Modelling of regional variable density groundwater flow in an area in New Mexico: importance of influencing parameters and processes

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Abstract A proposed repository location in New Mexico, USA, is in a bedded salt formation overlain by a series of aquifers and aquitards. Subrosion can take place at the surface of the salt formation and some overlying salt beds. The salt content can influence the groundwater density and the associated flow field. As one conceptual model, a two-dimensional vertical cross-section was considered in which all units above the salt formation were represented to allow vertical flow between these units. The density-dependent groundwater flow was simulated until a steady state was reached. A comparison of the computed density distribution, travel times and inflow rates with known data showed that the model was reasonable. The flow field was strongly affected by the permeability distribution. Significant vertical leakage occurred into the aquifers through the low permeability overlying and underlying aquitards. The density distribution was found to be of minor importance.

INTRODUCTION

The Waste Isolation Pilot Plant (WIPP) site is located in the southeast of New Mexico, USA. This site has been chosen as a potential location for a radioactive waste repository in a bedded salt formation. A test case based on the results of the extensive investigations carried out around the site was defined for the international INTRAVAL project (SKI/NEA, 1996). The test case provided an opportunity of addressing the choice of a conceptual model, as well as other important issues relating to groundwater flow and transport models. Most of the site-specific investigations on groundwater movement considered the Culebra Dolomite: the most permeable, relatively thin, but extensive member of the formation overlying the salt formation. These investigations involved two-dimensional horizontal groundwater models. The Culebra dolomite is of interest from a long-term safety point of view because it is the first high permeable layer above the potential repository location.

As an alternative, a two-dimensional vertical cross-section was considered in which all units above the salt formation were represented. This allows vertical flow between the units modelled, which was neglected in the areal models. The objectives were to simulate the density-dependent regional groundwater flow until a steady state was
reached, and to show that the model is reasonable, by comparing the results with measured groundwater salinities, isotopic data and inferred paleo-precipitation rates. The intention was also to look for answers to important issues such as the kind of model which has to be used to describe the system (two-dimensional horizontal, two-dimensional vertical, or three-dimensional, steady state or transient) and the important processes which influence the flow system (effect of density variations).

HYDROGEOLOGICAL SITUATION

The area surrounding the WIPP site is relatively flat. A local rise in the east, called "The Divide", which possibly forms a regional water divide, two smaller ridges of hills in the east and west and another one in the north combine to give a basin-like topographical structure (Fig. 1). West of the WIPP site, a large depression, the Nash Draw, is found, with a gentle slope in the topography inclined towards the Pecos River, which is the river draining this area. In the Nash Draw, a salt lake is found as a result of groundwater discharge.

The stratigraphy of the area is well known as a result of the intensive investigation programme. The potential location for the planned repository is approximately 660 m below the surface in the Permian Salado formation, which is a bedded salt formation. The Salado formation is overlain by the Permian Rustler formation. West of the WIPP Site, subrosion processes have formed a silty to clayey residue at the top of the Salado formation, the Rustler Salado contact zone. This is the first permeable layer above the Salado formation. Often there is no sharp interface between this zone and the overlying Rustler formation.

**Fig. 1** Topography in the WIPP region with the location of the WIPP site and the line of the vertical cross-section (height in feet).
The 100-150 m thick Rustler formation can be divided into five different members, the upper three of which outcrop at the surface in the area of the Nash Draw. These members are from bottom to top (cf. Holt et al., 1991):
- the low permeability unnamed lower member is composed of siltstones, anhydrite/gypsum and halite. The latter can only be found east of the WIPP site. It is replaced continuously to the west by a dissolution residue.
- the permeable Culebra Dolomite member is approximately 8 m thick everywhere in the investigation area. Especially in the western part of this area, it is a highly permeable fractured aquifer.
- The overlying very low permeability Tamarisk member is formed by two thick anhydrite layers, separated in the eastern part by a halite layer and, further to the west, by the silty dissolution residue of this layer.
- The Magenta Dolomite member is similar to the Culebra Dolomite. It has nearly the same thickness, but is not as permeable as the Culebra Dolomite.
- The low permeability Forty Niner member lies at the top of the Rustler formation. Like the Tamarisk member, it is composed of two anhydrite layers separated by a silty layer or a halite layer.

The Rustler formation is overlain by the Dewey Lake Red Beds of the Upper Permian. This layer consists almost everywhere of low permeability siltstones, claystones and sandstones, with prevalent vertical fractures generally filled with gypsum. Although water was found in boreholes in the Dewey Lake Red Beds, it was not possible until now to define a water table in this layer.

East of the WIPP site, the Dewey Lake Red Beds are overlain by the Late Triassic Dockum group. In the main this is composed of low permeability claystones, siltstones and sandstones. However, an interbedded aquifer is found in the Dockum group in the eastern part of the WIPP region. The Dockum group, and where absent, the Dewey Lake Red Beds, are overlain by thin Quaternary sediments which are of minor importance to the regional groundwater model.

The database on the interesting hydrogeological units for the groundwater model in the region around the WIPP site varied considerably in detail. A very good database existed for the Culebra Dolomite (cf. Caufman et al., 1990) and a reasonable database was available for the Magenta Dolomite, but for the low permeability layers of the Rustler formation the database was relatively small, and almost no data was available for the layers overlying the Rustler formation, apart from the hydrogeological description.

A great deal of information could be derived from a correlation of the site-specific data. There was a strong connection in the Rustler formation between the occurrence of halite in the aquitards and high salinities in the surrounding permeable layers (see Fig. 2). The high salinities are found in the eastern part of the regional groundwater system. Another interesting result could be derived from the measured permeability data of the members of the Rustler formation. The permeability increased generally in these layers from east to west.

CONCEPTUAL MODEL AND MODEL STRUCTURE

Most of the investigations on groundwater movement and solute transport have only considered the flow in two-dimensional models of the Culebra Dolomite (cf. Davies,
Fig. 2 Location of the halite margins of the members of the Rustler formation (ULM means unnamed lower member) and measured water densities in the Culebra Dolomite (sizes of the symbols are proportional to the density).

1989). Underlying this sort of model is the assumption that the permeabilities of the units above and below the Culebra Dolomite are so small that vertical flow can be neglected. Results of chemical analyses (Chapman, 1988), two of the latest model calculations for the WIPP area (e.g. Davies, 1989) and experience from model calculations carried out to model the deep groundwater movement in northern Germany (Schelkes et al., 1991) justified using another conceptual model. In this alternative "groundwater basin model", all units above the Salado formation were represented. The entire regional flow system was modelled taking the limits of the domain at assumed water divides and at the Pecos River. The top of the Salado formation was used as an impermeable boundary at the bottom of the model. It was assumed that the unknown position of the water table was close to the surface. This avoids some of the difficulties associated with the choice of boundary conditions in the two-dimensional areal models. Decisions concerning these boundary conditions are replaced by assumptions in the groundwater basin model, which seem easier to justify with respect to the location of the water divides and the position of the water table. In the model, groundwater inflows and outflows are only possible at the upper boundary, which represents the land surface. It was important for the model to take the salinity, and therefore the variable density of the groundwater, into account.

In principle, such a regional model is three-dimensional. However, for the conditions of the site, a reasonable approximation to the full three-dimensional model is given by a two-dimensional vertical cross-section model for a line running from the regional high point at The Divide, to the Nash Draw (see Fig. 1). This line runs parallel to the steepest surface gradient, and is normal to the margins of the halite layers in the Rustler formation which represent a potential source of salinity (see Fig. 2). The line runs from east to west through the southernmost part of the WIPP site.

All available data were incorporated in the model, but nevertheless many parameters had to be estimated. This was done, where possible, in a manner consistent with the
geological settings. Vertically averaged values for the permeabilities and porosities were used for each of the five members of the Rustler formation. That means the vertical heterogeneities within these layers were not explicitly considered. Only in the unnamed lower member were the upper and lower part distinguished, corresponding to the two different halite layers in this unit. Plausible values for permeability and porosity were used for all of the other formations. The trend of a permeability increase from east to west in some of the layers was also taken into account. The groundwater in the halite beds, as well as at the lower boundary on top of the Salado formation, was assumed to be saturated brine.

The finite element program ROCKFLOW (Kröhn, 1990) was used for the calculations. Various preliminary simulations with simplified models were undertaken to investigate the effects of discretization, density variations and permeability contrasts, prior to setting up a physically and numerically realistic model. Most of these calculations used combinations of a homogeneous or inhomogeneous hydrogeological model with fresh water or fresh/salt water conditions. A lot of information could be derived from these preliminary model studies which assisted in the development of a reasonable model.

It could be shown that element aspect ratios should not exceed 100. The calculations gave reason to choose small grid lengths in areas with strong curvatures of the stream lines as well as areas with high concentration gradients. At the margins of the halite, which were assumed to be sharp and vertical, horizontal pressure gradients were generated, possibly giving rise to convection cells, which needed a finer grid to resolve. The use of a realistic permeability distribution led to an erratic velocity distribution due to the high permeability contrasts (up to more than four orders of magnitude) between aquifers and aquitards. The differences in permeability were therefore smoothed so that the contrasts did not exceed two orders of magnitude between two elements. The use of the topography, which was linearly interpolated between measured elevations at several borehole locations, as a fixed pressure boundary condition at the top of the model led to an unrealistic flow field, especially near changes in surface slope. This problem was resolved by modifying and smoothing the theoretical groundwater table so that the infiltration rates showed acceptable values.

STEADY STATE GROUNDWATER MOVEMENT

The model which was finally used is shown in Fig 3. The permeability distribution representing a first approximation of a realistic distribution was a result of the data analysis in combination with the preliminary numerical calculations. A transient simulation of the density-dependent groundwater system was carried out until a steady state situation was reached. Fresh water conditions in the whole system were assumed as the initial condition for the transient calculations. A fixed concentration of saturated brine was assumed in the halite layers and as the boundary condition at the bottom.

It was found that steady state conditions were only approached very slowly. This was caused by the time dependent behaviour of the salt distribution. Whereas the flow field did not change very much during the transient simulation, the convergence of the concentration to a stable salt distribution was very slow, especially at the eastern part of the model domain. Figure 4 illustrates the modelled flow field after 4 million years,
which was taken to be close to steady state. The measure used to define this situation as steady state was that the 2% concentration contour line did not change significantly over a longer period of time.

Infiltration occurs over almost all of the top boundary of the model, except for the western part in the Nash Draw. The infiltration rate was found to be less than
60 mm year\(^{-1}\) which is consistent with inferred paleo-precipitation rates. The infiltration represents about 10\% of the precipitation rate during the last glacial maximum 20 000 years ago (Swift, 1991). East of the WIPP site, it is almost less than 1 mm year\(^{-1}\). This suggests that the climatic changes since the last ice age would only have had a minor impact on the eastern half of the system. The groundwater largely flows around the halite zones in the eastern part of the model. The flow is almost vertical in the low permeability layers. The flow in the Culebra Dolomite outside the zone where halite beds are observed in the Rustler formation is several orders of magnitude higher than that in the halite zone. A small convection cell can be observed at the end of the lower halite layer in the unnamed lower member.

The salt concentration is loosely related to the halite zones. The salt plume reached the surface in the eastern part of the model, but is quite narrow west of the WIPP site. The steep concentration gradients in the Culebra Dolomite recorded in the field are matched by the model (Fig. 5). The model also has nearly fresh water in the Magenta Dolomite at the positions where it was measured. Unfortunately, all of these wells in the Magenta Dolomite lie close together.

Interpretations of groundwater chemistry (carbon 14, stable isotopes) suggest that the water in the Culebra Dolomite in the WIPP area may be more than 12 000 years old (cf. Siegel et al., 1991). This estimate was compared with groundwater ages calculated by tracking back along pathlines from the ground surface to the Culebra Dolomite directly below the WIPP site (Fig. 6). The tracks produced ages of 29 000 years for the groundwater on the western boundary of the WIPP site, and 22 million years for the groundwater on the eastern boundary. Because the calculations did not take into account diffusion and dispersion, these travel times provide only an indication of the groundwater age.

These results suggest that the model is reasonable. It should be noted, however, that the model was not fully calibrated. As mentioned above, the permeabilities used were based on a first estimate of realistic parameters.

Overall, the stationary two-dimensional vertical model showed a regional groundwater system fairly typical of deep, layered, regional groundwater systems, with nearly vertical groundwater movement in the aquitards and horizontal movement in the
The transport of salt in the eastern part of the region is dominated by diffusion, and the flow and the velocities are very low. The salt plume does not spread too far west of the halite zones into the dolomites. Density effects only have a minor effect on the flow field, as confirmed by further investigations. The main factor affecting the flow field is the distribution of permeability, with its large heterogeneities.

One important result of the study is that significant vertical leakage occurs into the Culebra Dolomite virtually over the whole distance between the halite zone and the Nash Draw. Figure 7 shows the vertical flux through the Tamarisk member and the horizontal mass flux in the Culebra Dolomite. The calculated vertical fluxes through the Tamarisk member below the WIPP site, and to the east of it, are low (less than 1 mm year\(^{-1}\)) and increasing to the west to up to 600 mm year\(^{-1}\) (taking into account the local water density). These fluxes cause an increase of the horizontal flux in the Culebra Dolomite from almost zero at the eastern boundary to more than a million kilograms per year at the Nash Draw. This shows that the groundwater flow through the aquitards overlying and underlying the Culebra Dolomite should be considered as a very important factor when calculating the flow in the Culebra Dolomite.
The study of groundwater movement in a two-dimensional vertical cross-section has shown that the groundwater basin model seems to be a good alternative conceptual model to a two-dimensional horizontal confined aquifer model. The results are compatible with measured data and values determined from this data, e.g. water densities, groundwater ages and infiltration rates. Although the study was not intended to determine what kind of conceptual model will provide the best representation of the groundwater system, the results could stimulate additional ideas regarding the treatment of this important issue.

REFERENCES


