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SIMULATIONS OF PARADOX SALT BASIN

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Purpose

This report documents the preliminary NRC in-house modeling of a bedded salt site. The exercise has several purposes:

- 1) to prepare for receipt of the site characterization report by analyzing one of the potential salt sites;
- 2) to gain experience using the salt related options of the SWIFT code; and
- 3) to determine the information and level of detail necessary to realistically model the site.

Background

The Department of Energy is currently investigating several salt deposits as potential repository horizons. The sites include both salt beds and salt domes located in Texas, Louisiana, Mississippi and Utah. Site investigations will be occuring in all locations until receipt of the Site Characterization Report.

In order to narrow the scope of this preliminary modeling effort, the staff decided to focus their analysis on the Paradox Basin. The site was chosen principally because of the level of information available about the site. At the time this work began, two reports on the Paradox had just been received by NRC: Permianland: A Field Symposium Guidebook of the Four Corners Geological Society (D. L. Baars, 1979), and Geology of the

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Paradox Basin, Rocky Mountain Association of Geologists (DL Wiegand, 1981). This in conjunction with the data information from topographic map of Paradox area (USGS Topographic Maps) and the Geosciences Data Base Handbook (Isherwood, 1981) provided the base data necessary for the modeling exercise. The primary goal of all numerical modeling performed to date was to simulate the contoured piezometric distribution seen on maps as compiled by Thackson (1981).

The Paradox Basin, located in southeastern Utah and southwestern Colorado, is underlain by a sedimentary sequence including thick salt units (Figure 1). The basin itself is defined by the zero salt line which is the axis separating areas of salt formation from nondepositional areas. Within the basin, intrusion of igneous features and faulting associated with dissolution has modified the distribution of the sedimentary layers (Figure 2).

Two rivers flow through the basin, the Colorado and the Green. The Colorado River is one of the principal sources of water for the region. During preliminary studies sites were being investigated both north and south of the Colorado River (Figure 3). Recently, however, the preferred sites have been narrowed to an area near Gibson Dome (ONWI 291). The region selected for modeling is centered around this smaller area.

Use of this basin also provided a parallel effort to the Sandia site description of the Permian basin. When the modeling began, data collection on the Permian basin was in the preliminary stages. Sandia had not developed the conceptual hydrologic flow field and the boundary conditions remained uncertain. For this reason Paradox represented a simpler site for modeling purposes. Most of the values selected for

 \blacksquare Figure 2. \blacksquare \mathcal{L} (Ref. Wiegand, 1981)

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material properties will be reviewed following receipt of the Permian basin site definition. It is expected that the basic set up will be transferable to the Permian basin.

Hydrostratigraphic Units

These analyses have been done on a three dimensional gridding system. This allowed both examination of the flow in the plane of each layer and the potential for interaction between layers.

For the initial exercise, three layers were used. These layers correspond to the three hydrostratigraphic units outlined by Thackston (1981). The upper hydrostratigraphic layer corresponds to the Permian and the upper Pennsylvanian strata (Figure 4, 5). The character of the beds varies from a fairly productive sandstone aquifer in the Permian to a tight shale layer, the Honaker Trail, overlying the salt. The variation in conductivity relates to the facies transitions as well as the fractures associated with igneous intrusions. For initial modeling, this layer was assigned a thickness of 1500 feet and a conductivity of .5 ft/day.

The middle hydrostratigraphic layer corresponds to the middle Pennsylvanian units. These include the lower Hanaker Trail and the Paradox Formation. The rock types are principally shales, salts and interbed layers. The layer was assigned a thickness of 1500 feet and a horizontal conductivity of 10^{-5} ft/day. The lowest layer corresponds to the lower Pennsylvanian and Mississippian age formations. The lower Pennsylvanian units, the Molas and the Pinkerton Trail formations, are

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Figure 4.
(Ref. ONWI 290)

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Figure 5.

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low permeability units while the Mississippian Leadville Limestone is moderately transmissive. This layer was given a thickness of 1000 feet and a conductivity of .5 ft/day.

For brine simulations, the three layer stratigraphy was subdivided into five layers. The upper layer was divided into two to represent the Permian and the Pennsylvanian Honaker Trail formation. The thickness and properties of the middle hydrostratigraphic layer, the Paradox salt, remained unchanged. The lower layer was also divided into two layers to represent the Pinkerton Trail and the Mississippian formations. The units have the following thickness, conductivities and brine concentrations:

1) Layer 1, 1200 ft, .5 ft/day, 0 brine concentration 2) Layer 2, 300 ft, .5 ft/day, .5 brine concentration 3) Layer 3, 1500 ft, 10^{-5} ft/day, 1.0 brine concentration 4) Layer 4, 300 ft, .5 ft/day, .8 brine concentration 5) Layer 5, 700 ft, .5 ft/day, .8 brine concentration

Description of Geometry

The gridding system used is shown in Figure 6. The northwest boundary has been extended past the river to ensure that water is not forced into that discharge point. The northeast and southwest boundaries correspond approximately to the zero salt lines. They were designed to incorporate the potential recharge areas along the Abajo and La Salle Mountains. The choice of the southeast boundary is more arbitrary and is located inside the zero salt line.

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Wells with constant bottom hole pressure were used to simulate recharge in the mountains. One well was used in the Lasalles and 4 in the Abayos. For the preliminary study the upper and lower hydrostratigraphic units are assumed to have no interconnection. Wells are either completed in the upper or lower hydrostratigraphic unit.

The river is also simulated using wells with constant bottom hole pressures. The water level in the river was approximated from the topographic surface map. Future work will require more accurate measures of the water elevation along the river. No increase in conductivity was assumed either along the river or around the intrusives.

The pressures assigned to the boundaries are interpolations of the contours given by Thackston. The number of control points vary a great deal from boundary to boundary (Figure 7, 8); aquifer influence functions were used to simulate these boundaries (Figure 9, 10). The salt layer because of its low conductivity and lack of continuous flow was assigned a no flow boundary.

Steady State Analysis

Initial runs were performed as steady state. The contours produced correspond fairly closely to Thackston's contours (Figure 11 a-f). Flow in-the upper layers were generally toward the Colorado river from both the north and the south. One exception is the area, south of the La Salle Mountains where water is moving radially away from the recharge zone toward the boundary. This reflects our choice of the boundaries as interpolations of contours rather than structural breaks to flow.

Figure 7. Potentiometric Surface of Upper Hydrostratigraphic Unit (Ref. Wiegand, 1981)

Figure 8. Potentiometric Surface of Lower Hydrostratigraphic Unit (Ref. Wiegand, 1981)

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Pressure Distribution In Feet

Figure 11b. CRSEC Plots Of Layer 1

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Figure 11c. SWIFT Output For Layer 2 Steady State Analysis

Pressure Distribution In Feet

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Figure 11e.

SWIFT Output For Layer 3 Steady State Analysis

Pressure Distribution In Feet

Figure 11f. CRSEC Plots of Layer 3

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Flow in the lower unit does not reflect as strongly the topography and structures of the area. This is due to the presence of the salt layer which buffers the effects of the overlying units. The lower unit reflects a larger flow sytem which extends beyond the limits of the Paradox Basin (Thackston, 1981). The only exceptions to this pattern are the areas of interconnection along the structures.

The contours produced did not always correspond to the reported contours. The principal difference occurred along the intrusives (recharge wells) where calculated heads were higher than those observed. To correct this, the number of wells simulating recharge was reduced but the calculated heads still remained high. This could be further corrected by increasing the conductivity or changing the well index to reflect higher k values around the recharge zone. This would be consistent with the tectonic induced fracturing pressumed in the area. Additional refinement may be obtained by more precisely correlating the locations of wells in the grid.

Modeling of Brine

Salt concentrations in the Paradox Basin groundwaters cause density gradients within the overall system, which in turn impacts the groundwater flow regime. Inclusion of brine in the SWIFT simulations is an.1mportant step toward creating a more realistic numerical and conceptual model. In the five layer system the lower four layers contain varying concentrations of brine while the top layer is considered to be fresh.

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The SWIFT steady state flow model was altered to allow the inclusion of the brine. The first alteration was done by initializing each of the five layers to a brine concentration and specifying constant brine concentrations on all boundaries. The middle layer, representing the salt (Paradox fm), was assigned initial and boundary brine concentrations of 1.0. Dissolution of the salt layer was not accounted for since the dissolution parameter contains time units not compatable to steady state flow.

Results of this simulation were not satisfactory since the brine concentrations were not correct. Brine concentrations in all layers were zero, indicating that salt was purged from the system despite constant concentration boundary conditions. The mass balance calculated on brine was approximately 1%. This indicated that considerably more salt was leaving rather than entering the basin. The problem appears to be the introduction of fresh water in the recharge wells. The analysis will need to be rerun with brine introduced into the wells.

The next phase in the study was to modify the previous SWIFT set-up to be a transient simulation. A transient simulation would allow for inclusion of a salt dissolution term and would enable the SWIFT treatment of brine to be monitored. First a non-saline steady-state flow regine was established to initialize flow, and then a transient solution using saline boundary conditions and a salt dissolution term for the middle layer was implemented.

In the transient runs, brine remained in the system but resulted in a poor mass balance. When SWIFT was allowed to choose its own time step, the smallest specified step (0.01 days) was chosen with only slightly

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improved results. It should be noted that the mass balances obtained are consistent with results obtained by Sandia (Finley and Reeves, 1982) and other SWIFT users performing brine studies (Personal Communications). Clarification is needed from Sandia on what would constitute an acceptable value.

Variations on the brine dispersion coefficient were included in an attempt to correct the poor mass balance. Previously, the dispersivity of brine was assumed to be zero and thus grossly violated the numerical criteria for brine transport (Reeves and Cranwell, 1981). In order to satisfy the criteria, the dispersivity coefficient would need to be at least one half the length of a grid block, or three miles. It should be noted, however, that the vertical dimensions of the grid blocks are approximately an order of magnitude smaller than the horizontal. A dispersivity coefficient chosen on the basis of the numerical criteria will result in too much dispersion in the vertical direction.

Simulations were performed where the dispersivity criteria was violated, and also where it was exceeded. Brine mass balance improved with increased dispersivity values. Where the dispersivity was equal to one half the horizontal grid block length (satisfying the criteria), the mass balance was poor. However, at this value complete mixing occurred in the top two layers contaminating all of the fresh water, and contaminating the river wells.

Further evaluation of the above results needs to be performed before the SWIFT modeling study proceeds. A smaller scale study using smaller grid blocks may be one way of avoiding the brine transport problems

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encountered above. Incorporation of different logitudinal and transverse dispersivity will also be useful.

USGS Code

The USGS Trescott, Pinder, Larson (1979) flow code was employed to check the SWIFT code. SWIFT requires a very complex data set; the results obtained from the much simpler USGS code would give confidence in the analyses using the more complicated methods. Although both are finite difference codes, the different treatments of boundary conditions and recharge/discharge locations within the respective codes will probably be revealed in the results. These differences, should they occur, will be beneficial in analysis and subsequent data calibration.

A steady-state simulation with the USGS code was performed on the top layer of the steady-state 3 layer SWIFT simulation. The grid configuration and hydrologic parameters used were identical to those used with SWIFT. Boundary conditions and recharge/discharge locations were set by indicating a constant head over each of the specified elements. This differs from SWIFT where boundary conditions are set by assigning constant head values to element edges and recharge/discharge locations are simulated by injection/production wells. The input used for the codes is contained in Appendix A.

Reasonably good results were obtained with both codes, however, the USGS code yielded a closer approximation to the real field data (Figure 12). Preliminary analysis indicates that the head discrepancies are due primarily to the SWIFT well index values used at the recharge locations

Figure 12. Head distribution from USGS simulation.

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which is allowing excessive amounts of fluid to be injected for a specified pressure. Further work needs to be done on isolating the discrepancies.

Recommendations

- 1. A decision must be made on the level of effort devoted to modeling the salt sites. The alternatives are either to model each of the salt sites on a limited scale or to concentrate on one location. NRC should attempt to find out how much reliance will be placed on modeling for selection of a salt site. This will determine how many sites it is necessary to model.
- 2. Before conclusions can be reached from this modeling exercise, a more extensive data base should be used. Once additional data has been compiled, the model would need to be altered to include: (1) smaller grid blocks around structures to provide better resolution; (2) inclusion of more layers to reflect the changes in stratigraphy; (3) spatially variable conductivity to reflect despositional sequences and structural deformations; and (4) inclusion of structures such as Lockhart Basin and the Needles dissolution zone.
- 3. To improve the model given current data limitations, the Siting Section would need to review the data and recommend the best characterization of the material. The Siting Section should also review the head distribution in the drill holes to aid in making more reasonable estimates of boundary conditions. The recent

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Figure 13. (Ref. Wiegand, 1981)

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receipt of ONWI 290 should provide a better data base for future model studies.

- 4. A smaller scale model should be developed to analyze faults and dissolution areas like Lockhart Basin and Shay Graben (Figure 13). Various interpretations have been proposed to explain the interactions in the areas. Modeling may be able to aid in interpreting these collapse features.
- 5. The USGS code has been successfully used to simulate flow in the upper aquifer. Since this code has been shown to be simple to use, use of this code should be expanded to simulate regional flow in the lower aquifer as well. Such simulation might identify areas of hydrologic uncertainties and support assumptions that will be made on boundary conditions in smaller scale simulations.
- 6. Current contours of flow in the lower aquifer indicate apparent movement into the region beneath the Colorado River. If correct, flow could be moving in a more permeable channel beneath the river, or migrating upward into the river. Such migration would be introducing salt into the Colorado. SWIFT should be used to determine the amount of salt that would be transported into the river by this mechanism' if upward migration would occur. SWIFT should also be used to investigate the hydrological effects, if any, that would be caused by more permeable zone underneath the river. A comprehensive water balance analysis should be performed to determine the amount of flow from both units seeping into the river as well as its salt contribution.

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7. The errors associated with the brine mass balance in SWIFT need to be reviewed to determine the problem. SWIFT must be able to provide reasonable mass balance to ensure reliable representations of salinity concentrations.

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Appendix A

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Input Deck for GS Code

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