mathematical formulation first involves the generation of the basic equations for groundwater flow and solute transport. These are shown in conceptual form in Table 1. These basic equations are complex differential equations with non-linear characteristics. In essence, equations (1) and (3) are variations on the Law of Conservation of Mass, (ie. they are continuity equations) while equation (2) is an expression of the work necessary to cause groundwater flow. Any simplifying assumptions to suit analysis requirements are introduced into the equations at this time. Due to the complex nature of most real groundwater hydrology problems it is usually impossible to find solutions which satisfy the basic equations at all points within the flow regime.

TABLE 1BASIC EQUATIONS USED IN THE GROUNDWATER COMPUTER PACKAGEHYDRAULIC SOLUTION

$$\left\{ \begin{array}{l} \text{Net rate of inflow} \\ \text{to an element} \end{array} \right\} = \left\{ \begin{array}{l} \text{Material Storage} \\ \text{Coefficient} \end{array} \right\} \times \left\{ \begin{array}{l} \text{Rate of Increase} \\ \text{of Pressure Head} \end{array} \right\} \quad (1)$$

The flow rate is calculated using Darcy's Law, which relates the seepage rate to the head gradient:-

$$\left\{ \begin{array}{l} \text{Seepage Rate} \end{array} \right\} = - \left\{ \begin{array}{l} \text{Permeability} \end{array} \right\} \times \left\{ \begin{array}{l} \text{Head Gradient} \end{array} \right\} \quad (2)$$

Equations (1) and (2) give the relations between

- (a) the pressures and the flow rates, and then between
- (b) the flow rates and the rates of change of pressure.

Together, these allow computation of the complete pressure-flow rate history of a groundwater flow problem.

SOLUTE TRANSPORT

$$\left\{ \begin{array}{l} \text{Net rate of solute transport} \\ \text{into an elemental volume} \end{array} \right\} = \left\{ \begin{array}{l} \text{Rate of increase of solute} \\ \text{concentration in the volume} \end{array} \right\} \quad (3)$$

Groundwater flow velocities are previously determined from the solution of equations (1) and (2) above.

This is where the finite element method enters as a useful procedure for computing an approximate solution to the governing equations. This is done, as previously described, by dividing the region of interest into a large number of elemental areas (or volumes), called finite elements, and assuming a simple form for the variation of pressure head or solute concentration over each element. Individual element solutions to the governing equations are found in terms of unknown nodal pressure heads or solute concentrations. Linearized global continuity equations are then produced by assembling these individual solutions in the same manner as the flow regime is synthesized from the finite elements. These global continuity equations are solved for the unknown nodal values by various solution methods depending on the type and temporal variation of the boundary conditions. The computed nodal values define the groundwater flow field conditions in space and time for the regime being modelled.

Groundwater flow problems in the general sense involve the solution of three-dimensional field equations. Although it is possible to generate full three-dimensional finite element continuity equations, it is a costly and time-consuming process to solve them. Many practical situations, however, have geometrical and/or geological configurations that allow the use of simpler two-dimensional and quasi-three-dimensional analogues to simulate groundwater flow conditions. Figures 1, 2 and 3 illustrate realistic finite element mesh idealizations for some practical groundwater flow situations. Figure 1 indicates the manner in which a layered aquifer system can be modelled using variable thickness elements, while Figures 2 and 3 indicate the use of standard two-dimensional planar and axisymmetric finite elements.

As the idealization of any flow regime is obtained by subdividing the original continuum into elements of appropriate sizes and shapes, all of the material properties of the original system are retained within the individual finite elements. One of the principal attributes of the finite element method is its ability to deal successfully with arbitrary material properties and geometries.

MULTI-AQUIFER HYDRAULIC FLOW (AFPM PROGRAM)

5

Figure 1

a) Aquifer Diagram

b) Finite Element Model

TWO DIMENSIONAL HYDRAULIC FLOW
(FPM PROGRAM)

6
Figure 2

a) PLANAR TWO DIMENSIONAL FLOW

b) FINITE ELEMENT MODEL

Date Feb. 77

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Project No. 7021226N (work)

RADIALLY OR AXI SYMMETRIC FLOW (FPM PROGRAM)

7
Figure 3

a) RADIAL FLOW

b) FINITE ELEMENT MODEL

High element densities (i.e., small finite elements) should be used in regions having high pressure head or concentration gradients, and larger elements should be laid out in other regions. Gradation of element sizes to suit analytical accuracy requirements is an attractive feature of the finite element method. The general rule is: the more elements, the better the solution. The cost of computing a solution increases rapidly with the number and complexity of elements involved, so the user can choose between a nominal cost solutions of limited accuracy and expensive solutions of increased accuracy. In groundwater hydrology problems, it is usually possible to achieve, at reasonable cost, solution accuracy compatible with the quality of the input data.

3.0 PURPOSE AND DESCRIPTION

The Groundwater Computer Package has been prepared to provide a practical capability for numerical modelling of flow quantity and quality in regional groundwater regimes. The package is an integrated suite of computer programs which incorporate the finite element method to simulate the hydraulic and solute transport characteristics of flow in groundwater basins. Auxiliary computer programs are included in the package for input data preparation, presentation of model results and calibration of model results with field data. The logical operational use of the component programs is illustrated by Figure 4.

The Groundwater Computer Package incorporates the finite element method variations for groundwater modelling discussed in the previous section. The package is capable of modelling hydraulic flow and solute transport in groundwater models having the geometry illustrated in Figures 1, 2 and 3, namely -

- (a) single and multi-layer regional aquifer systems,
- (b) planar 2-dimensional flow analogues, and
- (c) axisymmetric 2-dimensional analogues.

The general groundwater modelling capabilities of the groundwater computer package are indicated in Table 2, while the component programs and their specific capabilities are outlined below.

3.1 Hydraulic Analysis

There are two primary component programs in the package for hydraulic solution of groundwater flow problems. These programs, AFPM (Aquifer Flow in Porous Media) and FPM (Flow in Porous Media), are used to model aquifer layer and two-dimensional analogue flow regimes, respectively. They are based on the finite element models described previously and include the fundamental assumptions listed in Table 3. The various flow regimes simulated may be inhomogeneous, with many different material zones having material property relationships indicated in Table 4. A flow regime may also be analyzed as a confined or an unconfined problem, with the location of the phreatic surface being automatically calculated.

Primary Component Program Flow Chart

Date May '78

Revised

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TABLE 2GROUNDWATER COMPUTER PACKAGE - GENERAL MODELLING CAPABILITIESFlow Regime Models

- . single and multi-layer regional aquifer systems
- . two-dimensional analogues - planar flow
 - axisymmetric flow

Hydraulic Solution

- . confined, unconfined and 'leaky' aquifers
- . moving phreatic surface problems (including release or storage of water, and evapotranspiration effects)
- . steady-state or transient boundary and flow conditions
 - simulation of wells, surface inflow, etc.
 - including effects of material compressibility, and
 - interaction with surface flows

Solute Transport Solution

- . in one layer of a multi-aquifer system or in two-dimensional flow analogues
- . steady-state or transient boundary and flow conditions
- . including effects of - convection, dispersion, dilution, sorption and radioactive decay of pollutant.

TABLE 3FUNDAMENTAL LIMITING ASSUMPTIONS OF THE GROUNDWATER COMPUTER PACKAGE

- . Darcy's (linear) flow law is valid
- . the solid skeleton of the aquifer materials deforms in a linear elastic manner
- . the specific storativity and permeability of the aquifer materials are independent of fluid pressure and solute concentration changes
- . the fluid (water) obeys a linear equation of state
- . flow due to gradients of density, temperature or electric potential is negligible
- . solute concentration is small, so that fluid density is unaffected by concentration

TABLE 4
MATERIAL PROPERTY RELATIONSHIPS

Hydraulic Properties

- . Conductivity - linear isotropic, or
 - linear anisotropic
- . Specific Storage - zero (ie. incompressible), or
 - constant
- . Specific Yield - constant
- . Evapotranspiration - zero (ie. none), or
 - linear with depth (within limits)
- . Fluid Density - constant

Solute Transport Properties

- . Dispersivity - constant longitudinal and transverse
 coefficients for an isotropic media
- . Retardation - constant sorption rate
- . Effective Porosity - constant
- . Radioactive Decay - constant exponential decay rate

The AFPM computer program determines fluid potentials and fluid pressures, as well as flow rates, quantities and directions in both steady-state and transient three-dimensional multi-aquifer flow regimes. The groundwater flow regime must be capable of being approximately represented as a layered system of confined, unconfined and leaky aquifers (see Figure 1(a)). Interaction of subsurface groundwater flow with streams, rivers, or lakes on the ground surface can be modelled. As illustrated in Figure 1(b), the flow regime is arranged in aquifer layers which are subdivided into triangular and quadrilateral elements of prismoidal shape. These layered finite elements (see Figure 5) have appropriate material properties assigned, may vary in thickness and may be inclined from the horizontal. The potential head in a layer element is presumed to be constant in the vertical direction. Different aquifer layers may be separated by aquitards through which leakage may occur. Leaky aquifers can thus be modelled by specifying leakage conditions between layer elements. Leakage may also occur through an aquitard between a layer and a 'reservoir'. Boundary conditions of either known flow rates or fluid potentials (pressures) may be applied (and altered at any time for transient hydraulic analyses).

The FPM computer program determines fluid potentials and fluid pressures, as well as flow rates, quantities and directions in both steady-state and transient planar and axisymmetric flow regimes. The groundwater flow regime must be capable of being approximately represented as either a planar or axisymmetric flow system (see Figures 2 and 3). Interaction with surface water systems such as streams, rivers, or lakes can be modelled. The vertical face of the flow regime is subdivided into triangular and quadrilateral shaped elements as illustrated in Figures 2 and 3. These elements are of constant thickness for planar flow analysis, and have toroidal volumes for axisymmetric flow analysis (Figure 6). The elements are assigned appropriate material properties. Boundary conditions of either known flow rates or fluid potentials (pressures) may be applied and altered at any time for transient hydraulic analyses.

(a) PLANAR ELEMENTS

(b) AXISYMMETRIC ELEMENTS

For steady-state hydraulic analyses, the AFPM and FPM programs will automatically compute:

- the location of the water table (phreatic surface) for unconfined flow problems by iterative procedures (taking into account release or storage of water involved).
- fluid potentials and pressures at nodes throughout the flow regime.
- element flow rates and directions.
- leakage rates between aquifer layer elements (AFPM only).

For transient hydraulic analyses the AFPM and FPM programs will compute the above items for specified times as well as the net inflow-outflow of fluid to the regime (taking into account the effects of material compressibility). The results of both steady-state and transient hydraulic solutions can be stored on a permanent data file for subsequent reference by the AFPM (or FPM), FLOCON and SOLTR programs.

To minimize the computer time required to perform hydraulic solutions, the AFPM and FPM programs contain routines to:-

- re-number nodes and reduce the size of the conductivity matrix (minimizes computer memory and equation solution time requirements).
- increase or decrease the computer memory allocation based on the complexity of the problem to be solved.
- ensure convergence to a specified accuracy for any time interval.

In addition, the AFPM program uses an efficient out-of-core equation solver for all problem sizes.

The AFPM and FPM programs are also capable of producing simple printer plots of model results for both steady-state and transient solutions. More comprehensive plotting facilities are provided by the FLOCON computer program. The AFPM or FPM output data ('checkpoint') file containing model results is used as input to this plotting program. This same output file is used as input to the SOLTR program for subsequent calculation of solute transport by groundwater flow through the AFPM or FPM mesh. This output file can also be used to restart solutions from earlier runs.

3.2 Solute Transport

The SOLTR computer program (SOLTR is an acronym derived from SOLute TRansport) is a primary component in the Groundwater Computer Package (see Figure 4). It predicts solute concentration histories throughout a region of interest in a multi-aquifer (Figure 7) or two-dimensional finite element meshes (ie. planar or axisymmetric). Steady-state or transient hydraulic conditions within the meshes will have been previously calculated by either the AFPM or the FPM program.

The SOLTR computer program uses the finite element method to model the transport of a solute dissolved in flowing groundwater. While it is primarily intended to be used for predicting salinity changes in groundwater, it can also be used for simulating the movement of water polluted by fertilizers, insecticides, heavy metals, or radionuclides. Heat transport can also be simulated. The output of the SOLTR program is a prediction of solute concentration histories throughout the region of interest. Results are printed in tabular form, and contour plots of solute concentration levels can be prepared.

A typical use of the SOLTR program might be to simulate a situation where irrigation water was being pumped from a freshwater aquifer, and saline water was leaking down to the freshwater aquifer from an overlying saline aquifer. The SOLTR program would predict the future salinity concentrations in the freshwater aquifer, thus allowing water-use planners to optimize the allocation of pumping.

Part of the input to the SOLTR program is a description of the groundwater flow velocities. This input is provided by running either the AFPM or the FPM flow analysis program to compute the flow velocities and store the results in a "checkpoint" file on the computer. The SOLTR program reads this "checkpoint" file and then reads the additional information necessary to define the solute-transport problem to be solved.

After completion of any set of solute transport analyses, the user can direct the SOLTR program to produce contour plots of model results on the line printer. The user may also prepare a more precise series of plots on either a mechanical plotting device (ie. Calcomp) or the line printer using the FLOCON output display and plotting program. These plots are very often essential items in the modelling process as they present a comprehensive display of model results over a large portion of the model.

3.3 Input Data Preparation

The most cumbersome aspect of generating a multi-aquifer flow model is the preparation of the input data describing the spatial configuration and extent. The AFPM and FPM finite element analysis program must be provided with information relating to the nodes, elements and materials within the mesh. When a mesh contains hundreds of nodes and elements this task will represent a major portion of the total work effort required to solve the problem. If all node and element data has to be prepared manually and input via cards this task becomes tedious and time-consuming. In addition, a manual data preparation process is prone to error.

A computer program (called 'MLTMSH') is available to facilitate the preparation of finite element input data for single and multi-aquifer flow regime problems. Using the MLTMSH computer program, a user can generate a finite element mesh input data file in a format suitable for the hydraulic solution program AFPM.

The MLTMSH computer program provides a semi-automatic means of generating the system topology involved in a multi-aquifer finite element model. It is not a completely general program as the user is required to specify some information about the form of the finite element mesh desired. Mesh generation, whether manual or computerized, involves judgement for the effective placement of the nodes and elements within the flow regime. In addition, specification of boundary conditions and material properties requires considerable involvement on the part of the user.

The input to the MLTMSH computer program is in a problem-oriented-language format to facilitate usage by people who may be unfamiliar with computer techniques. Extensive data checking facilities as well as various plotting capabilities are incorporated in the program. The MLTMSH program produces an output data file containing the complete topology and geometry of the finite element mesh. Following this mesh generation operation, a post-processor program (called AFPOL) is used to assemble the remaining input data, including material properties and boundary conditions, required for an AFPM analysis.

The user still has the option to manually generate the finite element mesh and directly code input data for the AFPM program.

Finite element meshes must be manually generated for FPM program hydraulic analyses. Both the AFPM and FPM programs have simple node, element and boundary condition generation facilities to lighten the workload.

3.4 Output Presentation

The FLOCON computer program (FLOCON is an acronym derived from groundwater FLow COntouring) prepares finite element mesh, contour and vector plots of two- and three-dimensional groundwater flow hydraulic analysis results produced by the AFPM and FPM computer programs. It also prepares similar plots of groundwater contaminant transport analysis results produced by the SOLTR computer program. The FLOCON program is the output plotting and display component for the Groundwater Computer Package.

The primary component programs AFPM, FPM and SOLTR all have simple printer-plot facilities available for plot preparation at run time. The FLOCON program provides a capability for the preparation of specific and particularly high-quality mechanical (ie. Calcomp type) plots of model results subsequent to the actual analysis runs. In addition, the FLOCON program can prepare printer-plots of most of the machine-plottable functions.

The scale and plotting area of the FLOCON plot types can be set by the user, provided that certain dimensional limitations on total plot size are not exceeded. In addition, contour level values and intervals can also be specified by the user for all types of contour plots of all model results. For some types of plots, notably those involving multi-aquifer groundwater models, material layers and zone types must be carefully selected to ensure useful results. The user may also specify definition and boundary lines that can be included on mechanical plots to improve presentation and facilitate interpretation.

The input to the FLOCON program is in a problem-oriented language format designed to facilitate usage by staff members who may be unfamiliar with computer systems and programming techniques. Plotting capabilities are outlined in Table 5 for each type of groundwater flow or solute transport model available in the Groundwater Computer Package. All contour plots trace the calculated position of the function contour level through the individual finite elements in all or portions of the mesh. Most of the contourable functions vary linearly within a finite element and thus contours appear as connected straight-line segments. No smoothing of the contour lines is done by the FLOCON program, this is a function left to the user to perform. Figure 8 is a typical FLOCON mesh plot for a tailings dam seepage project, while Figure 9 is a composite of typical FLOCON output plots prepared for the resulting report.

TABLE 5
FLOCON PROGRAM PLOTTING CAPABILITIES

ANALYSIS PROGRAM			
	<u>AFPM</u>	<u>FPM</u>	<u>SOLTR</u>
<u>Mechanical Plots</u>			
1. MESH	YES	YES	YES
2. STREAM	NO	YES	NO
3. HEAD	YES	YES	NO
4. FLOWNET	NO	YES	NO
5. PRESSURE	YES	YES	NO
6. THICKNESS	YES	NO	NO
7. Z	YES	NO	NO
8. DEPTH	YES	NO	NO
9. CONCENTRATION	NO	NO	YES
10. VELOCITY	YES	YES	YES
<u>Printer-Plots</u>			
1. STREAM	NO	YES	NO
2. HEAD	YES	YES	NO
3. FLOWNET	NO	YES	NO
4. PRESSURE	YES	YES	NO
5. THICKNESS	YES	NO	NO
6. Z	YES	NO	NO
7. DEPTH	YES	NO	NO
8. CONCENTRATION	NO	NO	YES

PORTION OF FLOCON FINITE ELEMENT MESH PLOT

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Figure 8

TITLE OF ANALYSIS : TAILINGS DISTRIBUISHAL FLOW PROBLEM-RUN 1
 FUNCTION CONTOURED : MESH ONLY
 LEGEND : 9 - 0.
 PLOT ORIGIN (x) IS AT X = -1.000E+00 Y = 1.078E+03 X SCALE = 5.00E+00 M /INCH
 MATERIAL TYPES SELECTED : ALL
 11/12/78 16.26.49
 INTERVAL : 0.
 Y SCALE = 5.00E+00 M /INCH

FINITE ELEMENT SIMULATION OF STEADY STATE SEEPAGE

25
Figure 9

4.0 SETTING UP A FINITE ELEMENT ANALYSIS

The process of setting up and using a finite element model for groundwater flow and solute transport problems is straightforward. It requires considerable attention to detail and informed judgement on the part of the Engineer or user. The steps and tasks involved in generating a finite element model for a groundwater flow regime and subsequently using the Groundwater Computer Package to perform hydraulic and solute transport analyses are listed in sequential order in Table 6. As indicated in this table, once a region of interest has been outlined there is a considerable amount of preliminary work to be done before the finite element mesh generation can start. The user must be aware that a hydraulic analysis must be performed using either the AFPM or FPM program in order to use the SOLTR program for solute transport analysis. The finite element mesh used in the hydraulic analysis must also be suitable for solute transport analysis.

4.1 Problem Definition and Model Generation

4.1.1 Basic Geological and Hydrological Data Collection

Information relating to the geology of the region to be modelled has to be collected and interpreted. This information is necessary to define general topologies and geometries of the aquifers and confining beds making up the flow regime. Historical data on groundwater levels, pumping rates, anticipated infiltration, etc., must be collected in order to define realistic boundary conditions. Pump and other hydrologic test data must also be collected and reviewed to provide estimates or ranges of aquifer material properties such as transmissivity and specific storage. In addition to the information collected for the hydraulic analysis, the user must obtain and interpret data on solute sources and initial concentrations in the portion of the region of interest for solute transport. Material transport properties must also be obtained or inferred. This information is necessary to define the boundary conditions and transport characteristics of the flow regime. Prior to starting a finite element analysis, the user must have a reasonable understanding of the physical characteristics and nature of the flow regime he wishes to model. This phase is potentially the most time-consuming portion of the work involved in groundwater flow modelling.

TABLE 6

FINITE ELEMENT MODELLING OF GROUNDWATER FLOW AND SOLUTE TRANSPORT

1. OUTLINE REGION OF INTEREST
2. COLLECT GEOLOGICAL AND HYDROLOGICAL DATA
3. STATE HYDRAULIC (AND SOLUTE TRANSPORT) PROBLEM TO BE ANALYZED
4. DEFINE REGION OF INTEREST AND ANALYSIS REQUIREMENTS
5. DEFINE APPROPRIATE FINITE ELEMENT MODELLING TECHNIQUE
6. DEFINE GEOMETRY OF MODEL
7. GENERATE FINITE ELEMENT MODEL
8. PERFORM HYDRAULIC ANALYSIS OF MODEL
 - (a) Define material hydraulic properties
 - (b) Define hydraulic boundary conditions
 - (c) Run hydraulic analysis using AFPM or FPM program
 - (d) Modify boundary conditions, material properties, etc.
 - (e) Run hydraulic analysis using AFPM or FPM program
 - (f) Repeat steps 8(d) and 8(e) as necessary
 - (g) Plot results (optional)
9. DEFINE (SUB) REGION OF INTEREST FOR SOLUTE TRANSPORT
10. REFINER (ie. WINDOW) FINITE ELEMENT MESH
11. PERFORM SOLUTE TRANSPORT ANALYSIS OF MODEL
 - (a) Define material transport properties
 - (b) Define solute transport boundary conditions
 - (c) Run solute transport analysis using SOLTR program
 - (d) Modify boundary conditions and/or material properties
 - (e) Run solute transport analysis using SOLTR program
 - (f) Repeat steps 11(d) and 11(e) as necessary
 - (g) Should solute transport analysis require new hydraulic solution repeat steps 8, 11(d) and 11(e) as necessary
 - (h) Plot results (optional)

4.1.2 Regional Plan Definition

A regional plan is set up with boundaries which extend beyond the limits of the flow regime to be analyzed. The plan must define the location of all bores, wells, other recorded drill holes and stream measurement stations. Surface hydrology features, such as streams and creeks, should also be indicated. The regional plan is used throughout the mesh generation process and should be carefully prepared. It is advisable to prepare a proper scaled drawing that can be copied, reproduced and modified.

Basic units should also be defined at this time, e.g., length and time and mass, if solute transport analyses are anticipated. Any system of units may be used but all input parameters must be specified in terms of a consistent set.

The fourth step involves a statement of the problem to be analyzed. This can vary from a simple simulation of existing groundwater behaviour to the modelling of alternative water resource usage plans. The user then goes on to define a region of interest and plots this on the regional plan as well as setting a series of grid limits. The region of interest must include those areas of the flow regime in which the user expects to see changes in flow rates, pressures or potentials, or pollutant concentrations. The boundary should be placed far enough from areas in which high pressure (potential) or concentration gradients are expected to occur to minimize the effects of the boundary values on the solution. The most preferable boundaries are those which coincide with natural features such as aquifer termination, major faults or heights of land, and river or creek channels.

4.1.3 Definition of Appropriate Modelling Techniques

Sufficient data will have been collected and interpreted to allow a reasonable understanding of the physical characteristics and nature of the flow regime. The user must now make a decision as to the most appropriate modelling technique to use. If the flow regime can be modelled

adequately and accurately by manual techniques or by the FPM program, then the user should choose the more appropriate of these simpler methods. If, on the other hand, the flow regime can only be realistically represented as a multi-aquifer AFPM model, then the user would continue setting up the three-dimensional finite element analysis.

4.1.4 Finite Element Model Generation

The next step in the analysis process is the generation of the basic finite element mesh data. Flow regime data is now organized into three basic categories:-

1. Aquifer and confining bed geometries.
2. Aquifer and confining bed material properties.
3. Flow regime boundary conditions.

In the finite element mesh generation process, each of these basic categories is treated separately. Initially, a detailed spatial description of the aquifers and confining beds that make up the flow regime is developed. Subsequently, material properties data and boundary condition values are added to the spatial description creating a two- or three-dimensional flow model that is ready for hydraulic analysis. The preparation of the input data describing the spatial configuration and extent is the most cumbersome aspect of generating a groundwater flow model. As indicated previously, both manual and automatic geometry definition procedures are available to accomplish this task.

Finally, material properties and flow boundary conditions are defined. Hydraulic conductivities and specific storage coefficients have to be assigned for confined flow layer materials. Unconfined layer materials also additionally require specific yield and (optional) evapotranspiration coefficients. Separator materials for multi-layer aquifer problems generally only require equivalent vertical or cross-bed conductivity to be input.

The specification of node boundary conditions can become quite involved. Sufficient boundary conditions must be applied to the finite

element mesh to permit a solution for the hydraulic characteristics. Nodes can have either known fluid-potential (or pressure) or known fluid inflow boundary conditions. Variations of these main types of node boundary conditions are available in the AFPM and FPM programs to handle linked potential conditions or to simulate surface features such as lakes and rivers.

For each groundwater flow problem studied, the input to the AFPM or FPM program can be divided into two parts - the problem description phase and the hydraulic solution phase. At this point the problem description data phase should be complete, i.e., the finite element mesh topology, geometry, materials and boundary conditions have all been specified.

4.2 Hydraulic Solutions

The hydraulic solution data phase of the input to the AFPM or FPM program is used to control the solution of steady-state and transient problems and to change problem geometry, materials or boundary conditions at specified times. Normally, the problem description data phase provides sufficient information and control for initial steady-state hydraulic solutions.

The hydraulic solution phase is directed by the user to produce the steady-state and transient solutions desired for the groundwater flow model. The user may change portions of the problem description data and subsequently run hydraulic analyses as many times as are required to produce the desired hydraulic solution results. In this way, for example, time dependent boundary conditions can be directly simulated. It is common practice to interrupt the solution of a problem during this phase and have the AFPM or FPM program produce an output "checkpoint" data file which can be used as the starting point for the next AFPM or FPM run.

After completion of a hydraulic analysis phase the user can direct the AFPM or FPM program to produce contour plots of model results on the line printer. The user may also prepare a more comprehensive series of plots using the FLOCON output display and plotting program.

For groundwater flow problems in which pollutant contamination is of interest, the AFPM and FPM program produces hydraulic solutions which are then used as the basis for solute transport analyses. This output data file is used as the initial input data file to the SOLTR program. The hydraulic solution completely defines the groundwater flow parameters to be used in the solute transport solution. Thus, care must be taken, when performing hydraulic solutions, to ensure that necessary simulations are carried out and the results saved on the checkpoint file. It is possible to input the results of additional hydraulic analyses to the SOLTR program during the course of a solute transport analysis. This method can be used when simulating solute transport through a transient groundwater flow system.

4.3 Solute Transport Analysis

4.3.1 Solute Transport Region Definition

The next step is to set up a regional definition of the area to be modelled during the solute transport analysis. The computer time required to solve transport problems is much greater than for hydraulic solutions of the same finite element mesh. It is thus sensible and, in some cases necessary, to refine (truncate) the basic finite element mesh for solute transport analysis.

The refined finite element mesh must include those areas of the groundwater flow regime in which the user expects to see changes in pollutant concentrations. The boundary of the refined finite element mesh should be placed far enough from areas in which high concentration gradients are expected to occur in order to minimize the effects of the boundary values on the eventual solution.

4.3.2 Boundary Condition Definition

The solute transport analysis is concerned with the amount of solute flowing within the refined groundwater flow regime. To maintain the 'mass balance' for the refined mesh, the amount of solute being input or extracted must be computed correctly. The specification of correct

boundary conditions can become quite complex as data for solute inflow specification is different from solute outflow specification. The user must have a very detailed understanding of the hydraulic characteristics (e. inflow and outflow) of the refined finite element mesh to be used in the solute transport analysis.

Sufficient (and correct) boundary conditions must be applied to the refined finite element mesh to permit a solution for the solute transport characteristics. The definition of correct boundary conditions for the refined mesh is the most critical task in solute transport analysis.

4.3.3 Material Transport Properties Definition

The last step in defining the solute transport regime is the definition of material transport properties. The user must determine dispersivity coefficients, retardation factors and porosities for each material type present in the refined mesh.

4.3.4 Solute Transport Solution

For each solute transport problem studied, the input to the SOLTR program can be divided into two parts - the problem description phase and the solute transport solution phase. At this point the problem description data phase should be complete, i.e. the finite element mesh has been refined, boundary conditions have been specified and material properties set.

The transport solution data phase of the input to the SOLTR program is used to control the solution of transport problems and to change problem boundary conditions, material properties and hydraulic characteristics at specified times. Solute transport solutions can be done for either transient or steady-state conditions. Transient solute transport solutions may be based on either steady-state or transient groundwater flow.

The transport solution phase is directed by the user to produce solutions desired for the solute transport model. This is achieved by direct input of transport solution control data to the SOLTR program. The user may change portions of the problem description data and subsequently run solute transport analyses as many times as are required to produce the desired solute transport results. In this way, time-dependent transport boundary conditions and/or hydraulic conditions can be directly simulated. It is common practice to interrupt the solution of a problem during this phase and have the SOLTR program produce an output "checkpoint" data file which can be used as the starting point for the next SOLTR run.

After completion of any set of solute transport analyses the user can direct the SOLTR program to produce contour plots of model results on the line printer. The user may also prepare a more precise series of solute concentration plots on either a mechanical plotting device (ie. Calcomp) or the line printer using the FLOCON output display and plotting program.

5.0 DOCUMENTATION

Four levels of documentation have been prepared for the Groundwater Computer Package. This documentation is available as required by users, programmers and management. The levels and items of documentation available are described below.

5.1 Management Summary

The Management Summary is intended to provide management and other personnel with non-technical instructive information about the package. This document is the management summary for the Groundwater Computer Package.

5.2 User's Manuals

User's Manuals describe in detail the capabilities of the individual component programs in the package, the procedures by which they may be used, input data requirements and formats, along with program operation instructions. In addition, for the analytical programs, the user's manuals provide:

- general sequence of events required to perform an analysis
- descriptions and interpretations of input parameters
- explanatory notes on program output and error conditions
- notes on auxiliary operations such as input data preparation and analysis results presentation.

The following User's Manuals are available.

1. Input Data Preparation for AFPM - Programs MLTMSH and AFPOL
2. Hydraulic Solution - AFPM Computer Program
3. Hydraulic Solution - FPM Computer Program
4. Solute Transport Solution - SOLTR Computer Program
5. Output Presentation and Plotting

All of the above User's Manuals have been written for use by engineers and geologists who are not necessarily familiar with computer programming.

5.3 Systems Manuals - Finite Element Theory

Systems Manuals contain the explicit mathematical formulations and fundamental assumptions for the variants of the finite element method incorporated in the Groundwater Computer Package. Users should familiarize themselves with the analytical details of the numerical methods to ensure correct interpretation of the modelling capabilities and limitations of the package.

1. Finite Element Theory - Hydraulic Solution
2. Finite Element Theory - Solute Transport
3. Salinity Solution Investigation Report

5.4 Programmer's Manuals

Programmer's Manuals contain the detailed logic and coding references of the component programs in the package. They are used by computer programmers and systems analysts for maintenance, enhancement and extension of the programs. The structure, functions, file organization, flow and control of each component program is detailed within the Programmer's Manuals. These manuals are intended to be read in conjunction with the actual (FORTRAN) coding of the component programs. The following programmer's manuals have been prepared:

1. MLTMSH and AFPOL Programs
2. Hydraulic Solution - AFPM Program
3. Hydraulic Solution - FPM Program
4. Solute Transport - SOLTR Program
5. Output Presentation and Display - FLOCON Program
6. Common System Subroutines and Functions

The above programmer's manuals have been written in a style comprehensible to individuals with an extensive scientific or engineering computing background.