Encl to 8-26-82 101
memo to Knapp.

COMPARISON OF MODEL STUDIES:

THE HANFORD RESERVATION

By Linda L. Lehman and Ellen J. Quinn

TABLE OF CONTENTS

LIST OF FIGURES

List of Figures (Continued) | Page

List of Figures (Continued) Page

LIST OF TABLES

COMPARISON OF MODEL STUDIES: THE HANFORD RESERVATION

By Linda L. Lehman and Ellen J. Quinn

INTRODUCTION

The U. S. Department of Energy (DOE), National Waste Terminal Storage Program, is currently assessing the feasibility of high-level nuclear waste storage at several locations in the United States. Of the sites now under consideration, the nuclear reservation at Hanford, Washington has received the most intensive study. A DOE Site Characterization Report (SCR) for Hanford will be submitted to the U. S. Nuclear Regulatory Commission (NRC) in September of 1982.

A thorough understanding of the dynamics of groundwater flow is essential to the development of both release scenarios and consequence analyses as required by 10 CFR 60. In response to this requirement, several groups of government and government contracted investigators have made independent efforts to formulate computer models which represent the groundwater flow system at the Hanford Reservation. The principal investigators are:

- Rockwell Hanford Operations (RHO)
- Battelle Pacific Northwest Laboratories (PNL)
- U. S. Geological Survey (USGS)

Several computer modeling efforts have been commissioned by RHO. Conducted under contract, three separate studies were made by Los Alamos Technical Associates, Intera Environmental Consultants, and Resource Management Associates. Additionally, a very recent in-house RHO effort is documented in the informal report RHO-BWI-LD-44, Arnett, et al. (1981).

The results of the PNL study are documented in the draft report PNL-3632, Dove, et al. (1979). The USGS modeling study has not yet been formally released for NRC review.

With the exception of the in-house RHO report, all these studies show a predominantly upward groundwater flow component which travels through the repository stratum and discharges at or near the Columbia River. The discordant RHO report describes a "near-horizontal" flow which would contain any groundwater contamination within the repository horizon (i.e., the Umtanum strata) with significantly longer travel times. Figure 1 and Table 1 summarize the pathways and travel times from the various reports.

In accordance with the NRC regulation 10 CFR 60, there must be a high degree of confidence in the direction of groundwater flow in an area designated for nuclear waste disposal. The most recent RHO report represents a significant deviation from all other computer simulations conducted for the Hanford site. These inconsistencies must be resolved in order to ascertain that the flow system is well understood. Consequently, the NRC has designated this flow path discrepancy as an issue of significant importance in its review of the Hanford site characterization program.

Since the groundwater flow path at Hanford is a critical issue, the NRC has undertaken an independent effort to evaluate the results obtained by the various computer simulations. The PNL and RHO models were selected for study. The PNL model was selected because it best represents the "traditional" concept of groundwater flow at Hanford; whereas the in-house RHO model presents a striking contradiction. Also, the difference between these particular flow paths may have important licensing implications. The purpose of this report is to describe the process by which the simulations were duplicated, compare boundary conditions, and identify areas which are of concern or where more data would be valuable for the purpose of achieving model capability.

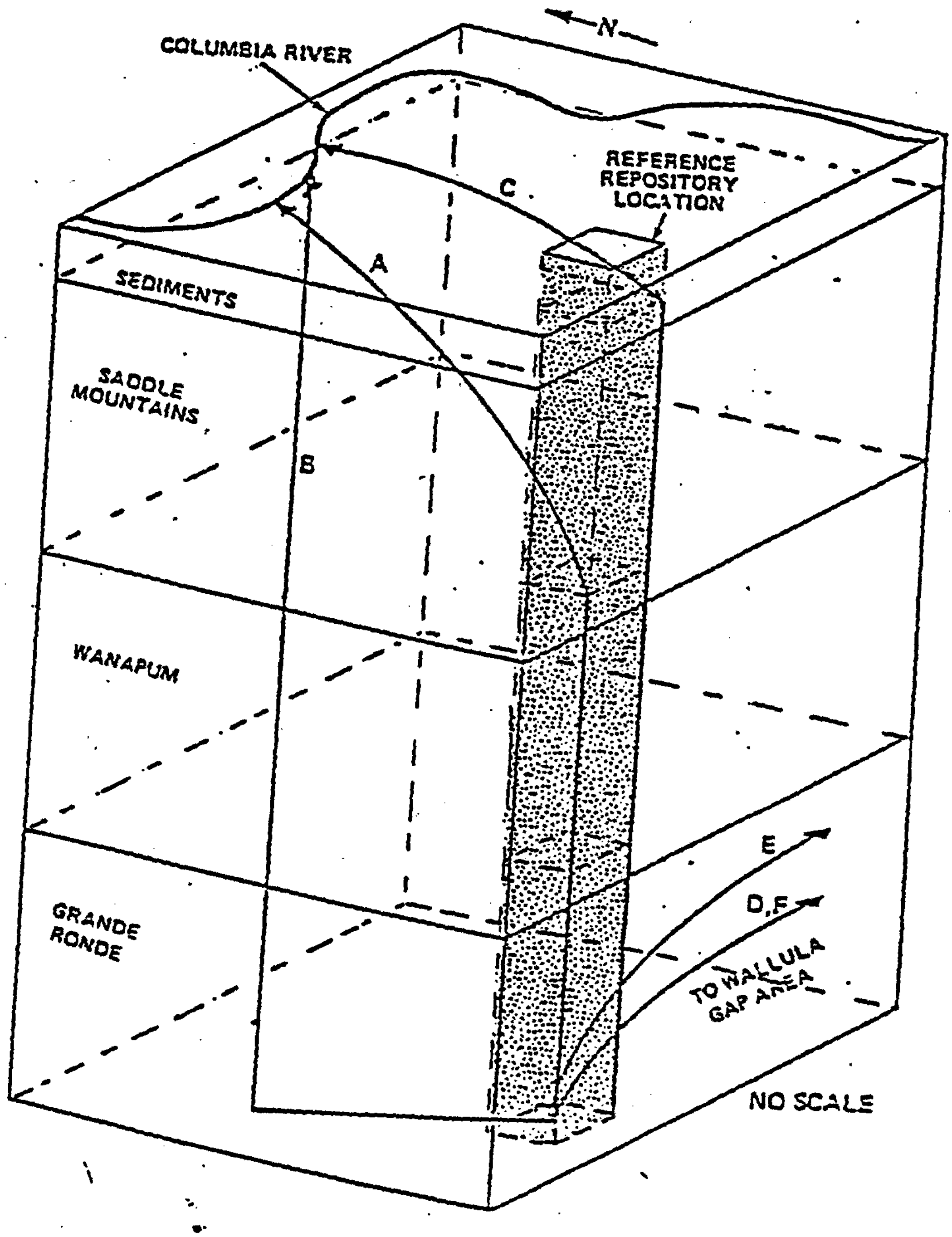


Figure 1. GENERALIZED REPRESENTATION OF SELECTED STREAMLINES (After RHO, Slide Presentation, September, 1981)

* Refer to Table 1 for explanation

Table 1

SUMMARY OF TRAVEL TIME ESTIMATES

FAR-FIELD

PATHLINE	STUDY	YEAR	DISTANCE TRAVELED**	TRAVEL TIMES (YEARS)
A	ROCKWELL	1979	~9 MILES	78,000
B	LATA/INTERA	1979	~6 MILES	34,000
C	PNL (AEGIS)	1979	~4-9 MILES	15,000-41,000
D	ROCKWELL/RMA	1981	~40 MILES	$>10^5$

NEAR-FIELD

PATHLINE	STUDY	YEAR	DISTANCE TRAVELED**	TRAVEL TIMES (YEARS)
E	ROCKWELL (THERMAL CONDITIONS)	1981	~2-5 MILES	10,000-30,000 TO NEAR-FIELD MODEL BOUNDARY***
F	ROCKWELL (NON-THERMAL CONDITIONS)	1981	~3-5 MILES	>8,000-12,000 TO NEAR-FIELD MODEL BOUNDARY***

**DISTANCE FROM REFERENCE REPOSITORY LOCATION TO COLUMBIA RIVER.

***BOUNDARY OF NEAR-FIELD IS TAKEN TO 2.7 MILES FROM OUTER BORDER OF REPOSITORY.

NEAR-FIELD - WITHIN THE THERMAL FIELD OF THE REPOSITORY, THIS IS PRINCIPALLY WITHIN THE GRANDE RONDE BASALT.

FAR-FIELD - AREA OUTSIDE OF THE NEAR-FIELD AND EXTENDING TO THE BIOSPHERE.

(After RHO, slide presentation, September, 1981)

NUMERICAL MODELS - BACKGROUND

Both the PNL and RHO computer models are finite element codes. In order to make a meaningful comparison of the PNL and RHO models, the boundary conditions and input parameters from each model were translated for use in the NRC finite difference code - SWIFT. Normalizing the numerical simulations to the same model in this fashion allows the results of each model to be compared within a common framework. It could be argued that the NRC model itself might introduce some bias to the results. This, however, has not been the case as the NRC simulations have duplicated the RHO and PNL results. This is not at all suprising as the three computer models being considered are quite competant to simulate a groundwater flow pattern given adequate and realistic input data, i.e., with the same input, each model should and will produce similar output. What is instructive in this study is the variance with which the input data has been selected by PNL and RHO, and the ramifications these selections have on the simulation results. Before addressing the results of the NRC model comparisons, it is first necessary to review the various models themselves and the underlying geologic and hydrologic assumptions.[1]

1/Translating the PNL and RHO input data for use in the NRC SWIFT model was not a trivial matter. In order not to distract the reader from the text, a detailed and technical discussion of how this translation was accomplished has been presented as Appendix A.

NRC FINITE DIFFERENCE MODEL

The NRC computer model used to compare the PNL and RHO simulations is the finite difference code SWIFT. The grid and layering scheme used to simulate the Pasco Basin was developed in-house by the NRC staff exclusively for this purpose. A detailed discussion of the scheme is contained in the NRC report "Mock Site Characterization Review of Basalt - The Hanford Site," L. Lehman and E. Quinn (1981), Attachment 1. A complete explanation of the internal workings of SWIFT will not be provided here. However, specific elements of the SWIFT code are addressed in the ensuing text when their explanation is appropriate and necessary.

ROCKWELL HANFORD OPERATIONS PASCO BASIN MODEL

The RHO Pasco Basin model uses the finite element code MAGNUM-3D. This code has neither been documented nor field verified at the present time. Plans for documentation are tentatively set for 1983. As a result, a thorough evaluation of this code is not considered in this report either, but will be addressed under NRC contract FIN NO B-6985, "Benchmarking of Computer Codes and Licensing Assistance."

Figure 2 shows the conceptual flow model of the Pasco Basin as presented by RHO in RHO-BWI-LD-44. The arrows indicate direction and magnitude of flow.

Recharge is occuring:

1) along the eastern boundary in all layers;
2) along the northwestern boundary in all layers;
3) along the northern boundary in the Grande Ronde Basalt; and
4) within the Rattlesnake Hills in the top two layers.

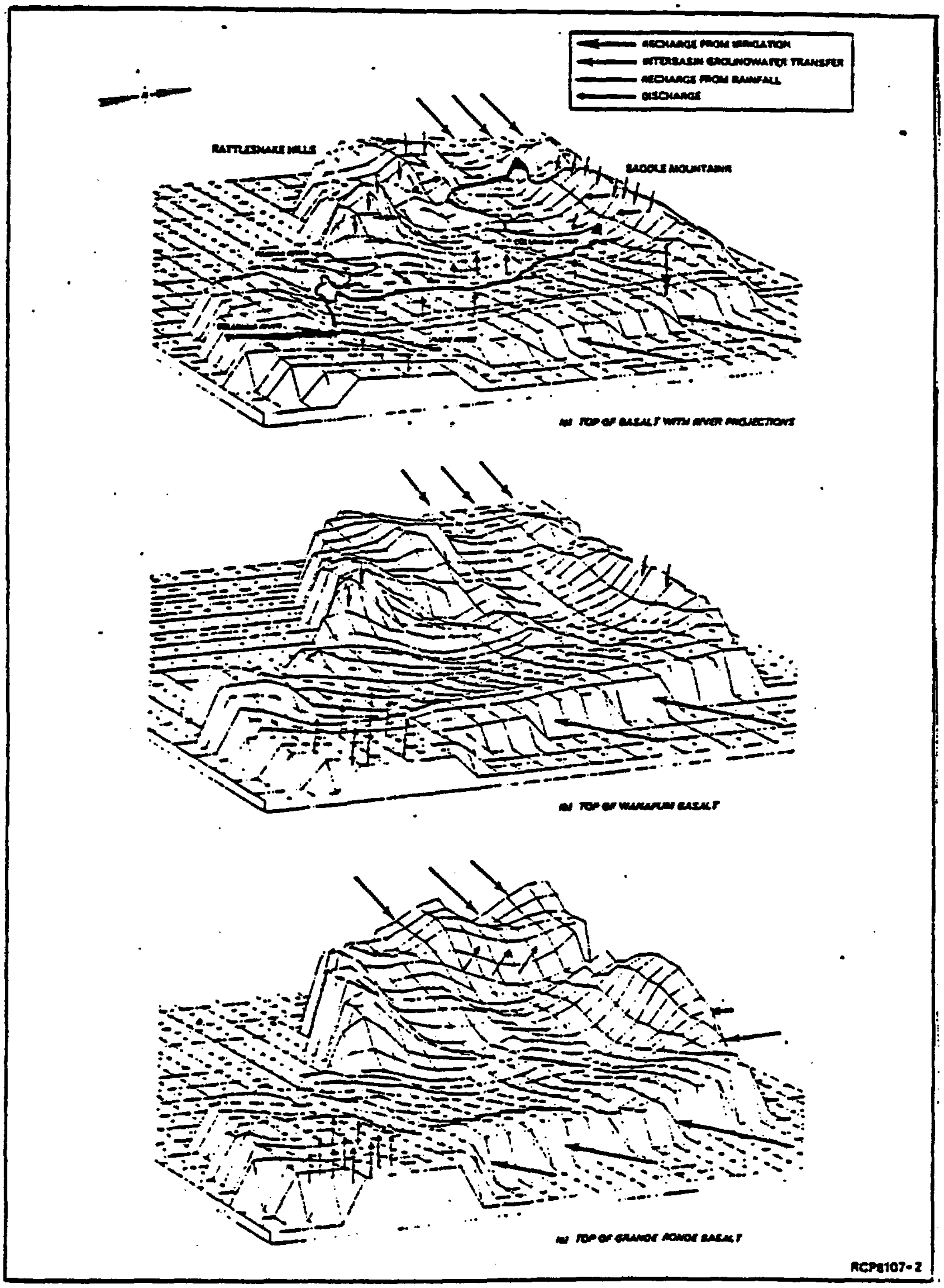


Figure 2. Pasco Basin Conceptual Groundwater Flow - RHO
(After, RHO- BWI-LD-44)

Discharge is occurring:

1) to the Columbia River in the top layer;
2) at the southeast corner (Wallula Gap area) in all layers; and
3) along the flanks of Rattlesnake Hills in the Grande Ronde Basalt.

Figure 3 shows the plan view of the Pasco Basin grid network used by RHO in their simulation. All numerical values are boundary conditions expressed as hydraulic head in meters above mean sea level. Along the eastern boundary a recharge condition exists in the conceptual model (as shown on Figure 2 but head values used for this boundary in the simulation indicate either horizontal flow (head constant with depth) or discharge (head increasing with depth). Since a recharge condition is not simulated, water flows out or rather than into the basin along that boundary. Conversely, the southeastern corner of the conceptual model is designated as a discharge area as shown in Figure 2; but in the numerical model heads either are constant with depth or decrease with depth as is typical of recharge head distributions. These inconsistencies in the formulation of boundary conditions have resulted in a lack of discharge in the modeled area for Rockwell's simulations.

Additionally, Rockwell has forced the water table to maintain a specific configuration through the use of constant head boundaries.

The following discussion regarding boundary conditions is taken directly from RHO-BWI-LD-44:

> The boundary conditions for the initial MAGNUM-3D simulation were developed in part from the broad criteria listed below.
>
> - The heads for the upper boundary nodes lying below the Columbia, Yakima, and Snake Rivers are assumed to be equal to the average river stages. By implication, the head in the unconfined region lying between the rivers and the basalt groundwater system is assumed to be hydrostatic. The average

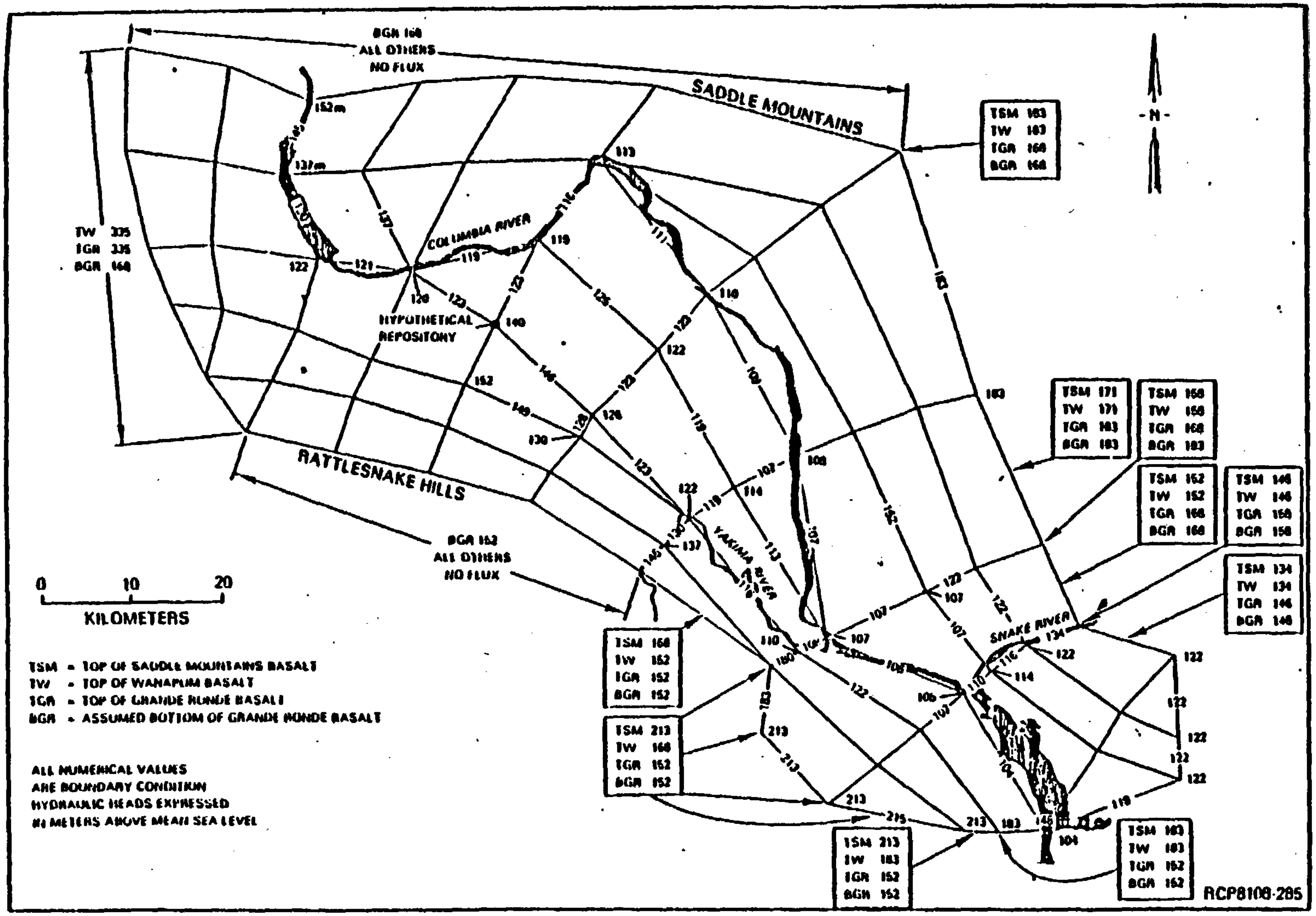


Figure 3. Plan View of Pasco Basin Rockwell Finite Element Grid
(After, RHO-BWI-LD-44)

river stages are obtained from Plate III-4 of Gephart et al. (1979).

- The heads for the upper boundary nodes lying below the unconfined sedimentary aquifer are assumed to be equal to the unconfined heads. The unconfined heads are assumed to be hydrostatic and are obtained from Plate III-4 of Gephart et al. (1979).

- The heads for the boundary nodes on the vertical sides of the system are estimated from borehole measurements reported in Gephart et al. (1979) and from other borehole data compiled by Rockwell. No-flux boundaries are assumed along the upper portions of the Rattlesnake Hills and Saddle Mountains anticlines. Elsewhere, the heads are assumed to be hydrostatic except in a few areas indicated in Figure 4-2. [Figure 3 of this report].

- The lower (bottom of Grande Ronde) aquifer boundary is assumed to be a no-flux boundary. This boundary is intentionally located sufficiently far below the surface (1,000 m below the top of the Grande Ronde) to be beyond the influence of recharge and pumpage. At this depth, the vertical head profile should be hydrostatic and vertical flow should be negligible.

- The surface fluxes (LT^{-1}) for the upper boundary elements lying below recharge areas are assumed to be proportional to annual rainfall. One fifth of the long-term average annual rainfall (3.7 cm/yr) is assumed to reach the basalt groundwater system. The recharge areas are defined in Plate III-12 of Gephart et al. (1979). [Figure 4 of this report].

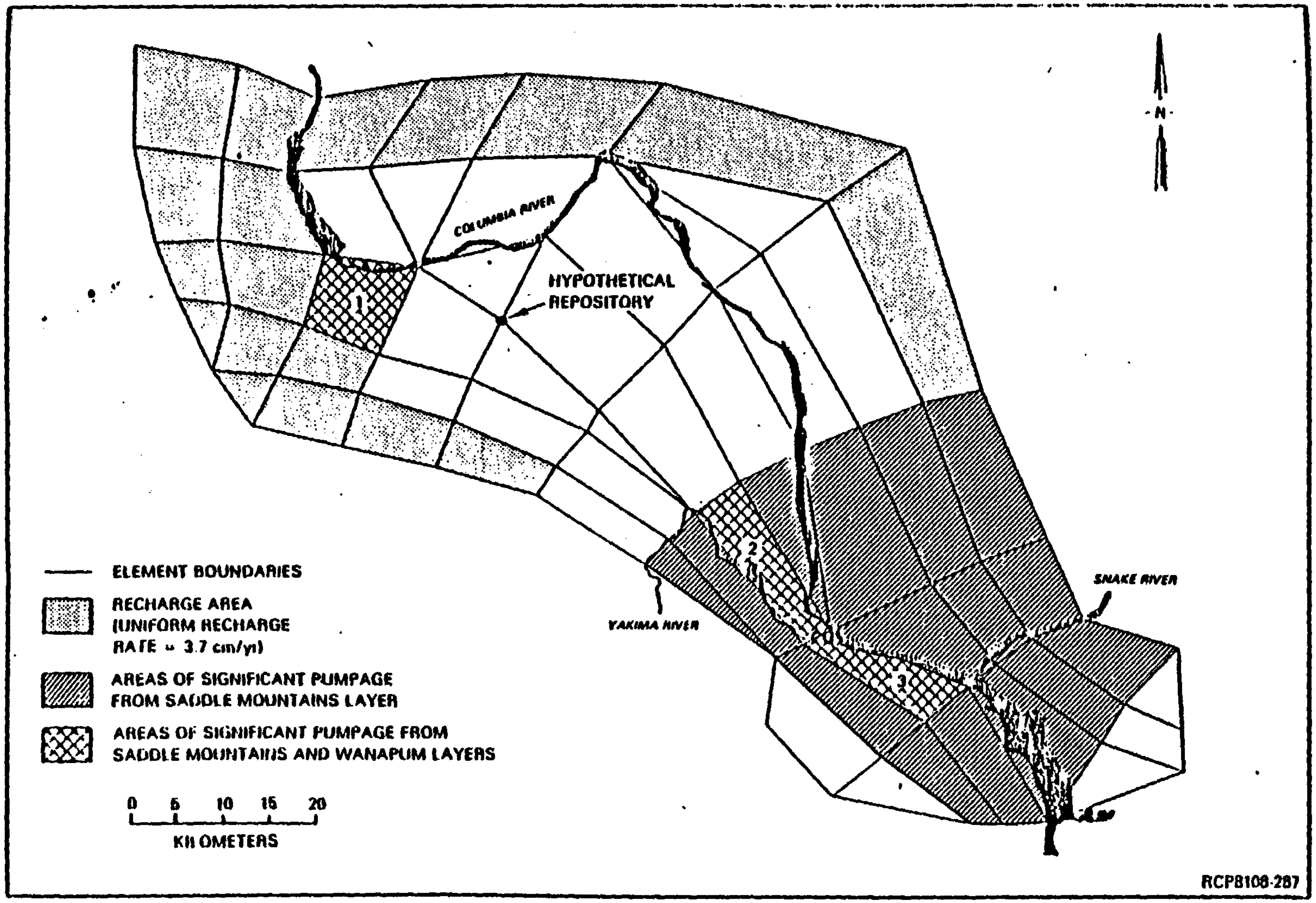


Figure 4. Distribution of Infiltration and Pumpage - RHO (After RHO-BWI-LD-44)

- Head values, in meters above mean sea level, for the various boundary nodes are indicated in Figure 4-2. [Figure 3 of this report]. The legends on this figure indicate where the hydrostatic assumption is made, where vertical variations exist between layers, and where surface-only boundary conditions are applied. The figure also indicates those regions where basalt extends above the sedimentary water table. Surface nodes in these regions are assumed to lie on a no-flux boundary and are not assigned specified head values.

Figure 5 shows the vertical layering scheme used by RHO in their simulation. The layering separates the geologic section into three main hydrostratigraphic formations, i.e., the Saddle Mountains, Wanapum and Grande Ronde formations.

Permeabilities and hydraulic properties of these units are provided and discussed subsequently in this report.

<u>Results from RHO-BWI-LD-44</u>

The flow path RHO derived from their simulation is shown in Figure 6. This path runs from the repository southeastward, crosses under the Columbia River north of Richland crosses under the Snake River near Ice Harbor Dam and continues on to the south.

A cross-sectional view of the Pasco Basin (Figure 7) shows that a particle released from the repository will remain in the Grande Ronde Formation. No vertical component of flow exists along this streamline. However as will be shown subsequently this is a consequence of the establishment (fixing) of a 1099 foot head along the 25 mile northwest corner of the grid (see page 37, item 1) and of the fact tht 25 miles of the eastern boundary were fixed at a head of 600 ft. and considered hydrostatic, constant head with depth precludes vertical flow in the vicinity of such as boundary. A similar statement applies to the south

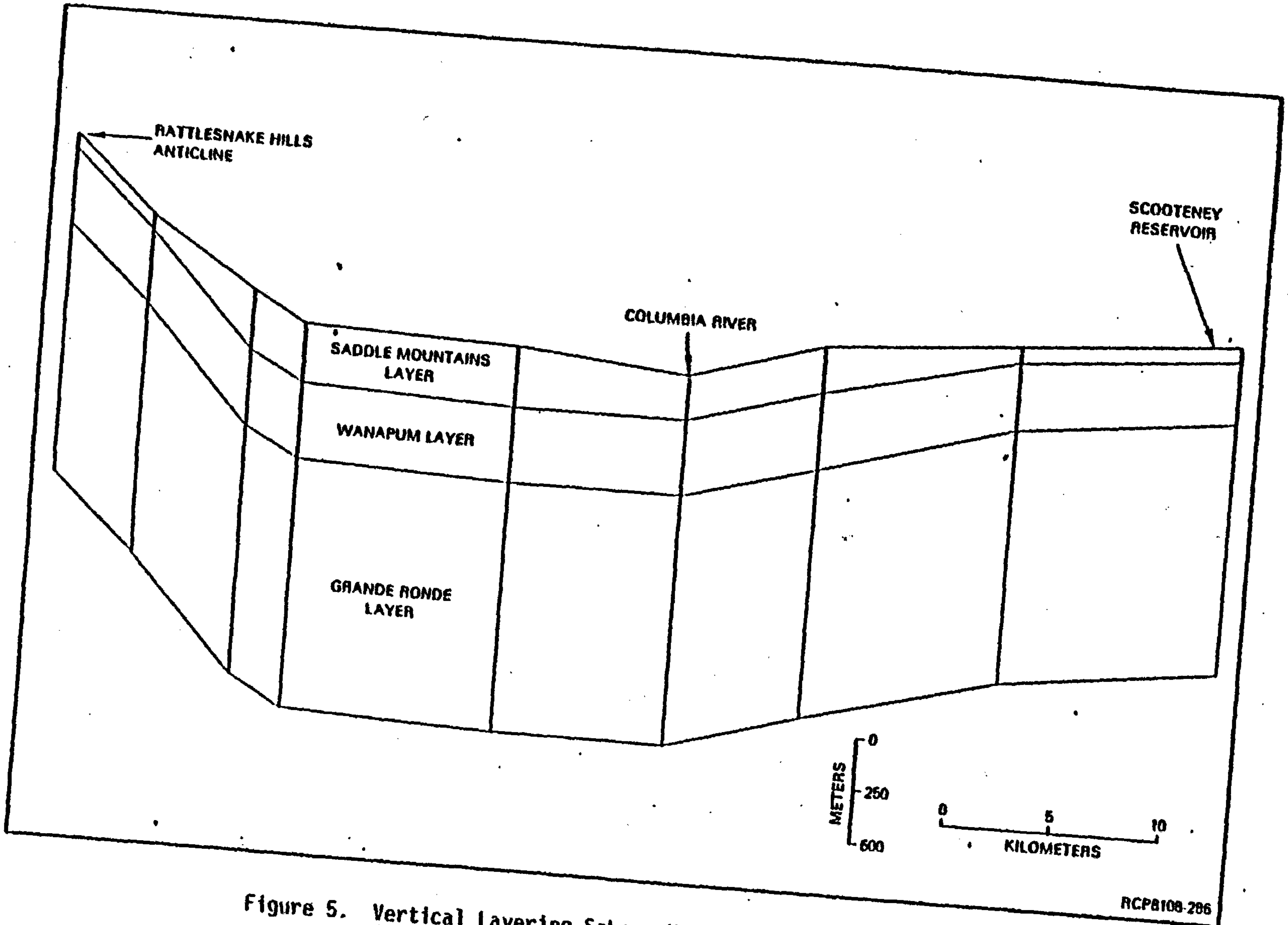


Figure 5. Vertical Layering Scheme Used By RHO
(After, RHO-BWI-LD-44)

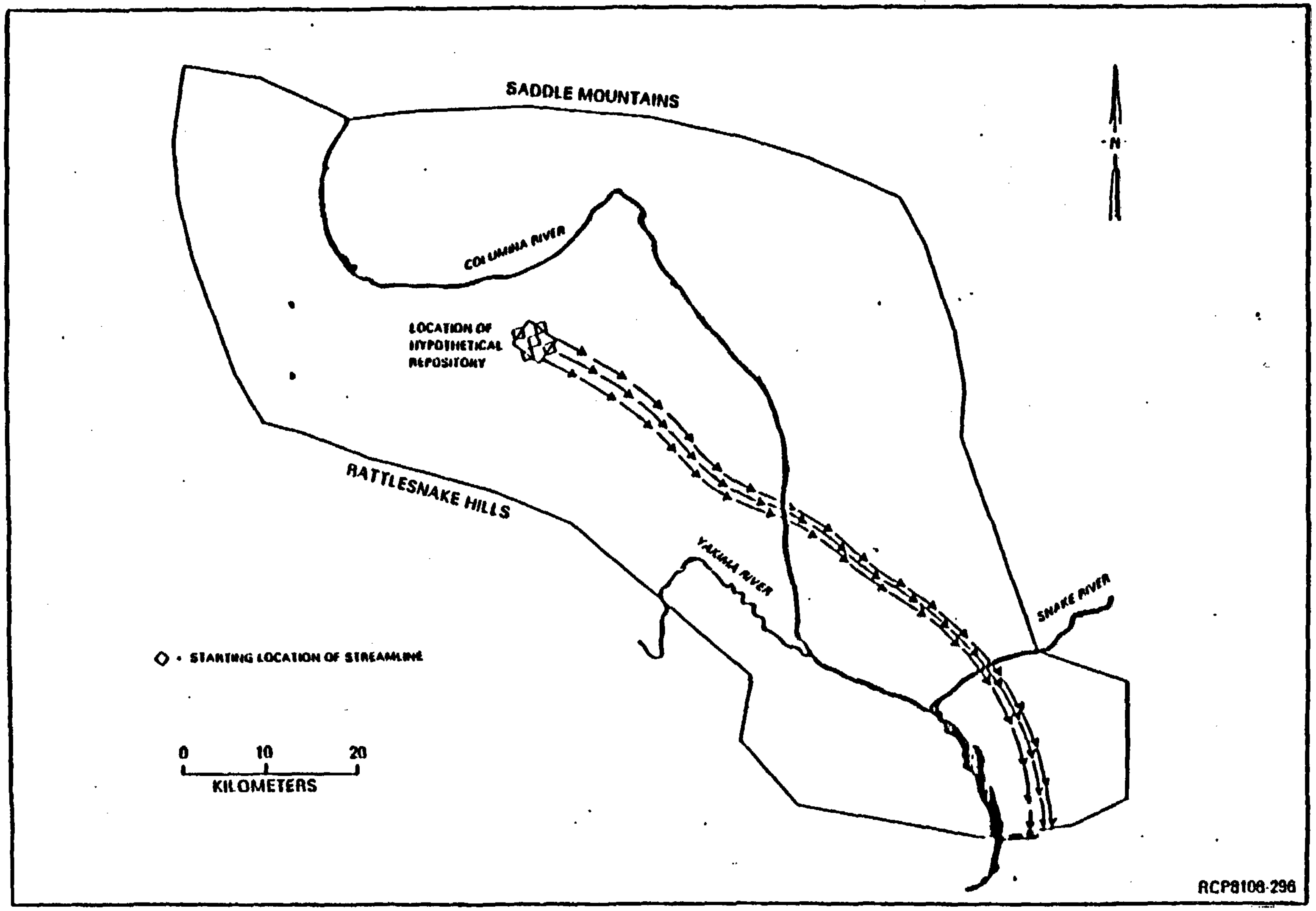


Figure 6. Flow Path Derived From RHO Simulation
(After, RHO-BWI-LD-44)

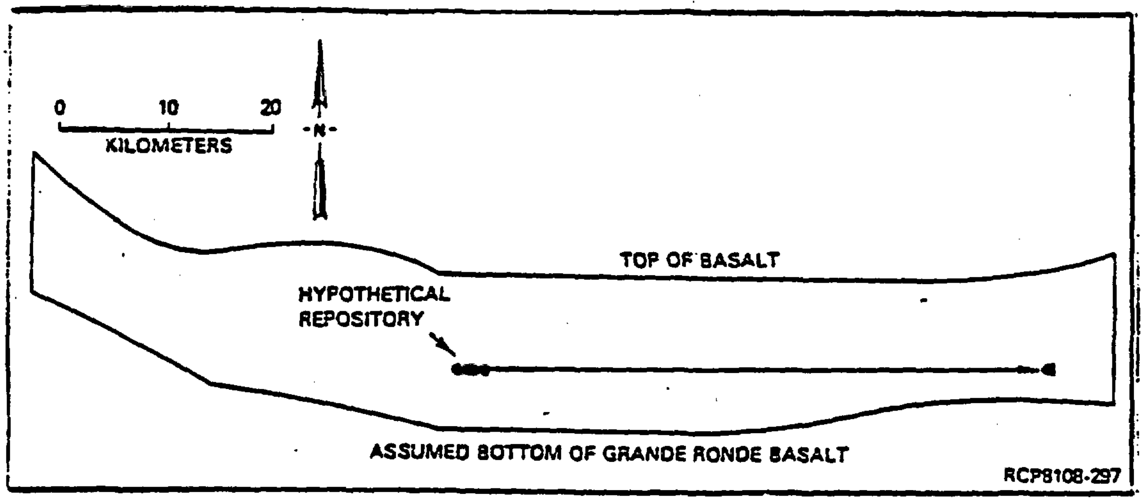


Figure 7. Cross sectional view of Pasco Basin showing through the RRL streamline.
(After, RHO-BWI-LD-44)

12 miles of the eastern side of its grid where the head was fixed at 400 ft. No vertical flow can occur there either.

Conclusions drawn by RHO include:

1. The hydraulic head patterns generated in this simulation show only a limited upward gradient.

2. Streamlines calculated by the model extend from a hypothetical repository location to the edges of the model boundary and remain in the Grande Ronde basalt for the entire path length.

3. The overall travel time from the repository to the model boundary for a particle moving along the streamline was calculated to be well in excess of 100,000 years. This was true even though horizontal movement was assumed to occur in a material with the properties of the more conductive interflow zone. This low velocity is a consequence of very low gradients along the streamline; the low gradients in turn are a consequence of input boundary conditions.

BATTELLE PACIFIC NORTHWEST LABORATORIES MODEL

PNL's Conceptual Model is based on the hypothesis that the Pasco Basin is one of the main discharge areas for the entire Columbia Plateau. Concomitantly, flow in the Pasco Basin is predominantly upward from the deep basalts into the alluvial aquifer and the Columbia River.

The Conceptual Model is supported by PNL's regional scale modeling, which in turn is based in part on the fact that regional groundwater budget studies indicate a net discharge of water within the Pasco Basin. PNL has also used regional water level data to develop a model of groundwater flow in the Columbia Plateau. Figure 8 shows the cross-sectional view of the PNL Conceptual Model.

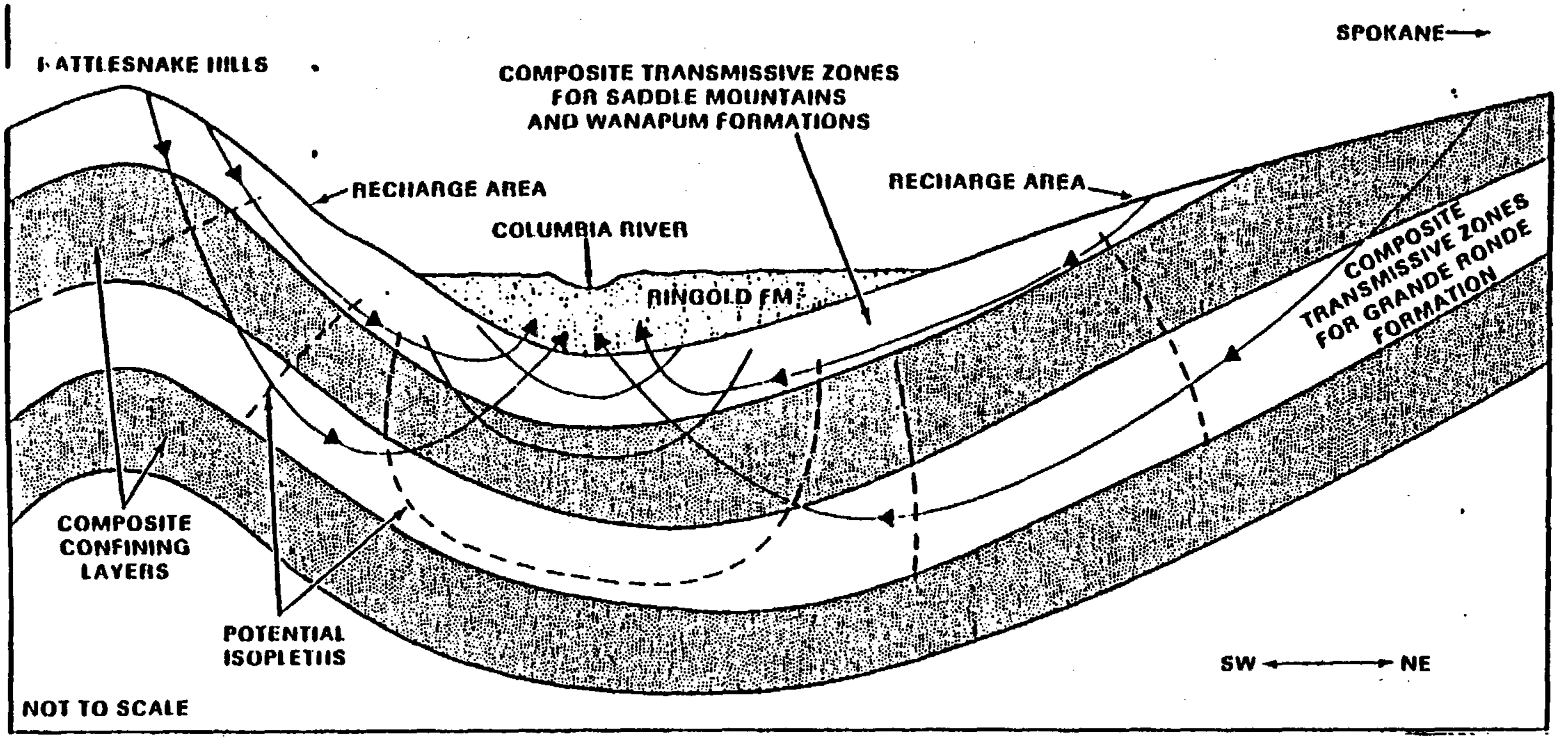


Figure 8. Cross-Sectional View of the PNL Conceptual Model (After, PNL-3632)

The PNL modeling effort began with the regional simulation of the Columbia Plateau to identify the boundary conditions for the Pasco Basin Model. While this procedure is not error-free, it does bring regional flow dynamics into consideration when examining local model boundary conditions. The Pasco Basin model simulates a sub-area of the regional model in greater detail. PNL selected the Finite Element Three-Dimensional Groundwater Model (FE3DGW) for the modeling exercise. The FE3DGW model uses the Galerkin finite element method with deformable quadrilateral elements. The Pasco Basin FE3DGW grid is shown as Figure 9. As with the Rockwell code, a complete examination will be addressed under NRC contract FIN No. B-6985.

The PNL model used 4 composite layers:

1. the alluvial water table aquifer;
2. the Saddle Mountains Formation;
3. the Wanapum Formation; and
4. the Grande Ronde Formation.

The PNL boundary conditions constitute a major deviation from those of the RHO model. The PNL boundary conditions include:

1. A water table that maintain a specific configuration through the use of constant head boundaries.
2. Flow boundaries (recharge) on the north and eastern sides of the basin.
3. No flow boundary (groundwater divide) on the west and southwestern boundary.

PNL Boundary conditions were not provided in graphic form as were the RHO boundary conditions. The values were reconstructed for the NRC simulation from original computer listings provided by PNL (Figure 10). The northern boundary is a flow boundary; the northeastern boundary is a recharge boundary (head decreasing with depth) and; the southeastern

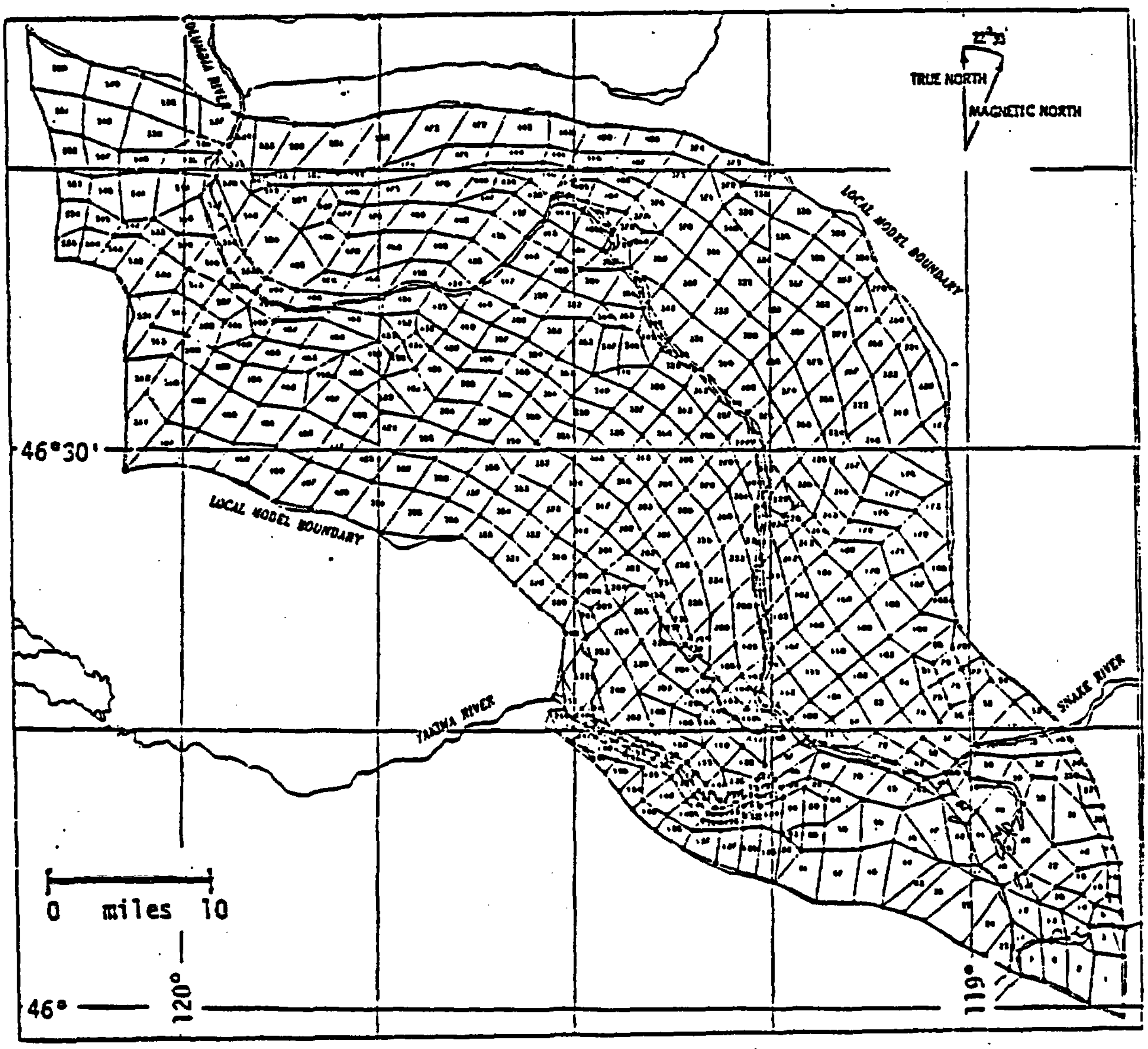
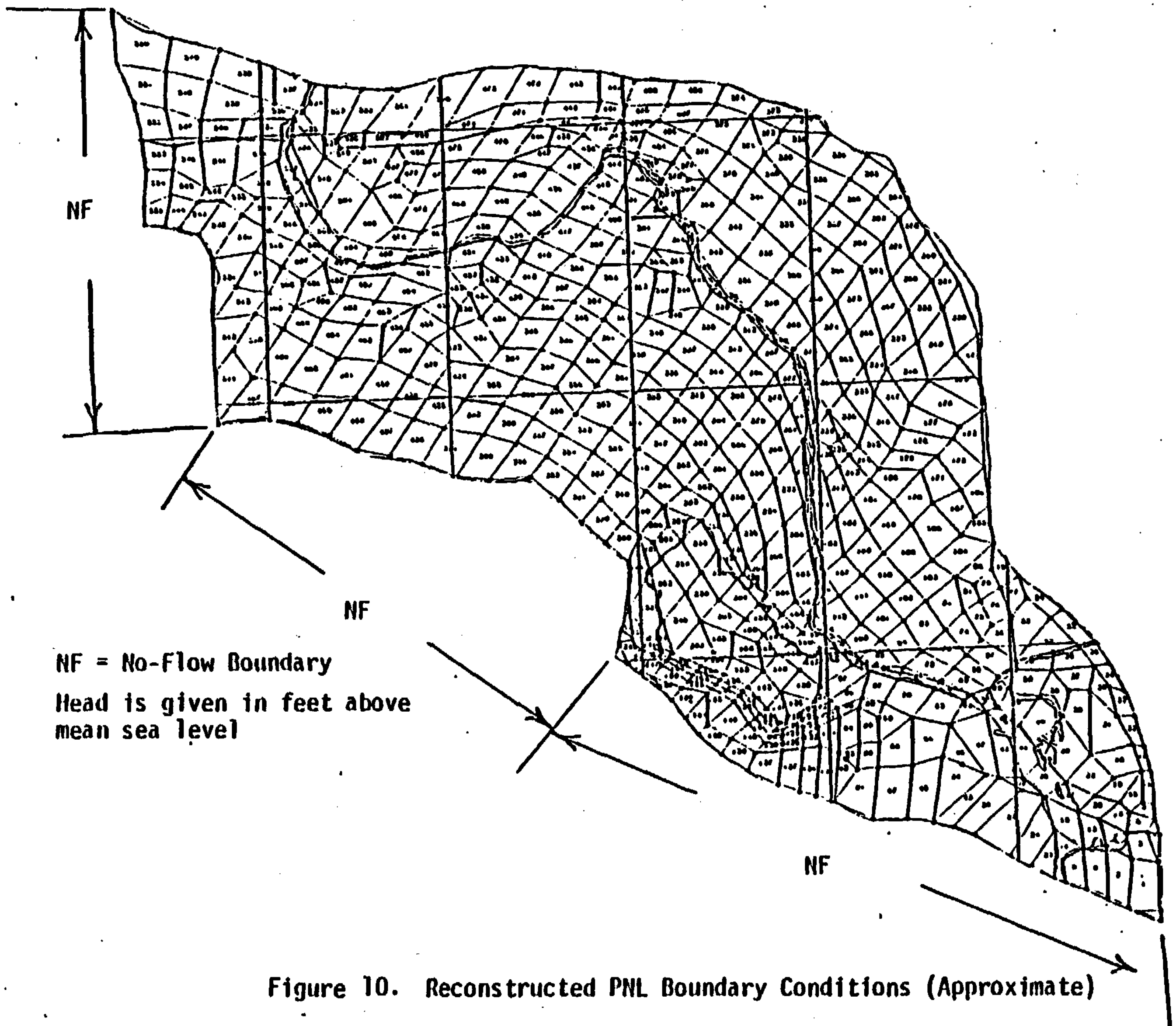


Figure 9. PNL Pasco Basin Grid Structure
(After, PNL - 3632)

TSM	NF	NF	NF	NF	NF	NF	NF	817	882	882
TWP	675	675	720	782	749	710	783	817	882	882
TGR	676	678	724	786	759	734	783	817	882	882
BGR	678	691	737	798	790	793	800	823	855	855



TSM TWP	TGR BGR
817 817	817 828
882 882	882 855
926 916	875 790
917 917	917 840
731 731	731 700
630 630	630 606
489 489	489 492
358 358	424 539
437 437	535 657

Figure 10. Reconstructed PNL Boundary Conditions (Approximate)

boundary is a discharge boundary (head increasing with depth). The numerical scheme is consistent with the Conceptual Flow Model.

PNL ran two significant scenarios; one using pre-man infiltration rates (before agriculatural development) and one of current conditions, which estimates run off and infiltration rates by crop types under development presently in the basin. Infiltration rates applied by PNL ranged from 6.5×10^4 ac. ft. per year for pre-man conditions to on the order of 10^5 acre ft per year under the current agricultural development scheme. The pre-man rates are very close to the infiltration rates used by RHO.

Results from PNL-3632

The PNL simulation indicates that the Pasco Basin is a discharge area over most of the basin. Discharge occurs: in areas where basalt formations make contact with surface water bodies, to the Columbia and Snake Rivers, and where the basalts contact saturated alluvium (where appropriate gradients are present).

PNL supports these results with the following reasoning:

- The very existence of an alluvial aquifer system in highly permeable sediments (in such an arid environment) provides some support for the discharge concept.

- Calculations indicate that under current conditions little if any natural recharge occurs in the area of the low lying alluvial systems. Artificial recharge is significant in the 200 East and 200 West areas of the Reservation.

- Historical evidence supports the existance of an alluvial groundwater system before man-induced recharge was supplied by Hanford Project activities and wide scale irrigation.

- A tremendous amount of flow system convergence would be required for discharge to occur only in areas where the basalt is in, or nearly in, contact with surface water bodies.

Particle tracking done by PNL shows:

1) that particles released from the repository would generally move upward and north to discharge at the Columbia River (Figure 1 line C)

2) particles released elsewhere in the basin move upward and inward toward the center of the basin

3) travel time calculations show that a particle leaving the repository would reach the river in 15,000 to 41,000 years (Table 1).

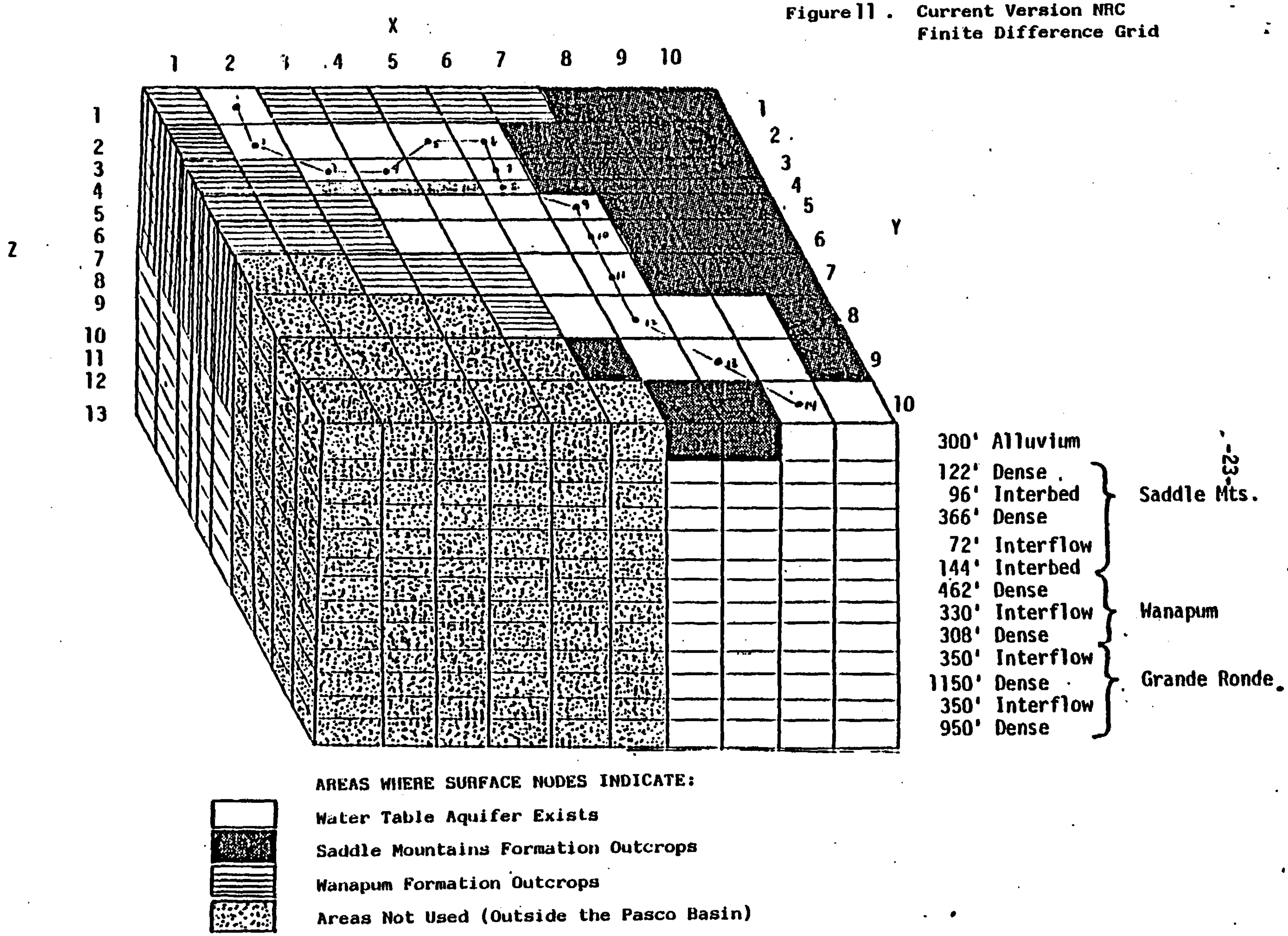
MODEL COMPARISON

As mentioned previously, in order to assess critically the modeling efforts of RHO and PNL, each numerical model was verified by applying the initial conditions used for these simulations to a finite difference grid structure of the Pasco Basin developed by the NRC. As a result of this process, initial boundary conditions and resultant flow paths could be compared meaningfully in the context of a common framework.

NRC Grid Structure

The NRC grid structure is shown in Figure 11. The three dimensional grid contains 13 layers. This structure represents the sequence of rock types and different hydraulic characteristics which we believe comprise the Pasco Basin stratigraphy in as much detail as can be derived form all available data. Layer 1 represents the alluvial aquifer, layers 2-6 comprise the Saddle Mountains Formation, layers 7-9 comprise the Wanapum

Figure 11. Current Version NRC Finite Difference Grid



Formation and layers 10-13 represent the Grande Ronde Formation. To be consistent with the RHO and PNL grids, all basin topography was simulated by elevated grid blocks. Elevating a finite difference grid introduces a slight error by increasing the transmissivity term. This error, however, is acceptable (or even desirable) because transmissivity probably increase within elevated structures in the Pasco Basin due to increased fracturing.

In raising the grid to match the topography, several assumption are necessary.

1. Hydrostatigraphic units were not thinned on the tops of anticlines or ridges.

2. The elevation change of hydrostratigrpahic units at the surface is continuous downward throughout the section.

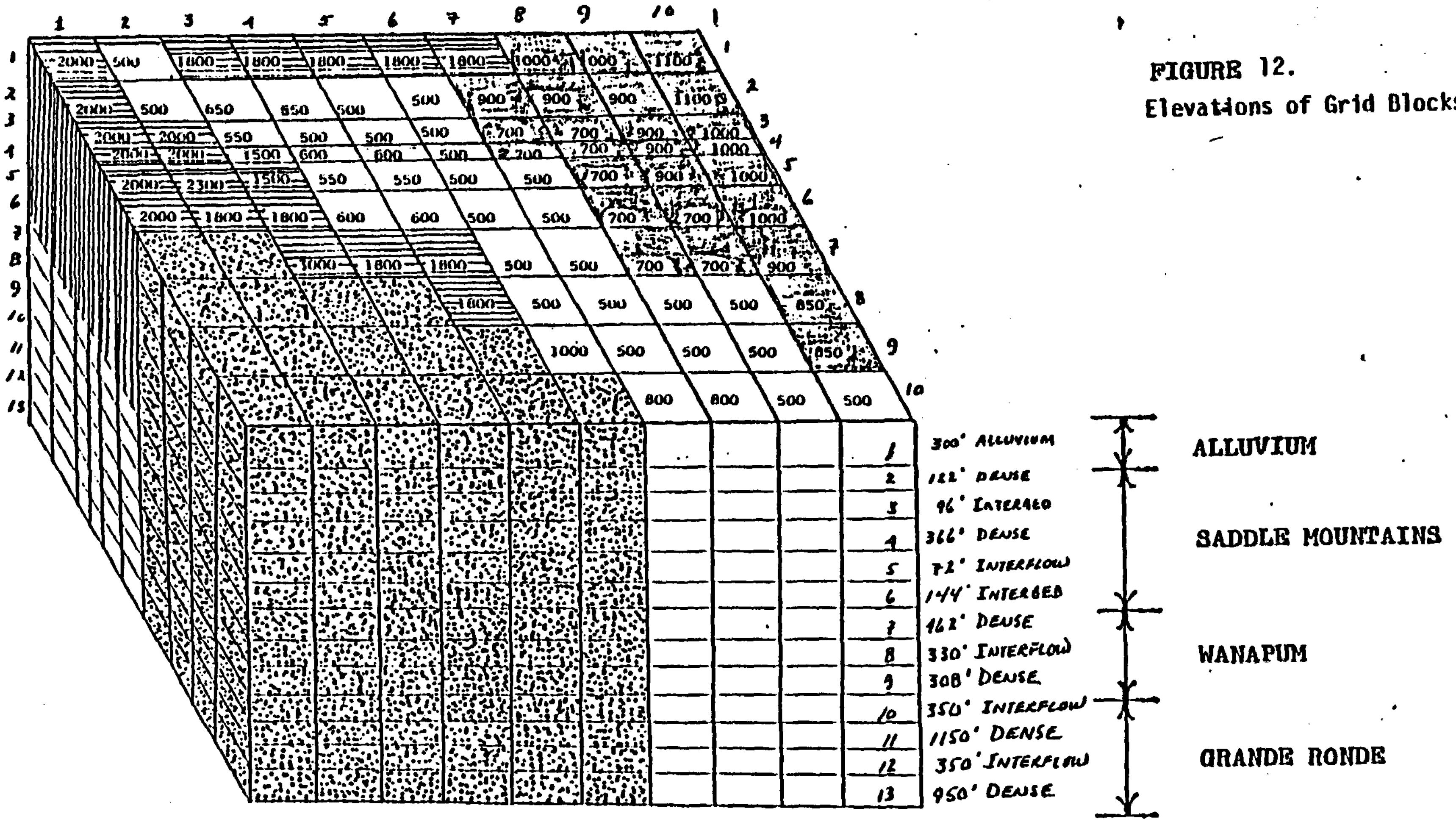
3. No erosion is assumed in areas where basalt units crop out; i.e., the entire thickness of the unit is present and constant over the entire basin.

Given the scale of the investigation and scarcity of data, these assumptions are not unreasonable. Some error may result from not thinning the hydrostratigraphic units but the error introduced is considered small compared to the overall uncertainty in the system. In addition the effort to change the grid was not justified by the minor increase in accuracy. Figure 12 shows elevation in feet above mean sea level of specific grid blocks.

Permeability and Permeability Ratios

In a steady state calculation for the determination of flow paths, actual permeabilities do not have to be identical in the two models. The critical requirement is that the overall permeability ratios, i.e., vertical permeability/horizontal permeability (K_v/K_h), be the same.

FIGURE 12.
Elevations of Grid Blocks



##NOT TO SCALE

AREAS WHERE SURFACE NODES INDICATE:

WATER TABLE AQUIFER EXISTS

SADDLE MOUNTAINS FORMATION OUTCROPS

WANAPUM FORMATION OUTCROPS

AREAS NOT USED (OUTSIDE THE PASCO BASIN)

RHO states in Arnett (1981) that the RHO model was executed using a $K_v/K_h = 10^{-4}$, but noted that better agreement could perhaps be obtained with a ratio of 10^{-3}.

PNL varied the permeability ratio according to structural deformation zones. (This process will be discussed later.) NRC duplicated the ratios and ratio distributions used by PNL and RHO when comparing the model.

In order to test the sensitivity of the model to K_v/K_h ratio, an initial analyses was conducted by varying the K_v/K_h ratio from 10^{-6} to 11. Selected hydraulic pressure gradient profiles are shown as Figures 13 through 16.

It can be seen that for ratios 11 to 10^{-2} hydraulic pressure gradients converge at the center of the basin. For ratios 10^{-3} and less hydraulic pressure gradients suggest that flow from the repository is horizontal and towards the Wallula Gap area.

When travel times of radionuclides to the accessible environment are being considered, it is of great importance to have the most accurate description of the hydrostratigraphy and reliable permeability values for the separate units. Therefore, in the interest of travel-time calculations the NRC grid was designed to allow for maximum flexibility by using the maximum number of layers numerically possible on the Brookhaven computer system. As mentioned previously, this number is 13 for this particular three-dimensional grid set up. Within these numerical constraints, the 13 layers were developed as accurately as possible to simulate the hydrostratigraphic sequence shown as Figure 17. The identity of the three major basalt formations, the Saddle Mountains, Wanapum and Grande Ronde was preserved and interflows and interbeds present within these formations could still be characterized hydraulically. The characterization procedures are discussed subsequently.

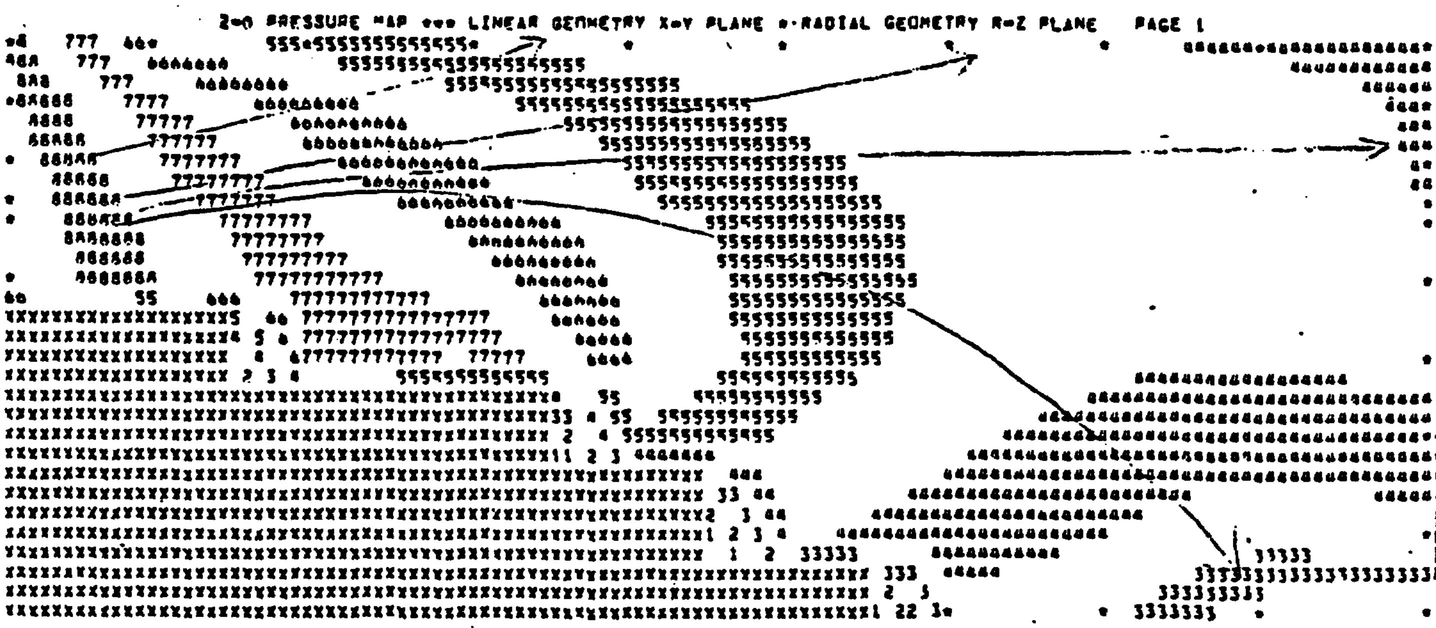


Figure 13. SWIFT Pressure Plots - Repository Horizon (Plan View) $K_v/K_h = 10^{-5}$

Figure 14. SWIFT Pressure Plots - Repository Horizon (Plan View) $K_v/K_h = 10^{-4}$

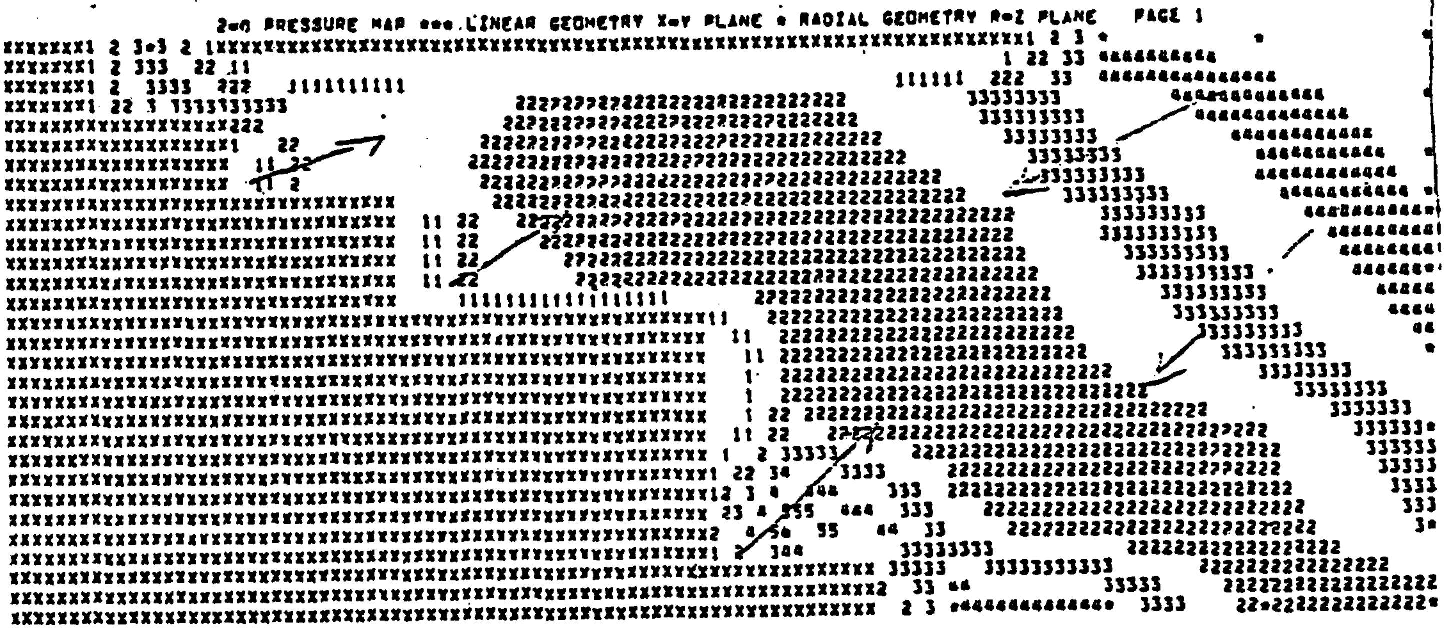


Figure 15. SWIFT Pressure Plots - Repository Horizon (Plan View) $K_v/K_h = 10^{-2}$

Figure 16. SWIFT Pressure Plots - Repository Horizon (Plan View) $K_v/K_h = 1$

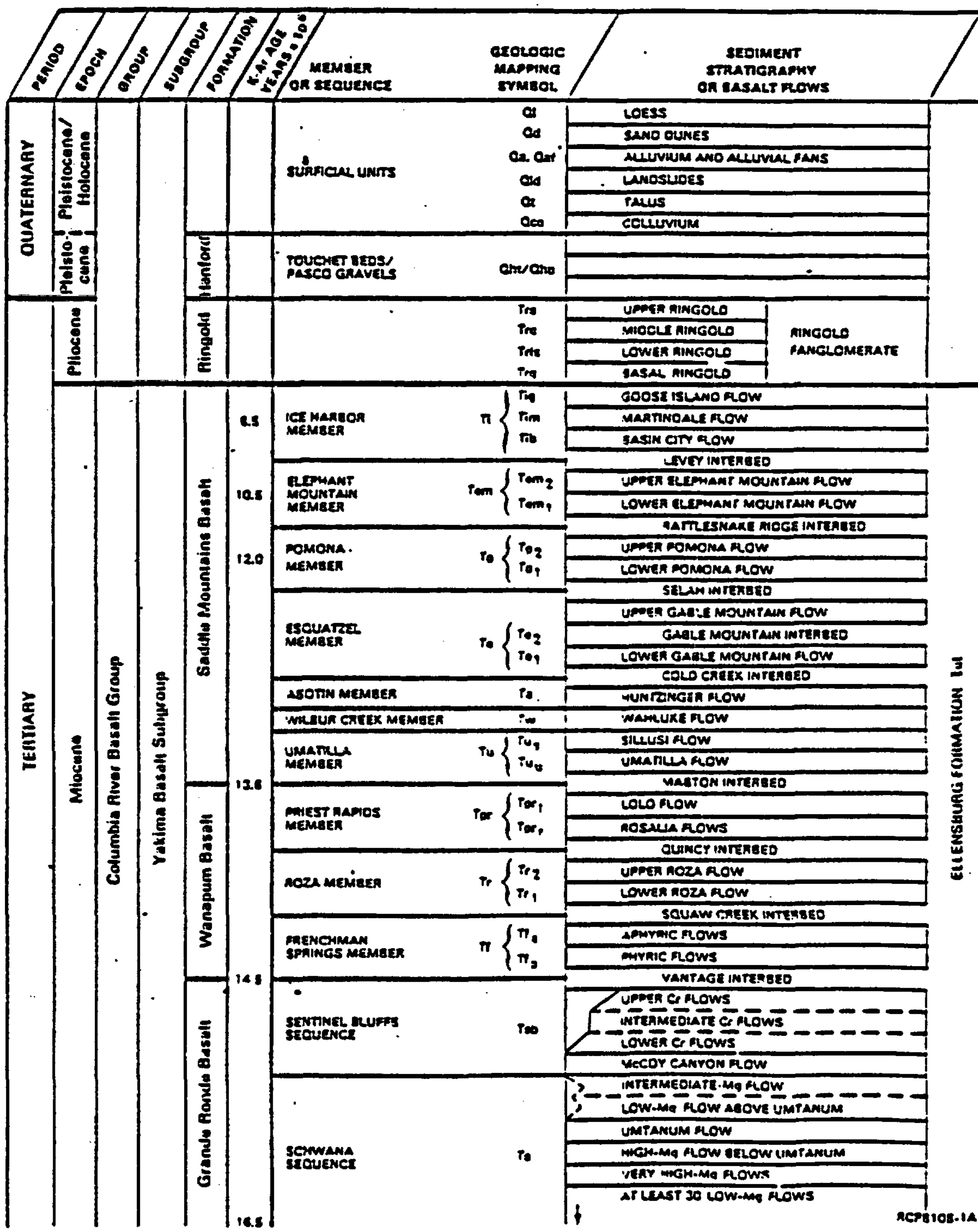


Figure 17. Pasco Basin Stratigraphic Nomenclature
(After, RHO-BWI-LD-44)

The three-layer version used by RHO lumped together the separate permeabilities of the dense units with those of the interbeds and interflows to form one composite permeability for each of the three main basalt formations. This technique is acceptable and cost effective for flow path determinations - but can result in severe under-estimates of certain travel time calculations. This is especially true in the horizontal plane. RHO has stated that their travel time calculations indicate a need for more layers in their future modeling work to overcome this limitation.

PNL also used a composite premeability value for each of their layers. However, the method used to assign permeabilities was quite complex. The first step was to prepare transmissivity maps for each of the four layers. The transmissivity maps for the Saddle Mountain and Wanapum formations were developed from existing contour maps; the Grande Ronde map was developed from three data points in the basin. In the upper units data from a wide variety of sources was used. For this reason, all the transmissivity values reported may not represent the same combination of aquifers. An interpolation routine was next used to assign hydraulic conductivity values to each node in the model. The spatial variability of the conductivity, in part, reflected the zones of structural deformation and tectonic fracturing. The permeability (K) was then computed using the relationship K=T/b, where b was the saturated thickness at each node and T was the transmissivity. The permeabilities varied from element to element over each surface, and from layer to layer vertically. Figures 18 through 21 are the transmissivity maps upon which the permeabilities were based.

The K_v/K_h ratio determination was similarly complex with several iterations required to select the best match with available head data. The process began with the assumption that K_v was related mainly to the degree of geologic deformation in the basin. (No fundamental relationship between K_v and K_h was assumed to exist). Structural maps of the top of the basalt and top of the Grande Ronde were next used to identify zones of equal deformation, Figure 22. Based on changes in

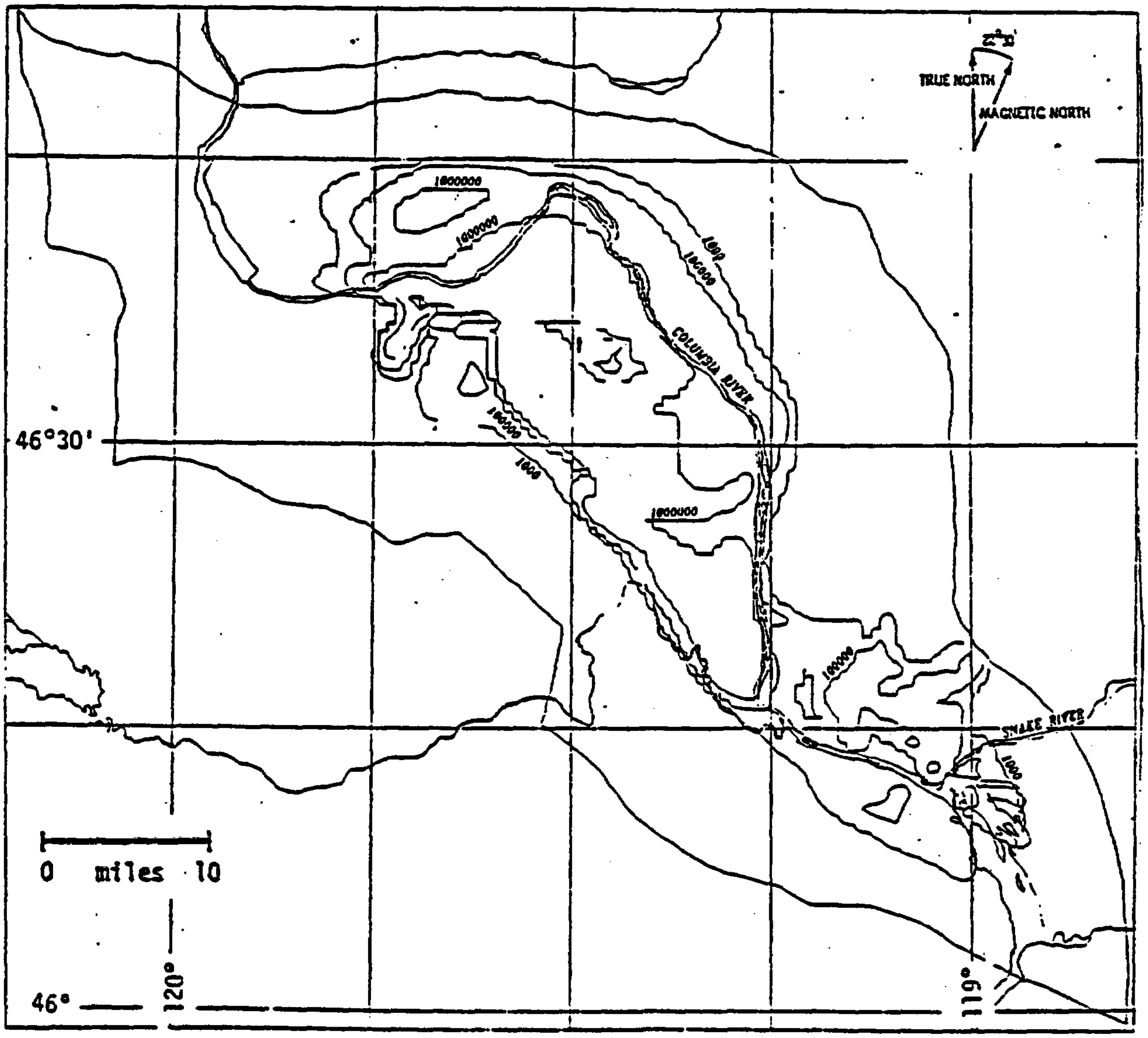


Figure 18. Transmissivity of the Alluvial Aquifer (gpd/ft)
(After, PNL - 3632)

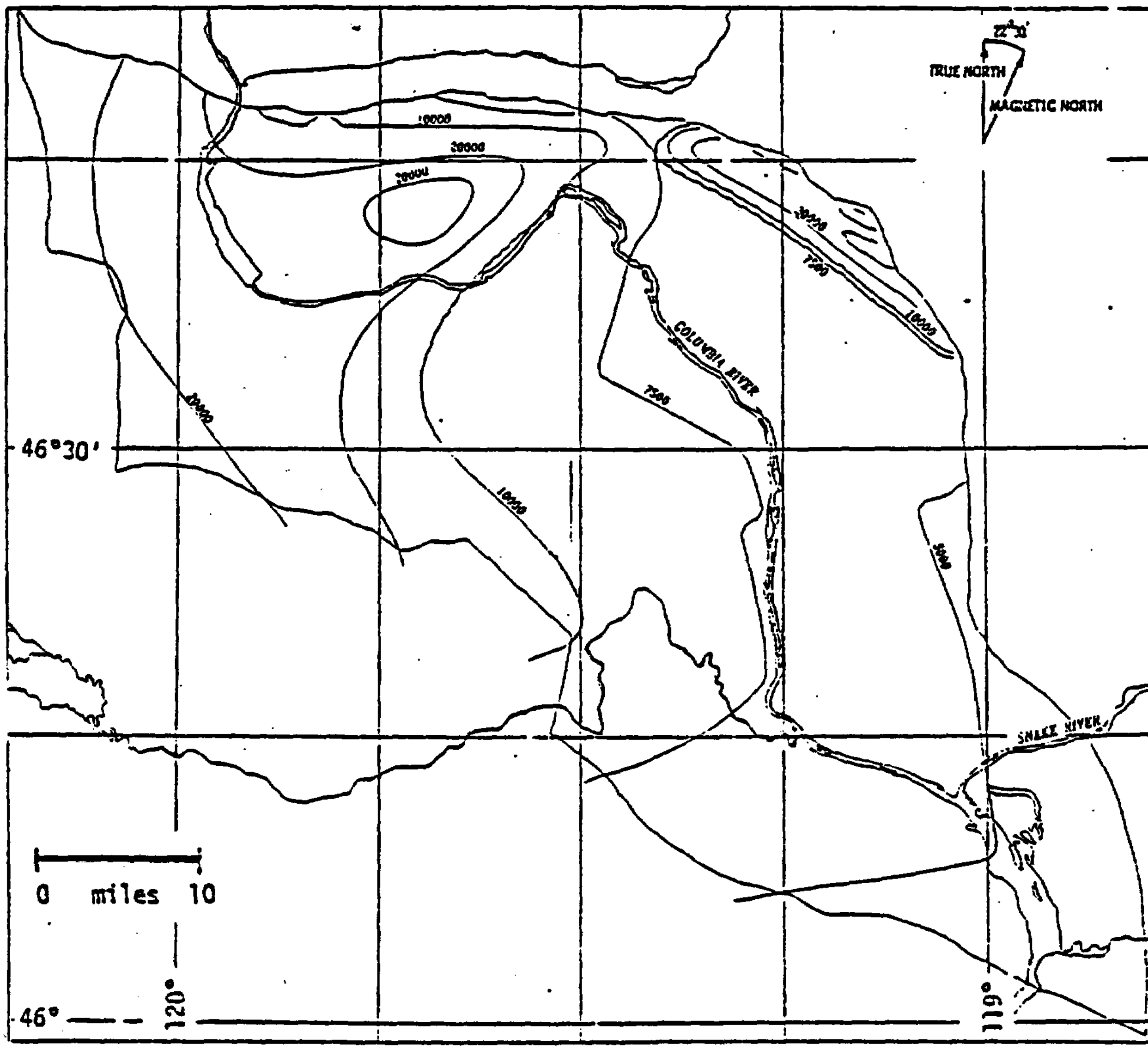


Figure 19. Transmissivity of the Saddle Mountains (gpd/ft)
(After, PNL - 3632)

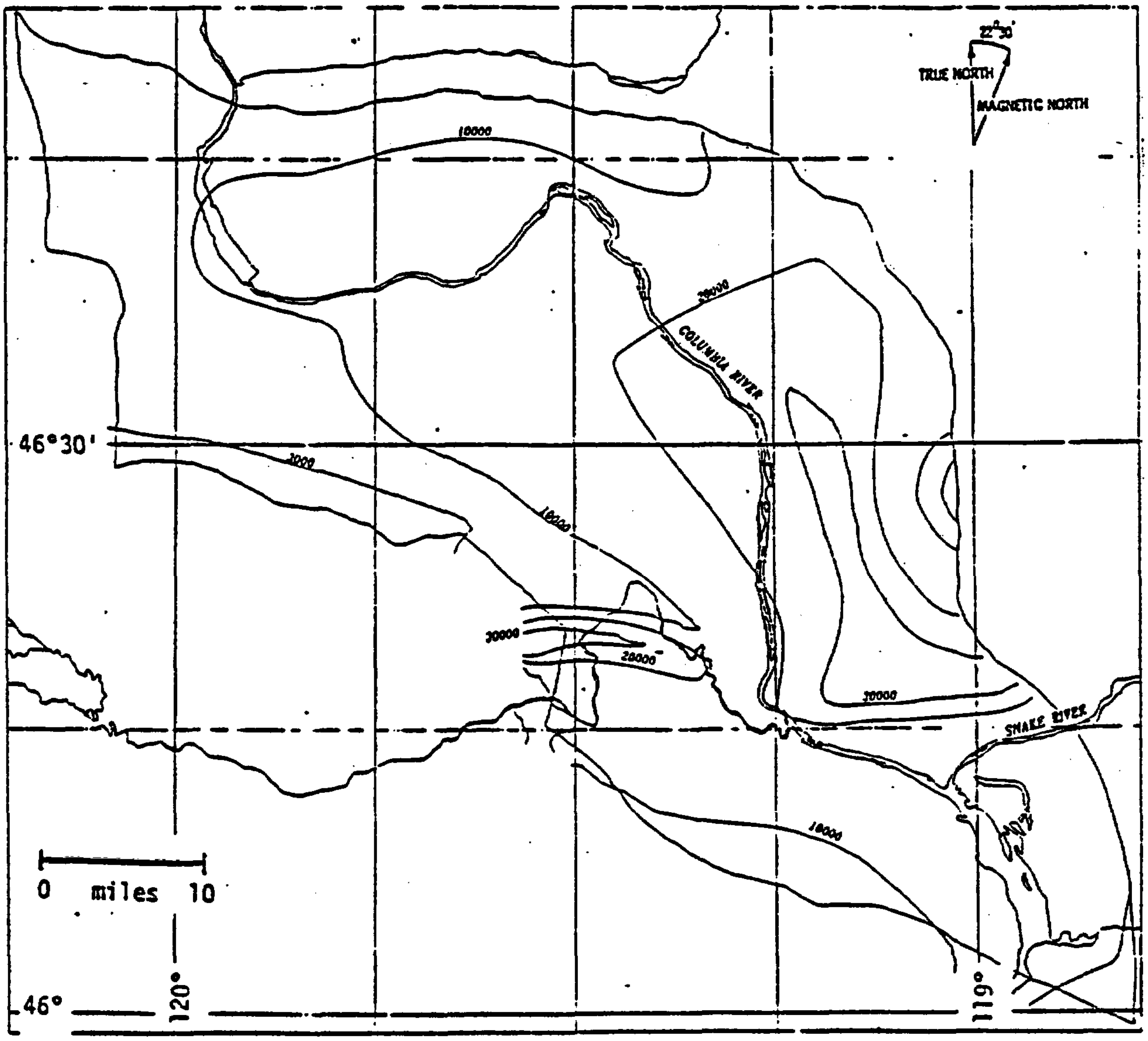


Figure 20. Transmissivity of the Wanapum Formation (gpd/ft)
(After, PNL - 3632)

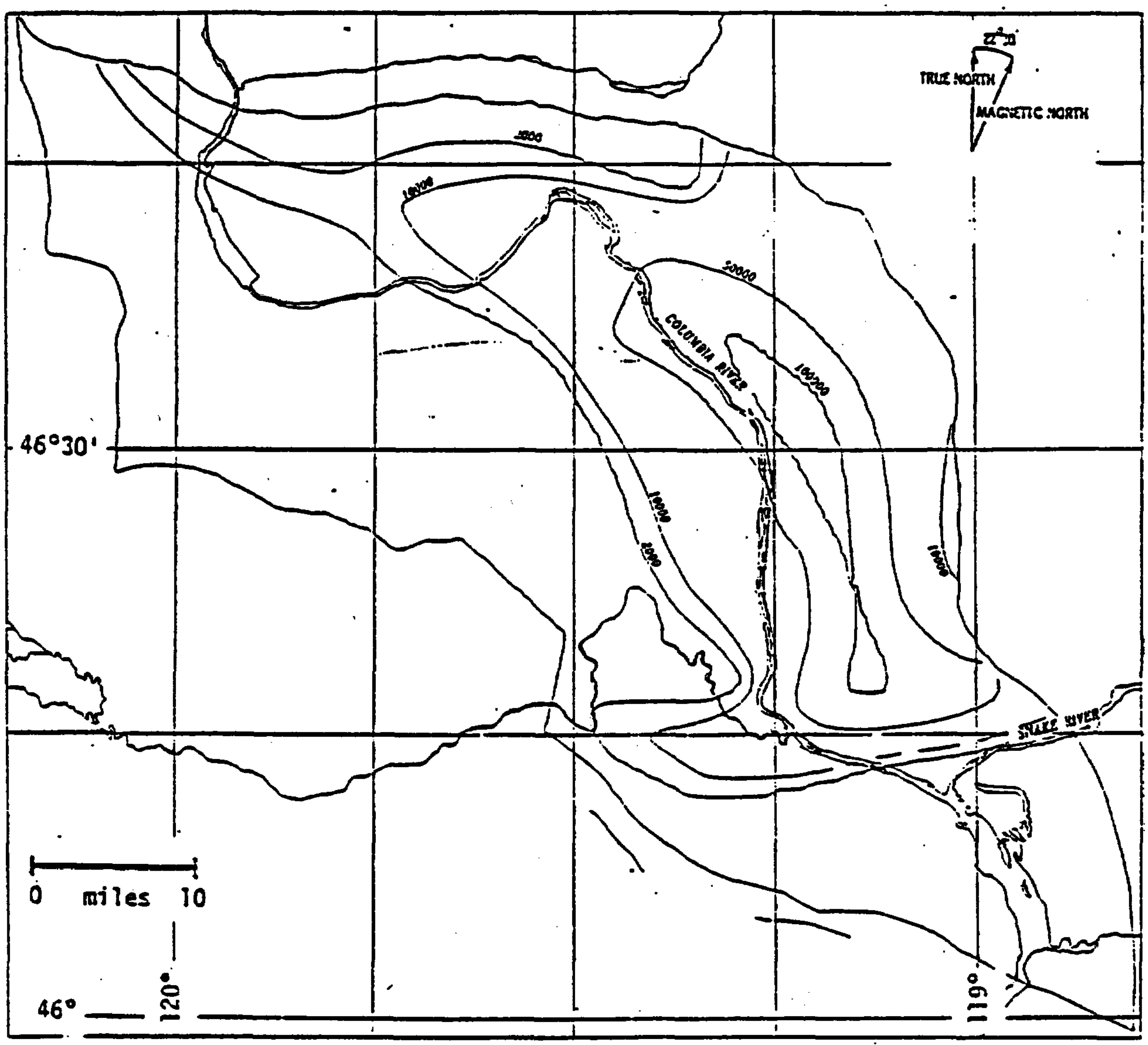


Figure 21. Transmissivity of the Grande Ronde (gpd/ft)
(After, PNL - 3632)

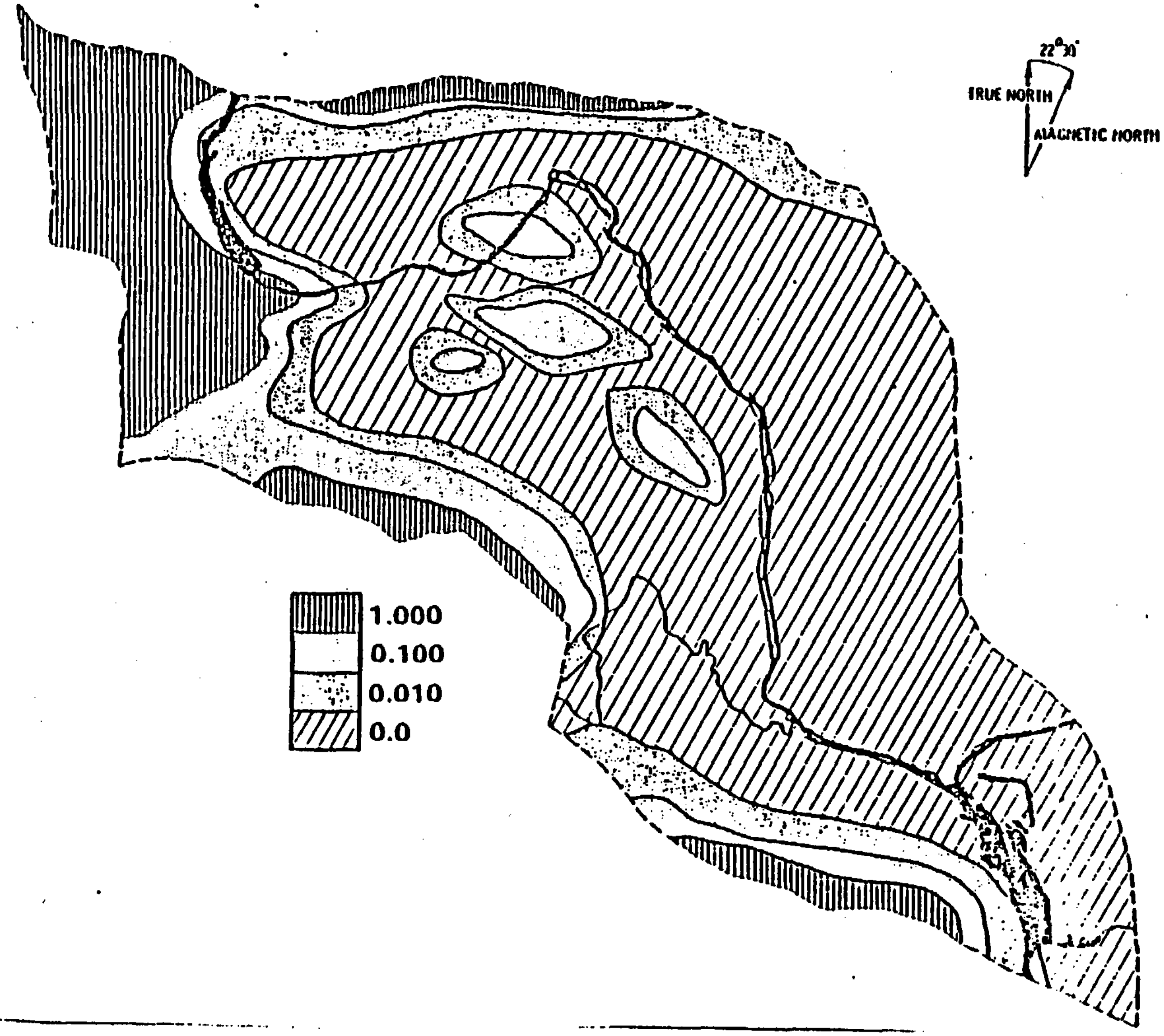


Figure 22. Inferred Zones of Structural Deformation
(After, PNL - 3632)

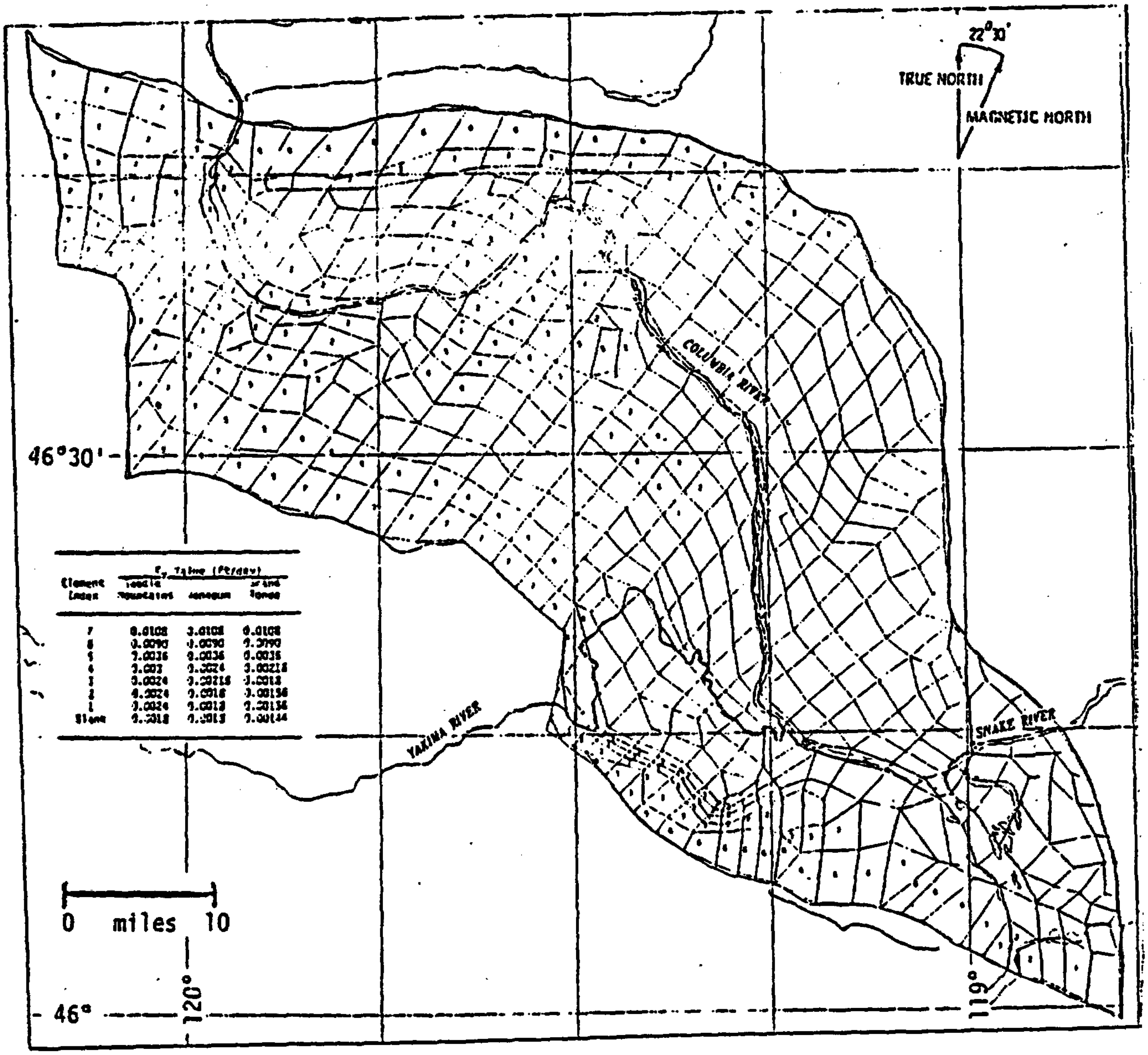


Figure 23. Distribution of K_v/K_h - PNL (After PNL-3632)

slope near the anticlines and synclines, the zones were rated from zero to one-with zero representing no deformation. Zones of greater deformation were assigned higher vertical permeability values. Final K_v/K_h ratios used in the PNL simulation are shown as Figure 23.

<u>Comparison of Boundary Conditions</u>

The boundary conditions used in the NRC simulations were the same pressures that were assumed to exist at the margins of the basin by RHO and PNL. The bottom surface in all cases was assumed to be a no-flow boundary. In simulating the RHO and PNL models, the NRC did not fix the water table configuration. Instead, the NRC simulations allowed the water table to equilibrate naturally in response to the boundary pressures. This resultant surface can then be used as a calibration tool generated by the model of field information.

The major differences between the boundary conditions of the PNL and RHO models are as follows:

1. The Rockwell model used a recharge boundary condition along the northwest corner of the grid for approximately 25 miles (Figure 24). The pressure head (1,099 feet above sea level) was significantly higher than than anywhere else in the model. This value, in fact, is so high that it caused all water to flow away from this area, across the basin, and out the eastern boundary. The eastward flow of water was exactly opposite to that of flow in the PNL model which depicted a westward and upward flow component.

   PNL chose a no flow boundary condition along the same 25 mile area *.

2. Rockwell set the head at the bottom of the Grande Ronde at 550 feet above sea level for approximately 42 miles along the northern basin boundary. No flow conditions were assigned to

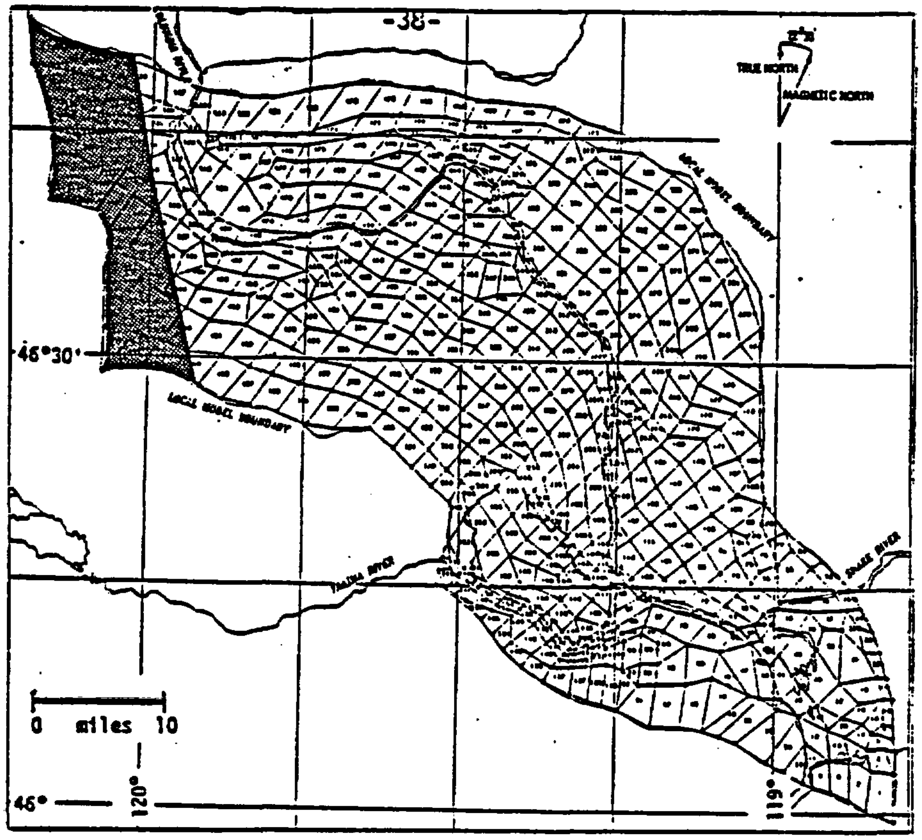


Figure 24. Major Areas of Model Input Disagreement (Northwest Pasco Basin)

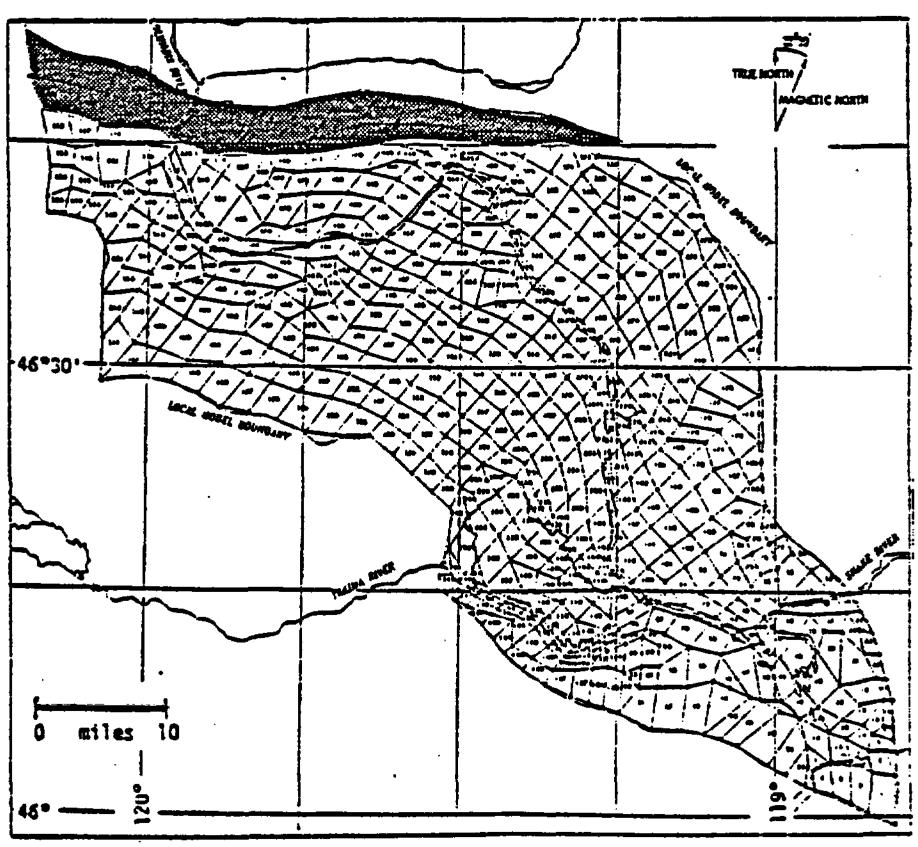


Figure 25. Major Areas of Model Input Disagreement (Northern Pasco Basin)

the northern boundaries of all units above this; thereby preventing flow from entering the basin from the north (see Figure 25).

PNL assigned a flow boundary along this area. Head values ranged from 675 to 880 ft. above sea level - increasing to the east. No-flow boundaries were assigned to the Saddle Mountains Formation only. The head difference between the two models ranged from 125 ft to 330 ft.*

3. The eastern basin boundary of the RHO model, from the northern edge for approximately 25 miles southeastward, was set at 600 ft; and was considered to be at hydrostatic equilibrium (head constant with depth, i.e., flow is horizontal along the boundary) (see Figure 26).

   The PNL heads along the eastern boundary, ranged from approximately 700 ft to 1100 ft above sea level-creating a head difference that ranged from 100-500 ft between the two models. Also, the PNL boundaries were recharge areas, i.e., head decreased with depth. It should be noted that in the PNL model the highest heads occured in this area.

4. In the RHO model, for approximately 12 miles along the southeastern corner to Wallula Gap, heads were set at approximately 400 ft, again with the hydrostatic equilibrium assumption horizontal flow along boundary (see Figure 27).

---

*In all cases the boundary choices of PNL were based on results from their regional simulations.

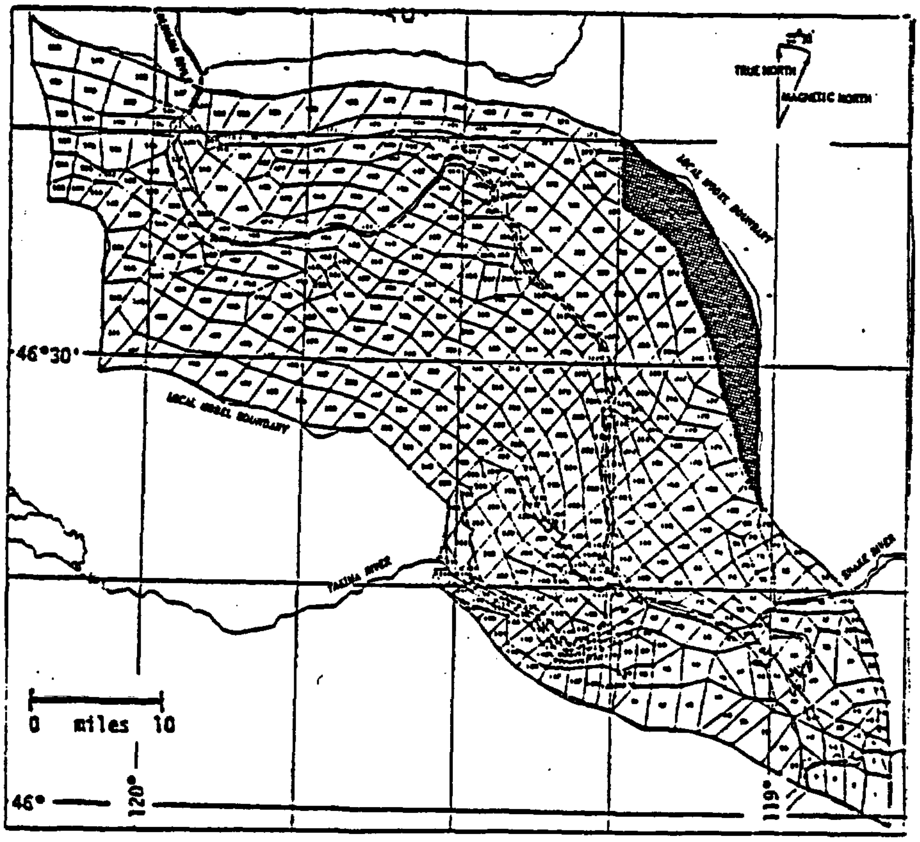


Figure 26. Major Areas of Model Input Disagreement (Eastern Pasco Basin)

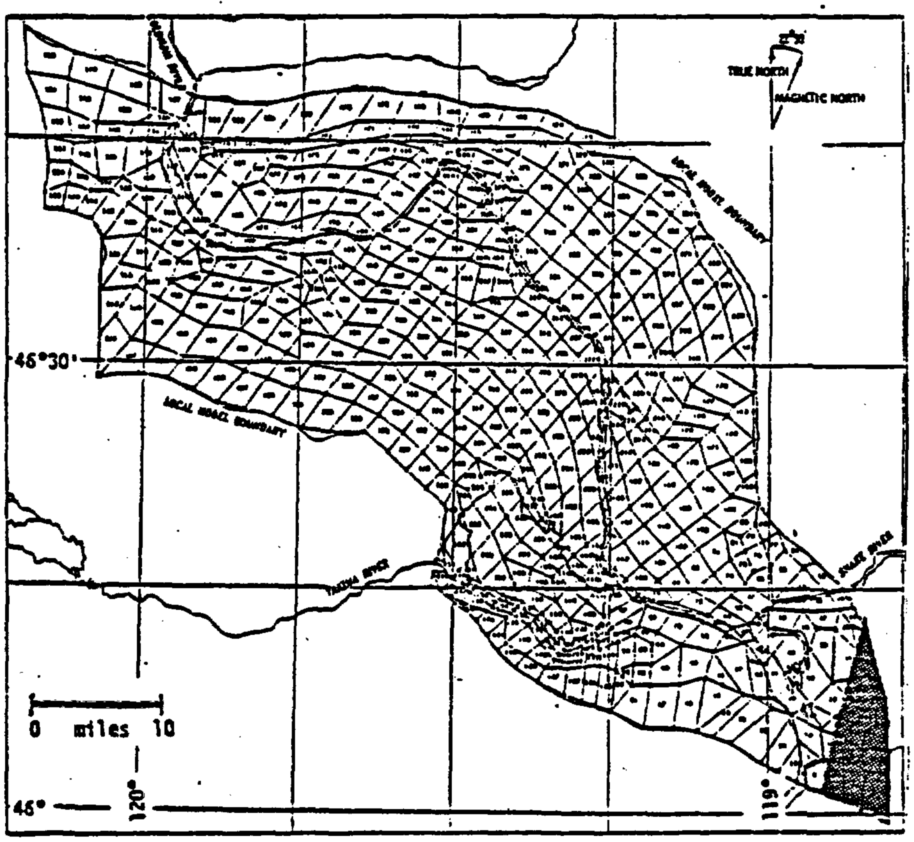


Figure 27. Major Areas of Model Input Disagreement (Southeastern Pasco Basin)

In the PNL model this area was a discharge boundary with heads in the lower units set at 650 feet and at the upper units 437 ft.

The head differences between the two models result in a discrepancy of approximately 250 ft in the lower units. Since the RHO model does not permit an upward gradient in this area, no upward flow can exist. This accounts for to RHO's conclusion that particles do not leave the Grande Ronde formation. The boundary conditions prevent particles form leaving the Grande Ronde.

---

*In all cases the boundary choices of PNL were based on results from their regional simulations.

5. In the RHO model, in the area beginning immediately west of Wallula Gap and continuing clockwise around the southwestern boundary for approximately 30 miles, a recharge boundary condition was imposed. Heads in this area drop from 700 ft in the upper units to 500 ft in the lower units. The gradient imposed in this region influences the flow of water in the entire southeastern portion of the model. The recharge boundary forces water downward in the Wallula Gap area, instead of upward as would be expected in a discharge area. (Figure 28).

   The PNL model assumed a no flow boundary condition along this same stretch.

The major similarities in the two models were as follows:

1. Water table surfaces were very similar and were both fixed by use of constant head pressures in both models.

2. River elevations were approximately the same in both simulations.

3. In the area of Rattlesnake Hills, both models had essentially a no flow boundary condition. (Figure 29).

4. In the area surrounding the Snake River (for approximately 12 miles) both models had discharge boundary conditions. (Figure 30).

<u>NRC Results - RHO Model</u>

The output of the NRC computer runs were particle tracking plots and pressure contours. Figure 31 shows that particles released east of the repository will follow RHO's stream line. Therefore RHO's results were successfully duplicated using their pressure boundary conditions on a

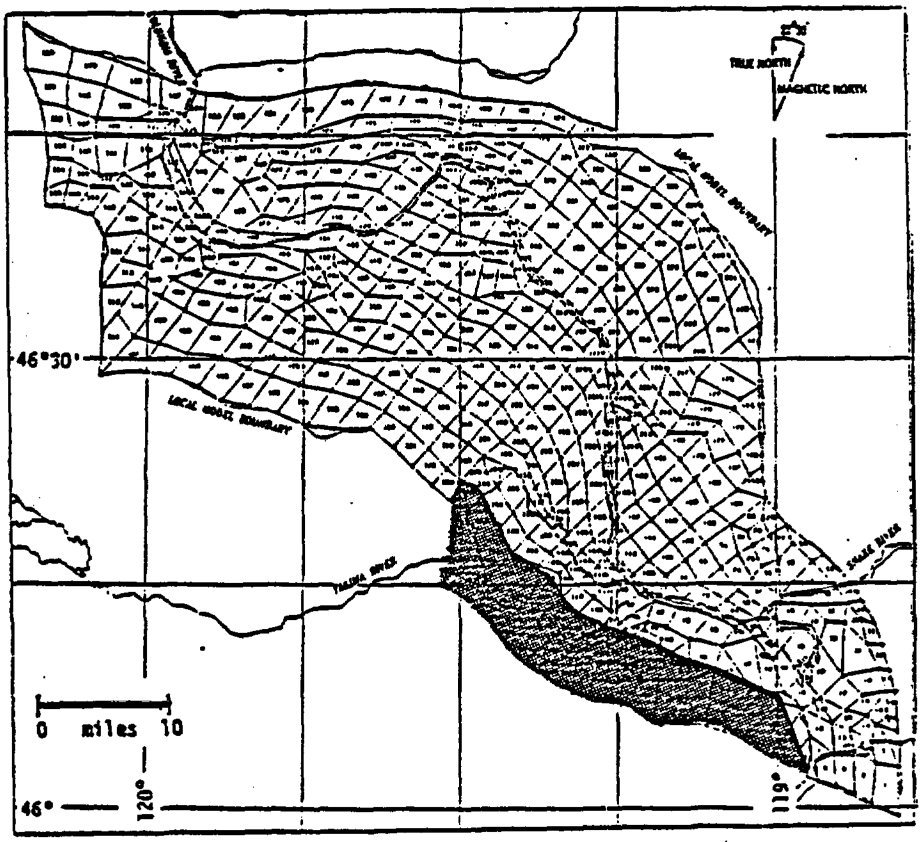


Figure 28. Major Areas of Model Input Disagreement (Southwestern Pasco Basin)

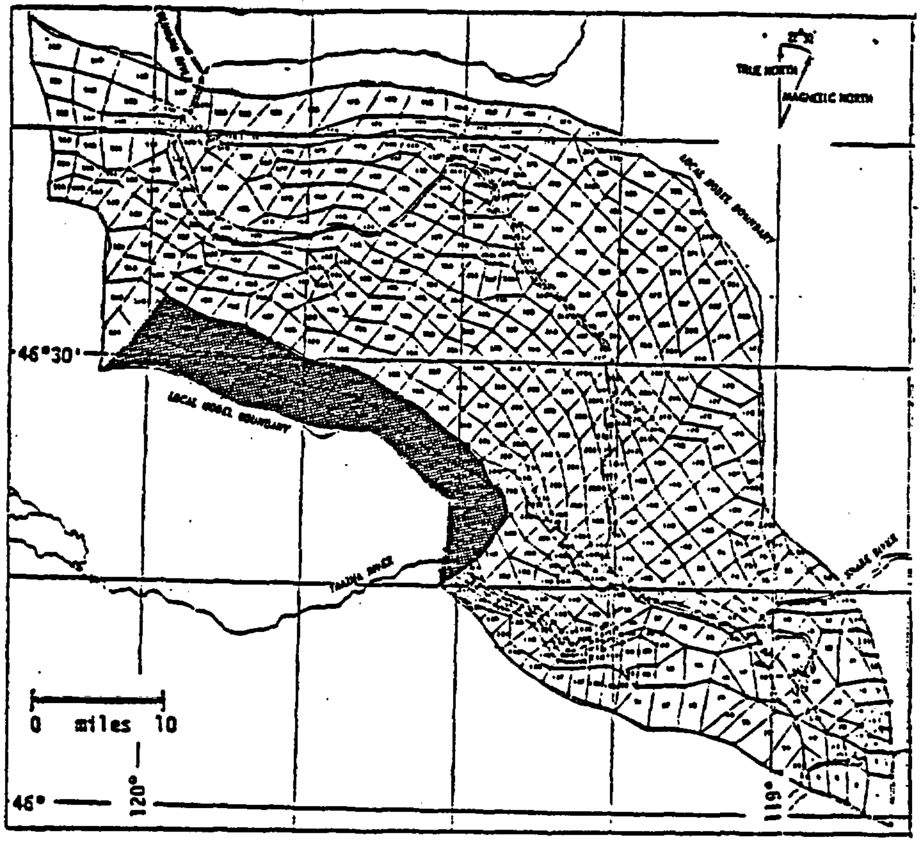


Figure 29. Major Areas of Model Agreement (Western Pasco Basin)

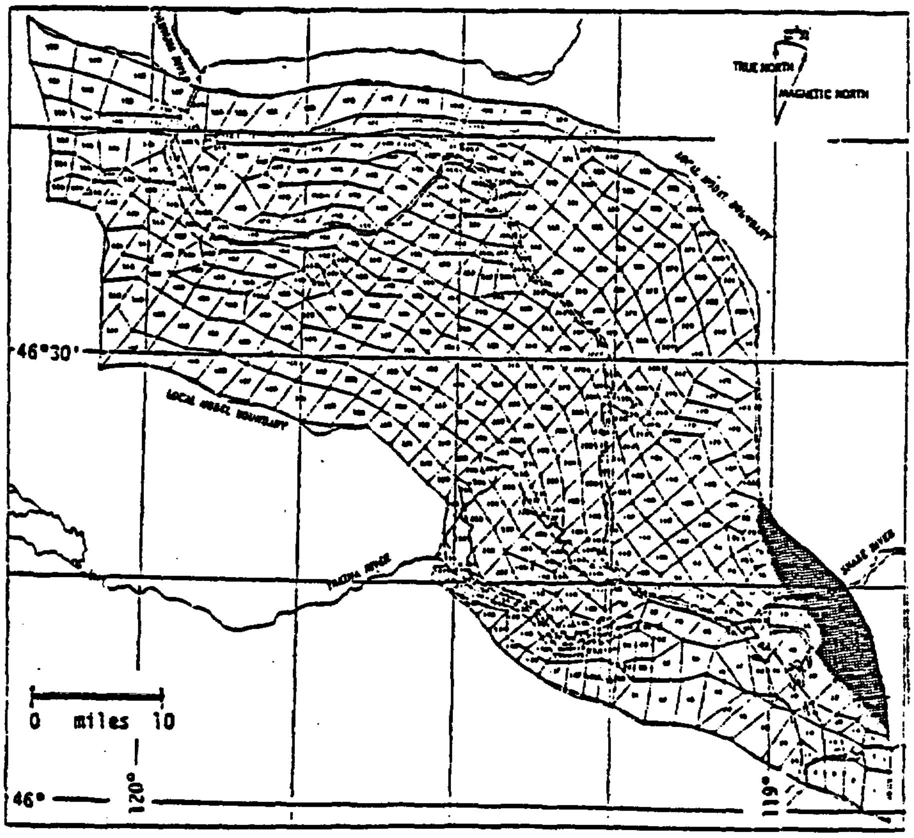


Figure 30. Major Areas of Model Agreement (Southeastern Pasco Basin)

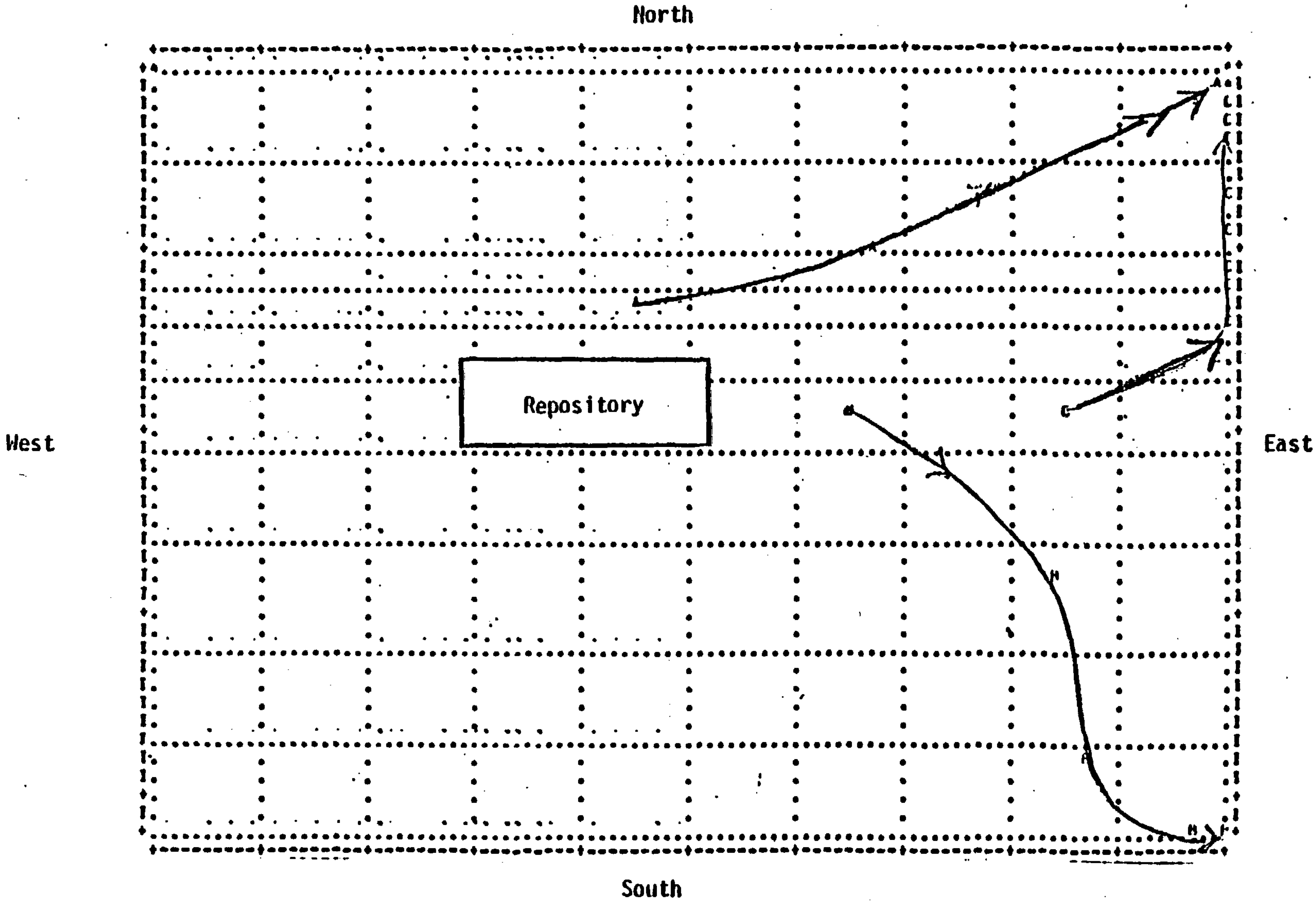


Figure 31. NRC Particle Tracking Results with RHO Boundary Conditions
Plan View

different computer grid. This at first appears to substantiate the RHO conceptual model. However, RHO does not discuss in RHO-BWI-LD-44 what happened to particles released elsewhere around the repository. In the NRC simulation, nost particles released in the vicinity of the repository actually moved either north or across the Columbia River and moved through the eastern basin boundary. While this characteristic is in complete harmony with the boundary conditions set in RHO's computer model, it is in direct conflict with RHO's conceptual model - which specifies recharge, not discharge, through the eastern boundary.

Additionally, the conceptual model clearly allows for vertical discharge in the southeastern part of the basin, the Wallula Gap area. The head distributions chosen in the numerical model are not consistent with the conceptual model and do not allow upward discharge to occur (Figure 28). Instead, particles in the vicinity of Wallula Gap were actually forced downward by the applied pressures. (Figure 32).

NRC Results - PNL Model

The particle tracking and pressure plots, produced by the NRC simulations using the PNL boundary conditions are shown on Figure 33. Flow originating in the area of the repository is seen to move predominantly northeast toward the Columbia River. Particles tracked in a north-south cross section also show the strong upward flow direction predicted in the PNL model. (Figure 34). Particles released elsewhere in the basin essentially track towards the river with a dominantly upward flow path. These results are in consonance with those of PNL and demonstrate that the PNL numerical model has been reproduced by NRC.

The PNL numerical model appears to be in good agreement with PNL's conceptual model.

WEST

EAST

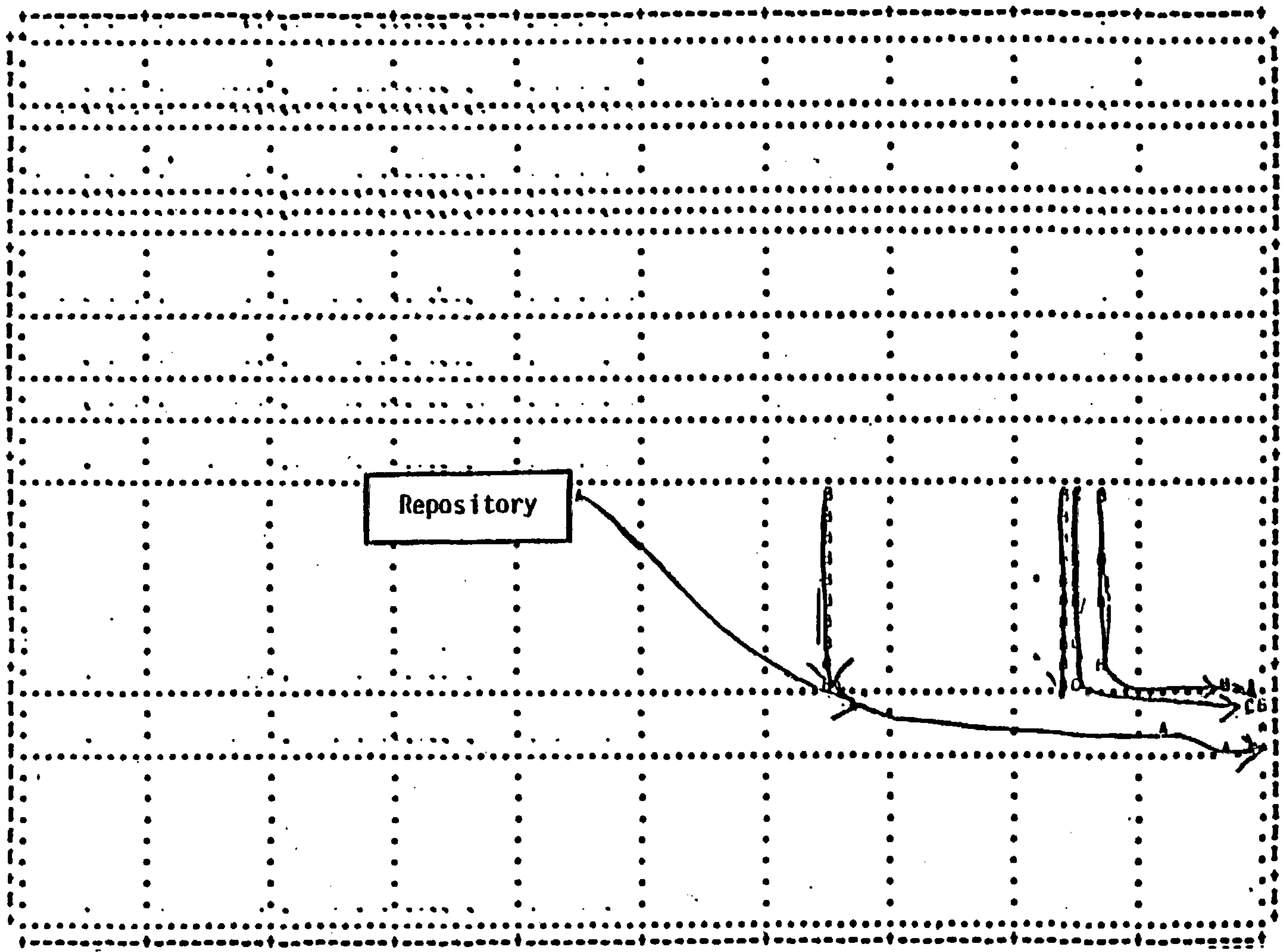


Figure 32. NRC Particle Tracking Results with RHO Boundary Conditions
East - West Cross-Sectional View

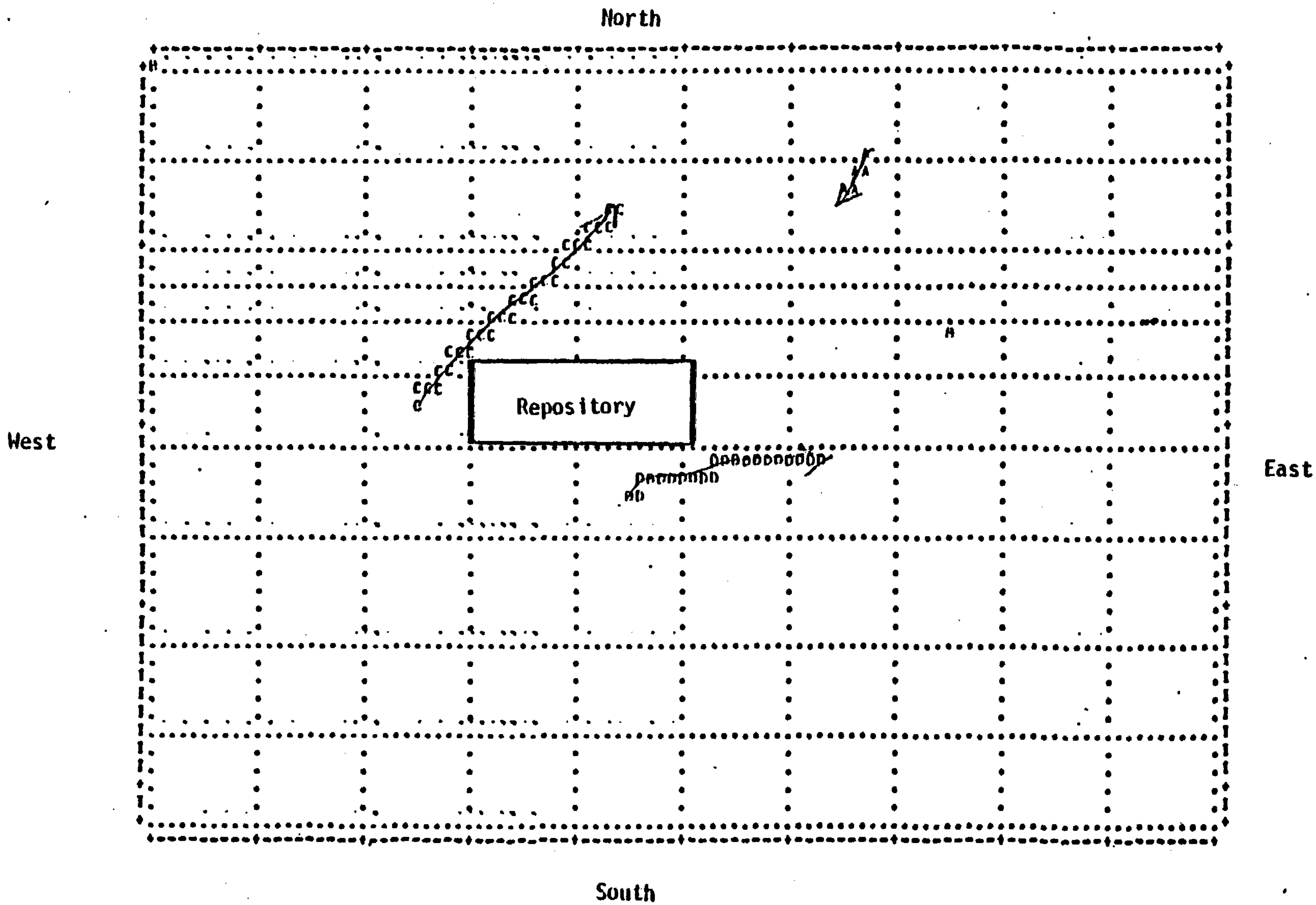


Figure 33. NRC Particle Tracking Results with PNL Boundary Conditions
Plan View

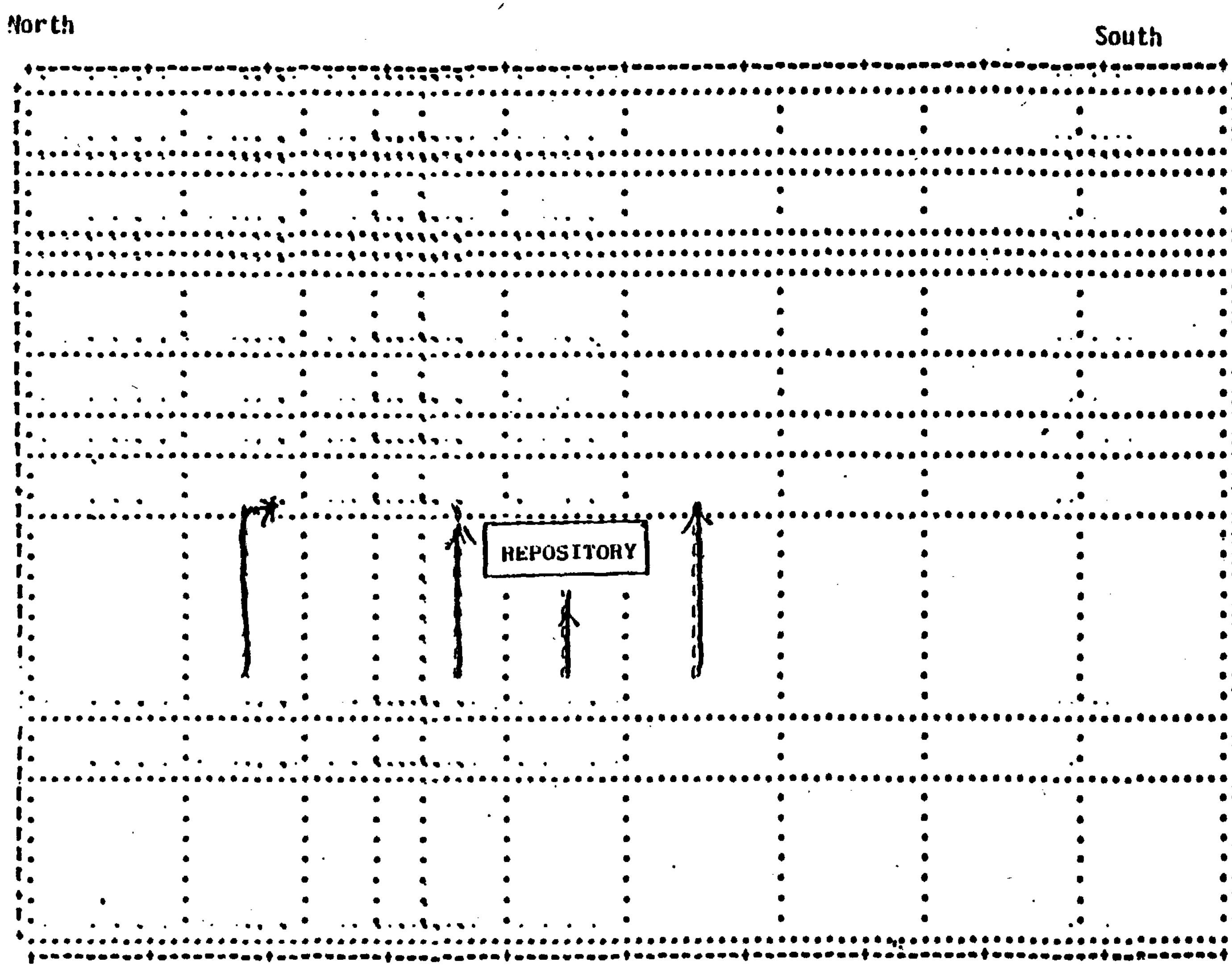


Figure 34. NRC Particle Tracking Results PNL Boundary Conditions
North - South Cross-Section

CONCLUSIONS AND RECOMMENDATIONS

Major conclusions derived from this study are as follows:

1. In the RHO simulation:
   a. The method used to determine boundary conditions was to preserve the downhole heads distribution by arbitrarily assigning numbers, both areally and vertically outward from the wells (Arnett, personal communication). While this is a valid approach, it will not necessarily provide a unique solution because there may be many combinations of side boundary pressures which allow the vertical head in a drillhole distribution to be preserved.

   b. The RHO numerical model is in conflict with their conceptual model in the following two areas:

      1. For the simulation the eastern boundary according to the resulting head distribution is a discharge boundary; the potential distribution is not appropriate for a recharge boundary as specified in the conceptual model.

      2. Vertical upward flow (discharge) in the Wallula Gap area is not permitted by the boundary conditions in the numerical model; yet this area is specified to be a discharge area in the conceptual model.

   c. K_v/K_h ratios have been held constant over the entire system. No increase in vertical permeabilities was assumed in the areas of structural deformation of the entire hydrostratigraphic section or portions of it.

2. In the PNL study:

a. The method of selecting boundary conditions was based on an analysis of the regional scale flow system.

b. K_v/K_h ratios were varied according to amounts of deformation within the system. All ratios used, however, must be considered as estimates.

c. The numerical model is in good agreement with the conceptual model.

d. Th downhole head distributions predicted by the PNL model generally agree with measured potentials, in that recharge or discharge is precicted correctly at most wells (Figure 35).

3. The hydraulic data base currently available to both RHO and PNL for the Pasco Basin is inadequate to allow the confident selection of computer boundary conditions and input parameters.

Boundary conditions and model parameters - in this case K_v/K_h ratio - are the most important input values required to model groundwater flow paths accurately. It is obvious that intelligent selection of this input is required to obtain accurate simulations. It is remarkable that two groups of investigators have made interpretations of the same basic data that result in profoundly different flow paths. Analyzing the differences in results is complicated by the difference in modeling schemes used by the investigators. This study has compared the flow paths predicted by the PNL and RHO models using the same mesh but a mesh that differs from both the PNL and RHO meshes.

It is obvious that "better data" are required to make more confident simulations. But it is not immediately clear what kind of data should be obtained, or what geographic areas should be emphasized. This study has identified the geographic areas where the two investigators have divergent opinions about boundary conditions or where internal inconsistencies exist. These preliminary analyses indicate that the

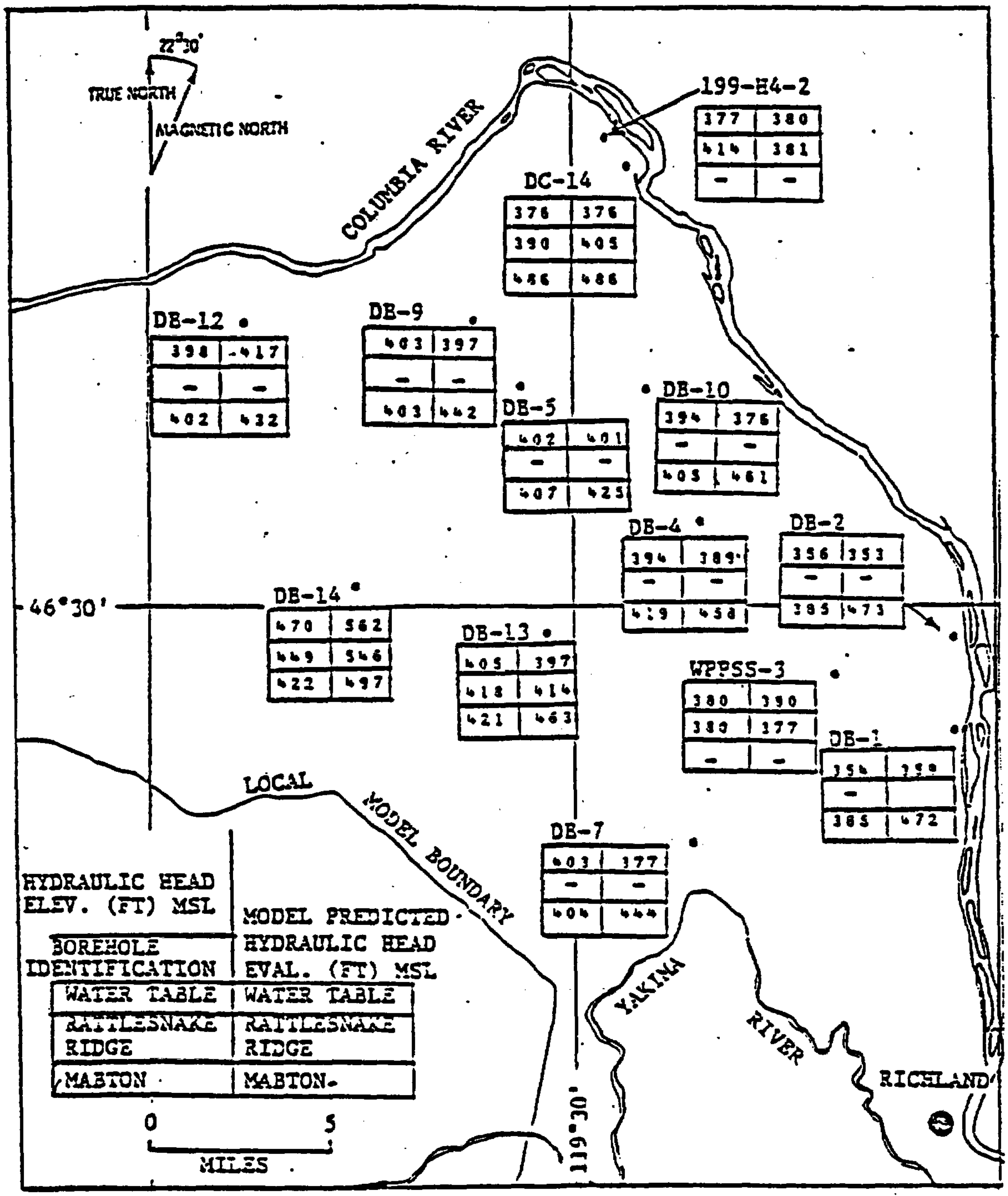


Figure 35. Comparison Between Model-Predicted and Observed Heads (After, PNL - 3632)

western and southeastern boundaries (Figures 24 and 28). Additional analyses will be required to determine the individual importance of these bounds. These areas, Figure 36, are recommended for future study to obtain agreement on the real hydraulic head configurations.

The sensitivity of the models to K_v/K_h ratio is critical. Maintaining constant RHO boundary conditions, NRC discovered that an increase in the ratio changed the potential for discharge from the Wallula Gap area to the center of the basin. It is recommended that testing procedures specifically address vertical permeability, not only in the Umtanum and Grande Ronde units, but the entire basalt sequence. Further, a good understanding of the areal distribution of this parameter will be required for dependable flow path determination.

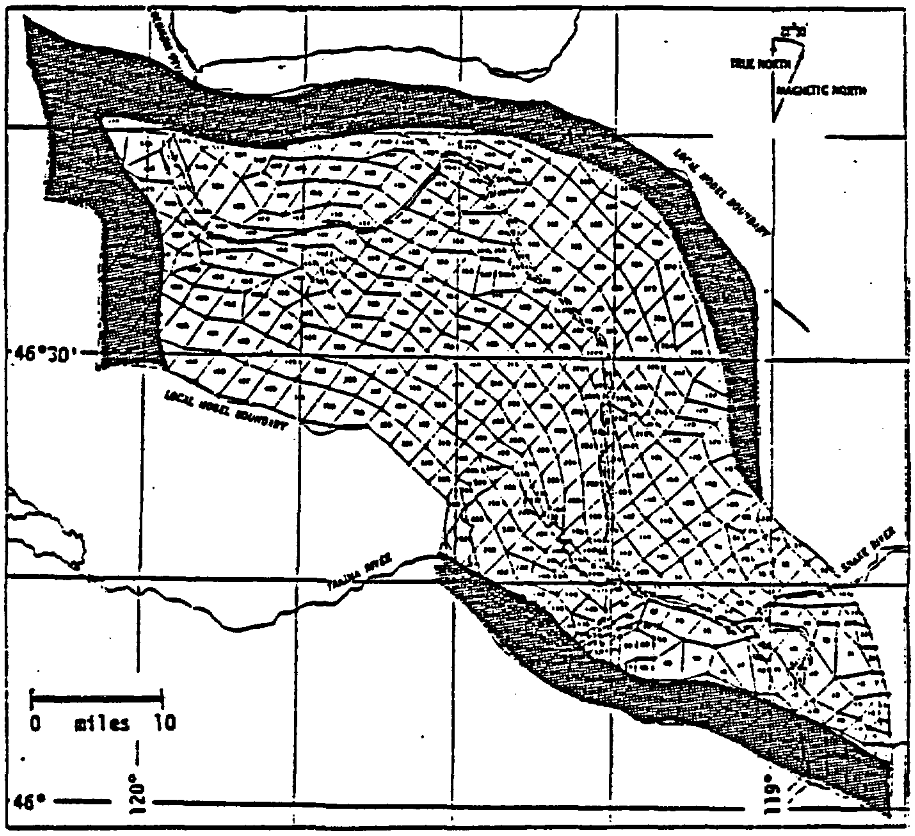


Figure 36. Areas of Divergent Opinion Regarding Boundary Conditions

APPENDIX A

Appendix A

This appendix describes actual model input changes which have occurred since described in Lehman and Quinn, (1981).

NRC Grid - Terrain Elevations

As of the last report (Lehman & Quinn, 1981), the Gable Mountain-Gable Butte anticline was the only structure which had been simulated by elevating grid blocks. This interior structure did have an effect on the distribution of pressure potentials.

Discussions with RHO indicated that the elevations used in previous simulations by the NRC in the Gable Mountain Gable Butte anticline were too high. NRC consequently reevaluated the data and used significantly lower elevations and a more gradual eastward slope. Row y=4 is the top of the anticline in Figure 12. The water table aquifer was left in place over the grid block 6, 4, but was thinned to 100' thickness to correspond more closely to the topography.

Since RHO and PNL had elevated their grids to simulated the terrain over the entire basin, the NRC decided to be consistent and also elevated the grid to match the topography throughout the basin.

In areas where the Saddle Mountains outcrops, all layers above the top of the Saddle Mountain unit have been set to zero-pore-volume. (By setting a cell to zero-pore-volume, no water can be contained within the cell, and consequently these cells are not used by the model). This has been done in areas where units are missing stratigraphically, such as near the basin margins where erosion may have removed the overlying units. In areas where the Wanapum is outcropping, all units above the top of the Wanapum have been set to zero-pore-volume and again are not used in the simulation.

Using a consistent set of boundary conditions, the model was run first with, and then without, elevated topography, to determine flow path sensitivity. Results indicated that elevating the grid around the margins of the basin had no effect on flow path.

Remove Aquifer Influence Blocks Which Simulate the Water Table

The next step in the simulation was to remove the aquifer influence functions which forced the water table surface via a constant pressure boundary (Lehman and Quinn, 1981). This was considered mandatory, as the water table is the only surface which is known well enough to calibrate against. RHO and PNL had forced the water table to conform in their simulation and left nothing to calibrate against except down hole pressure distributions.

The river wells which control the level of the river were allowed to remain as constant pressure boundaries.

RHO Simulation Initial Conditions

In order to evaluate the RHO model on a "first cut" basis, boundary conditions used by RHO in RHO-BWI-LD-44 were taken as input for the NRC grid. At first, these boundary conditions were applied as bottom hole pressures in wells. Since RHO had applied a different pressure at each major stratigraphic horizon, it was necessary to have multiple wells in each periheral grid block to duplicate the pressure distribution. Individual wells were provided for the Saddle Mountains, the Wanapum and the Grande Ronde and completed in each separate unit.

When pressures were applied in this manner, the following problems were encountered:

1. well shutin - wells which were to recharge did not have sufficient pressure head to do so, therefore were shut off by the code.

2. well index - numbers for well index had to be adjusted to approximate actual grid block pressures.

3. mass balance - mass balance was effected by well index values.

4. U tubes - flow would go into one well completed in a certain horizon within a grid block and be sucked out through a well within the same block from a different stratigraphic horizon.

To correct the well shutin problem, two updates were made to the code by Intera Environmental Consultants (IEC). The first one, FIXSIN, disables - the shutin algorithm, which for the steady state case was conditioned on the frequently unrealistic initial pressures. The second one, FIXPIN, corrected a bug in the code for the setup of initial pressures for overburden zero-pore-volume blocks (Reeves, Sandia Monthly Report for December 1981 for FIN A-1158).

The problem with the well index was two fold. First, if the well index was too small, the desired pressure control was not maintained. Second, if the well index was too large, bottom-hole and grid block pressures were sufficiently close to cause subtraction errors to occur in the mass balance. Thus, there was only a narrow range of values for well index which was acceptable. Usually, this range could not be known _a priori_, especially in rather complicated cases involving completion in multiple zones. (Reeves, 1981).

The problem involving U tubes was not overcome. As well index values and bottom hole pressures were adjusted, various amounts of interaction between wells occurred. Some of the wells which were expected to inject would produce, and thereby pull water away from adjacent wells. The resulting cones of depression and U tubes along the boundaries began to have a substantial effect on the general flow path. It helped to locate wells in different horizons of neighboring grid blocks, but in the end, all attempts to discourage injection wells from producing failed.

Due to this problem another approach to applying pressure boundaries was selected - this being the use of Aquifer Influence Functions.

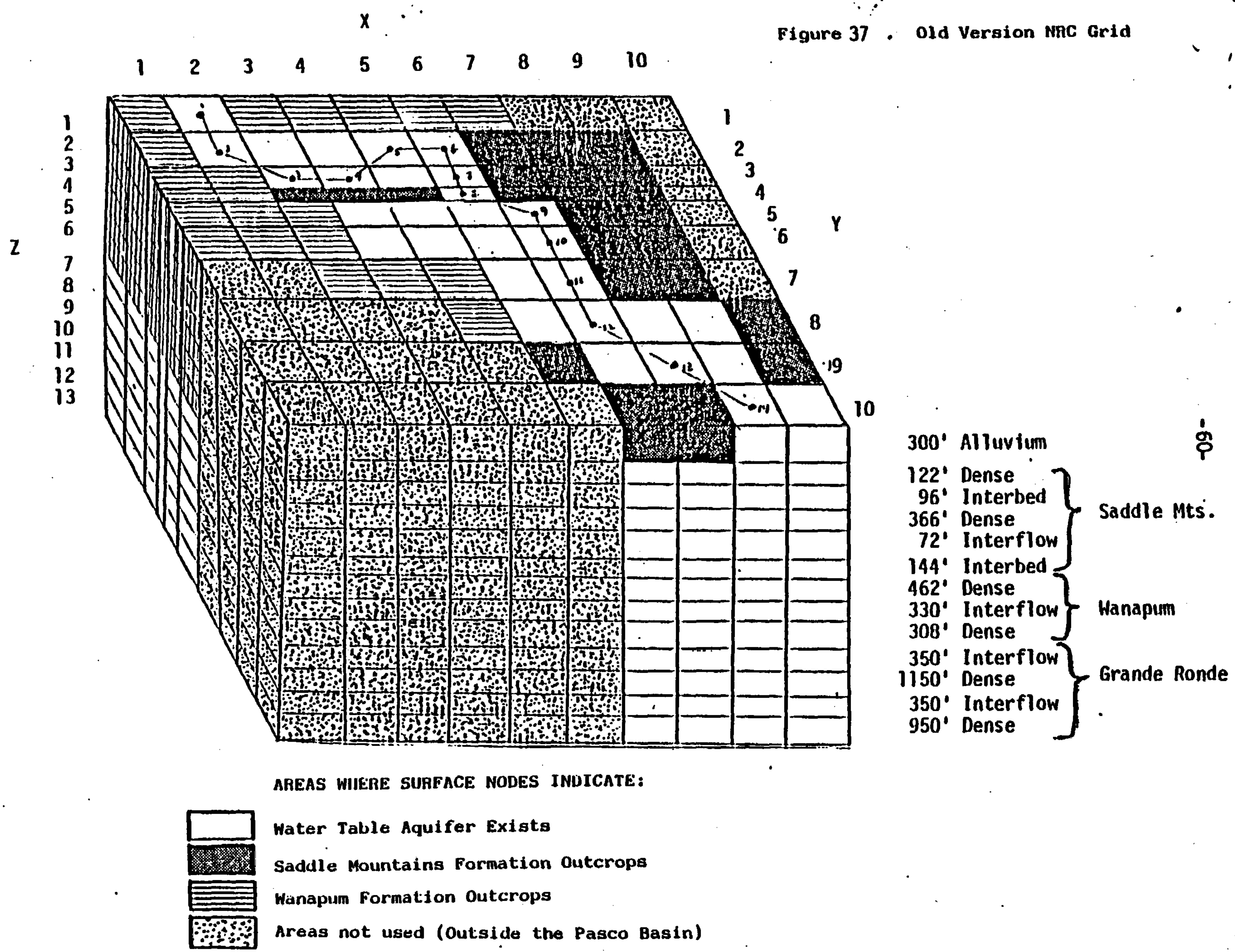
Use of Aquifer Influence Functions

The Aquifer Influence option in the code allowed the pressure to be applied at any specified outside edge of an outside grid block. (Aquifer influence block pressures cannot be applied to interior blocks.) In order to place the aquifer influence functions at locations to achieve the maximum coverage, the grid had to be slightly modified. The old grid is shown as Figure 37.

Figure 11 shows the expanded grid blocks. Notice that the blocks in the northeast corner are now being used. These seven blocks had previously been set to zero pore volume, but were changed for use as areas where Saddle Mountain basalt outcrops at the surface. This enabled the application of RHO's pressures to eastern and northern sides of the basin without using wells. This did create a problem in that the pressures were now applied further out: 6 miles in this case. Since the gradient was relatively flat, it was felt that the error caused by expanding the grid was neglibible.

If precise data were available at the original grid boundary, it would be possible to adjust the input pressure by multiplying by the hydraulic gradient across the expanded blocks to obtain the desired input.

Figure 37 . Old Version NRC Grid



Kv/Kh Ratio Under Ridges

Rockwell's simulation assumed a constant Kv/Kh ratio of 10^{-4} over the entire Pasco Basin. RHO did not use a different Kv/Kh ratio under the ridges and anticlines. Due to the amount of fracturing encountered in the anticlines, a partial sensitivity analyses was conducted which varied the ratio by a factor of 10 to a factor of 1000. The sensitivity analysis results showed that even small increases in permeability in the Gable Mountain-Gable Butte anticline allowed the free water surface to rise above the land surface. This is unrealistic and considered an artifact of the pressure boundaries selected by RHO.

Analyse Sensitivity to K_v/K_h Ratio Over the Entire Basin

For this simulation the 13 layer version was modified, in that hydraulic conductivities and porosities were changed to simulate 3 layers. Layers 1-6 simulate the composite permeabilities given by RHO in RHO-BWI-LD 44 for the Saddle Mountains Formation. Layers 7-9 use the composite values for the Wanapum and 10-13 simulate the composite values for the Grande Ronde. The values for permeabilties, layer thickness and K_v/K_h ratio for the SWIFT simulations are shown in Table A-1.

The flow path was extremely sensitive to this parameter as variations of only one or two orders of magnitude would change potential convergence to the center of the basin as opposed to the Wallula Gap area.

Analyze Sensitivity to Boundary Conditions in the Grande Ronde

When applying aquifer influence function boundary pressures it was noted that a large pressure drop occurred along the northern boundary from the western side of the basin to the eastern side (335 meters to 168 meters). Two different approaches were used to set up this northern boundary to see how the flow path was effected.

TABLE A-1

SWIFT INPUT FOR $K_v/K_h = 10^{-3}$

LAYER #	THICKNESS(ft)	K_h (ft/day)	K_v (ft/day)	POROSITY
1	300	1.0×10^{1}	1.0×10^{0}	.25
2	122	1.0×10^{-6}	1.0×10^{-3}	.05
3	96	1.0×10^{-3}	1.0×10^{-4}	.20
4	366	1.0×10^{-6}	1.0×10^{-3}	.05
5	72	1.0×10^{0}	1.0×10^{-1}	.25
6	144	1.0×10^{-3}	1.0×10^{-4}	.20
7	462	1.0×10^{-6}	1.0×10^{-3}	.05
8	330	1.0×10^{0}	1.0×10^{-1}	.25
9	308	1.0×10^{-6}	1.0×10^{-3}	.05
10	350	1.0×10^{0}	1.0×10^{-1}	.25
11	1150	1.0×10^{-6}	1.0×10^{-3}	.05
12	350	1.0×10^{0}	1.0×10^{-1}	.25
13	950	1.0×10^{-6}	1.0×10^{-3}	.05

RHO INPUT

LAYER #	THICKNESS(ft)	K_h (m/s)	K_v (m/s)	POROSITY
Saddle Mts.	984*	1.0×10^{-8}	1.0×10^{-11}	?
Wanapum	1150*	3.0×10^{-9}	3.0×10^{-12}	?
Grande Ronde	3280*	1.0×10^{-9}	1.0×10^{-12}	.01

*Approximate from graphics.

1) The Grande Ronde was held at 168 meters all the way across the basin and no-flux boundaries were applied to units above the Grande Ronde. 335 m was assigned to grid block 1, 1 in the Grande Ronde;

2) The average was taken between 168 meters and 335 meters and applied uniformly across the northern boundary except at grid block 1, 1, which was still held at 335 meters.

Changes in the boundary conditions influenced the flow direction slightly along this boundary. The higher averaged head values deflected the flow path farther to the east rather than north. A decision was made to comply as closely as possible to RHO's BC's so the 168 m boundary was held all the way across the northern boundary except at grid block (1,1).

PNL Simulation Initial Conditions

PNL boundary pressures were taken directly from their computer run which was suggested to the NRC. These pressures were applied through the use of aquifer influence functions around the basin perimeter, as were the RHO pressures. The grid structure was not changed.

K_v/K_h ratios were selected from Figure 23 which was taken directly from Dove, et al., 1981.

Obtain Computer Graphics

SWIFT did not have an adequate graphics capability to plot stream lines and pressure isobars. Therefore, an in house NRC program was developed to interface with SWIFT called CRSEC. CRSEC printed out pressure, temperature, and concentration contours, as well as velocity vectors. Additionally, a program called STLINE was made available by IEC. STLINE is a particle tracking code which enables stream lines to be plotted. With the aid of these two programs, a graphic display was produced that greatly enhanced the model's output.