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In general, the smaller the permeability considered in the model, the smaller the portion of the liquid zone affected by convective flow, leading to reduction of the rates of heat transfer. When a low permeability of 10^{-15} m² and an initial steam saturation of 25% are employed, conduction is the dominant heat-transfer mode in the liquid zone. Because heat released from the source cannot be efficiently dissipated by conduction, a two-phase liquid-dominated boiling zone develops immediately above it.

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Modeling Flow and Transport for Stripa Phase III: What Did We Learn?

J. C. S. Long

The Stripa Project represents a major milestone in the development of technology for the characterization of fractured rock for the purpose of predicting fluid flow and transport. There is probably no other *in situ* block of rock of similar scale that has been probed in so many ways with such intensity in such a brief period of time. An examination of what was learned at Stripa is nearly equivalent to an examination of what is currently knowable about flow and transport in crystalline rock.

This article reviews a few of the key findings that involved fluid flow and transport modeling. The analyses are based on the conceptual model described in Olsson et al. (1989), Black (1991), and Olsson (1992). This model included the definition of the major fracture zones in the Site Characterization and Validation (SCV) rock block. In particular, the conceptual model identified the H-zone as a subvertical zone that was the only major fracture zone to intersect the Validation Drift (VD).

This discussion of model predictions will refer to three hydraulic experiments. The first is the set of cross-hole interference tests (Black, 1991) that took place between packed-off intervals of the SCV boreholes. In particular, we concentrate on the C1-2 test, whose source was confined to interval 2 in borehole C1, which intersected fracture zone H. The second experiment was the Simulated Drift Experiment (SDE) (Black et al., 1991), which was meant to mimic the behavior of a drift from the hydrologic

point of view by placing six parallel boreholes within a ring. The third is the VD inflow experiment (Olsson, 1992), which was conducted from a drift excavated through one-half the length of the SDE boreholes. The SDE provided a unique study of the effects of excavation on hydrology.

The discussion will also refer to three sets of tracer experiments. The radar-saline experiments (Olsson, 1991a,b) consisted of combining a saline tracer test with radar tomography. In the first test, 30 l/min of saline was injected into the C1-2 interval and collected at a sink formed by opening the D-holes in the vicinity of the H-zone. The second test was a repeat of the first but took place after the excavation of the VD. The third set of tests consisted of tracer tests conducted after the excavation of the VD, where a variety of tracers were injected at very low rates from a variety of borehole intervals intersecting the H-zone and collected at the VD (Birgersson et al., 1992)

These experiments were used in the following ways. The C1-2 test was used to develop a model of fracture flow in the SDE based on the conceptual model of Black et al. (1991). The modeling approach used by LBL was to create hierarchical fracture systems through an iterative optimization procedure, or inverse method (Long et al., 1991, 1992a). In this approach, the fracture network is optimized so that it matches certain observations—for example, interference test results such as those from the C1-2 test. In

particular, this method obviates the need to measure the conductance distribution of individual fractures in the field. Simulated annealing is used as the optimization technique because the inversion problem is highly nonlinear and simulated annealing allows the optimization process to escape from local minima (Davey-Mauldon et al., 1993). A model annealed to the C1-2 test is first used to predict the SDE inflow results. The model is then annealed to both the C1-2 and the SDE results and used to predict the VD inflow. Finally, the ratio of flux to velocity in both of these models is calibrated such that the models will best predict the breakthrough curve for the first radar-saline test. These calibrated models are used to predict the second radar-saline test and the subsequent tracer tests.

THE IMPORTANCE OF THE CONCEPTUAL MODEL

A conceptual model is an interpretation of all the observations of a fracture system; it describes how flow and transport occurs and is the basis of numerical models that can quantify flow and transport. The conceptual model is built on the basis of interpretation of laboratory studies, field mapping, geophysical measurements, and *in situ* hydrologic tests. Building the conceptual model is the most important part of fracture characterization because the conceptual model is critical to making predictions. For example, suppose we have *in situ* measurement of transmissivity. The transport velocity we predict for this system will vary by many orders of magnitude, depending on whether we use a 3-D porous media approximation, a 2-D parallel-plate model for the fracture, or a 1-D channel model. The error associated with choosing the wrong conceptual model in this case is much more significant than the measurement error or the numerical errors.

Understanding the geometry of the fracture system and how that geometry controls flow is central to conceptual modeling. There are two types of fracture patterns that result in important flow paths: one is a well-connected cluster of open fractures, or a fracture zone. The other is an extension feature of significant extent. The former is apparently the case at Stripa. Nearly 100% of the flow is observed to occur in fracture zones.

Geophysics was extensively used to detect these fracture zones. Well testing can provide the proof that a geophysically identified feature is hydrologically important because a well can be drilled into the feature and used to test the flow and transport properties directly. Some success in identifying important fracture zones from borehole data was achieved at Stripa by using a variety of measurements together, each of which might be expected to be related to hydrologically important fracture features: e.g., transmissivity, fracture density, electrical conductivity, low acoustic velocity. A variable that was shown to be a good indicator

for important fracture features was the first eigenvector of the correlation matrix for these parameters (Black et al., 1991). Used together, these data provide a very good understanding of the likely location of major flow paths within major fracture zones.

The process of taking all of this information and turning it into a conceptual model is a process of abstraction. The analyst shapes the panoply of data using theoretical constructs and observational analogies to make a working description of the fluid flow system. The process should be fluid and interactive. As questions arise, further data collection is required to address these questions. It is very difficult to continue to make progress on understanding an earth science system when access to the field is cut off. This process was applied successfully at Stripa, particularly with respect to geophysics. In this sense, Stripa serves as an exemplar to those concerned with flow and transport in fractured rock.

The choice of an appropriate conceptual model also depends on the phenomena of interest. A simple prediction of flow rate as a function of time is not highly dependent on having a physically realistic conceptual model. Thus the prediction of inflow was insensitive to detailed conceptual modeling. If, however, one needs know where waste will migrate, a more complete understanding is critical. The purpose of the detailed conceptual modeling and development of sophisticated flow models was primarily to set the stage for the more complex transport modeling.

Some salient features of the conceptual model for the Stripa SCV can be briefly summarized as follows: The fluid flow is largely confined to fracture zones. There are approximately seven fracture zones in the block, including major zones whose location, orientation, and extent have been determined. The fracture zones are not uniformly permeable.

PREDICTION OF THE SIMULATED DRIFT EXPERIMENT

The conceptual model formed the basis of a series of numerical models for flow and transport. These models were formed by creating a lattice of conductors on each of the planes representing the fracture zones identified in the conceptual modeling exercise. Simulated annealing was used to conduct a random search through the elements of the lattice to find a configuration of elements that matches the hydraulic test data (Long et al., 1992a). Simulated annealing results in a solution that is constrained to agree with the hydrologic observations. The process can be repeated many times to get a series of models that all agree with the hydrologic observations. Although this was not done for the Stripa data, it is possible in this way to determine what constraints are placed on the model by the data.

Two kinds of models were created. One looked at the H-zone alone as though it were the only fracture zone to intersect the VD. The other represented all seven fracture zones (Figure 1). Each of these was annealed to the C1-2 data. Figure 2 shows the 2-D H-zone model annealed to the C1-2 data. Each of these annealed models was used to predict the inflow to the D-holes. The 2-D model predicted an inflow of 0.77 l/min, and the 3-D model predicted 0.95 l/min. The measured inflow was 0.77 l/min. These are highly encouraging results. The models are constrained by the conceptual modeling and a single interference test, and they predict a second test extremely well.

ISSUES THAT AROSE IN MODELING THE VALIDATION DRIFT

The next stage of the SCV project was to excavate the VD through the holes of the SDE. Prediction of inflow to the drift was to be accomplished with the models developed using the data from the SDE. The inflow measurement was meant to be used to test the predictive abilities of the models. Below we examine the reasons why this inflow measurement was inappropriate for this purpose but valuable as a measure of excavation effects.

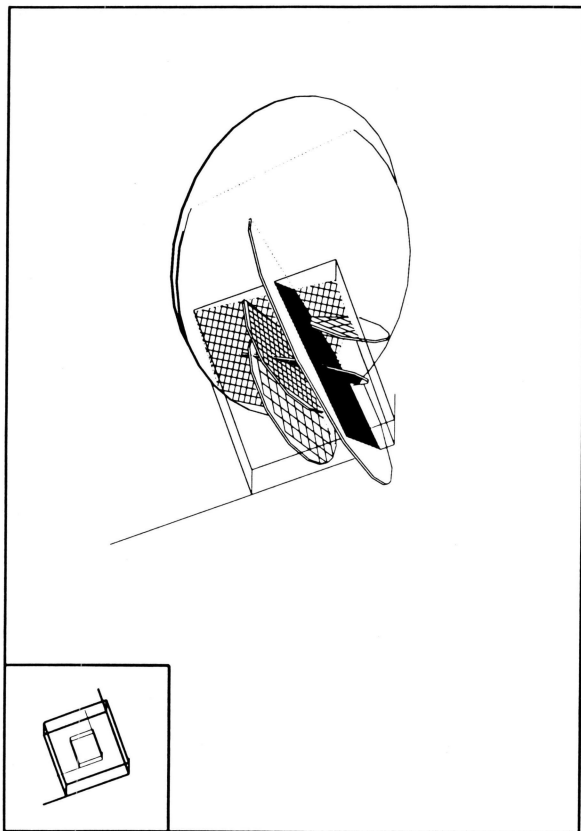


Figure 1. The 3-D model of the SCV, showing seven fracture zones represented by seven lattice structures. [XBL 921-5543]

2-D C1-2 annealed mesh (Dead-end elements dotted)

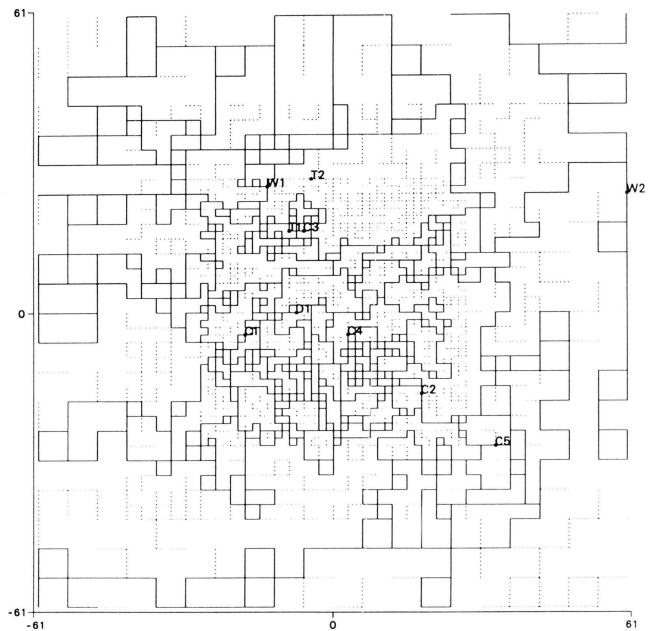


Figure 2. The configuration of the 2-D H-zone model that resulted from annealing to the C1-2 data. [XBL 9110-2207]

The SDE was conducted by lowering the pressure head in the boreholes in three separate steps. Lowering the head in the boreholes increases the gradient into the holes and increases the flow rate. In each step, the head was maintained for several weeks to develop steady-state conditions. Figure 3 shows the flow rate measured at the end of each step as a function of pressure head. During the last step, the pressure head in the boreholes was lowered to approximately 17 m above the elevation of the boreholes.

The shape of the isopotential boundary conditions imposed by the D-holes was almost identical to that imposed by the excavation (Black et al., 1991). Thus extrapolating the flow rates observed during the three steps of the SDE to the case for atmospheric pressure gives an estimate of the VD inflow, discounting any other effects due to excavation.

The total inflow to the D-holes consists of flow to the first 50-m sections of the boreholes, which were later excavated, plus the second 50-m sections, which were not excavated. Between the second and third steps, flow was redistributed among the boreholes as evidenced by the nonlinear flow plots shown in Figure 3 for each of these two borehole sections. However, the total flow is linear with pressure decrease, as expected. Extrapolating the flow rate from each of the three steps indicates that flow into the first 50 m of the boreholes was about 0.88 l/min (880 ml/min) at atmospheric pressure.

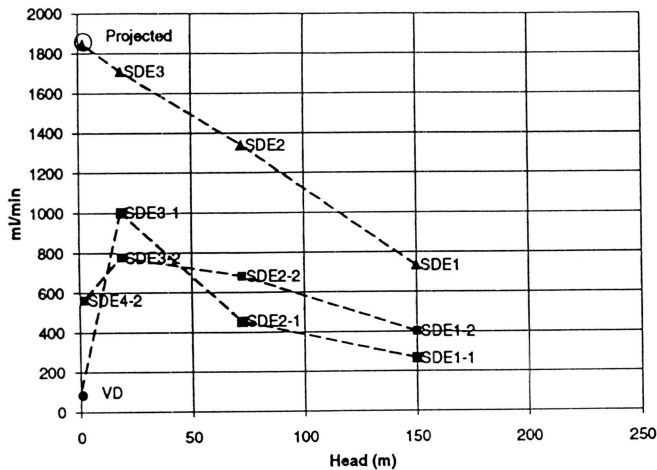


Figure 3. Inflow to the D-holes as a function of pressure head. SDE_x = total flow, SDE_x-1 = flow to 0 to 50 m, SDE_x-2 = flow to 50–100 m, + = flow to “average rock,” i.e., rock not in the H-zone. (The x denotes the steps of the SDE.) Validation Drift inflow is shown by a • symbol. [XBL 936-953]

The excavation of the VD reduced the pressure in the drift to atmospheric. Thus the flow into the excavation area should have increased and the pressures in the surrounding rock should have decreased. Pressures in the surrounding rock began to rise shortly after excavation commenced and continued to rise steadily during excavation. This means that inflow must have been decreasing. After excavation, the total measured inflow was approximately 0.1 l/min, roughly a factor of 9 lower than the SDE measurement.

A series of numerical analyses were conducted, first to simulate the SDE experiment and then, after the simulations were modified, to predict the VD inflow (Herbert et al., 1992; Dershowitz et al., 1991; Long et al., 1991, 1992a,b). Herbert et al. used an analysis of elastic, continuum stress changes due to excavation (McKinnon and Carr, 1990) to modify a discrete fracture model of the SDE to predict drift inflow. Herbert et al. used the computed change in normal stress acting on each fracture in the model and a relationship between stress and permeability derived from laboratory measurements (Gale et al., 1990) to change the permeability of the affected fractures. The net result was a small increase in inflow over that calculated for the SDE, contrary to what was observed. Dershowitz performed similar analyses in a stochastic mode and found increases in flow for some realizations and decreases in others.

Long et al. (1992a) used the equivalent-discontinuum models for the SDE described above, which included flow only in the fracture zones in the vicinity of the D-holes. Data on pressure distribution around a drift a few hundred meters to the west of the VD (the Macropermeability Drift)

were used to infer the magnitude of permeability decrease in a 5-m-wide zone around the drift. These data indicate that the permeability in the first 5 m is decreased on average by a factor of four (Wilson et al., 1981). When this permeability reduction was used in predictions of the inflow to the VD, the predicted inflows were high by a factor of about 5. To match the drift inflow, the permeability in the first 5 m had to be decreased by a factor of 40. Evidently the rock around the VD experiences a significantly less permeable skin than that observed during the Macropermeability Experiment (Wilson et al., 1981). The maximum reduction in permeability that can be inferred from the Macropermeability Experiment is a factor of 20. So the factor of 40 for the VD may not be unreasonable. The remainder of this section summarizes the possible causes examined by Long et al. (1992b) for this dramatic decrease in permeability in the vicinity of the VD. These are summarized below.

The effect of additional sinks drawing off an increasing proportion of the flow after excavation was examined numerically and shown to be unlikely to explain the decrease in Validation Drift inflow.

Drifts can significantly perturb the stress field and hence the fracture conductivity within a few diameters of the drift walls. The stress perturbation caused by the excavation of the VD was analyzed to examine the possible effect of VD inflow along the H-zone (Long et al., 1992a). The orientations of the VD and the most compressive far-field horizontal stress differ by only 4 ft. The stress state and the relevant geometries thus indicate that the change in stress on fractures perpendicular to the drift axis will be minimal. Therefore a 2-D plane-strain analysis is useful for analyzing the stress effects on the H-zone due to excavation. This analysis, based on the most recent stress measurements for the VD area, indicates that the maximum increase in normal stress will occur for fractures radiating from the drift. The compressive normal stress tangential to the drift wall should increase between 50% (at the drift walls) and 133% (at the roof and floor of the drift); these effects decay to less than 10% within a few meters from the drift. Experimental work on laboratory core samples suggests that the ratio of the change in fracture hydraulic conductivity to the change in normal stress varies as σ/N^α , where α most likely is in the range -0.2 to -1 (Gale et al., 1990, Makurat et al., 1990). Accordingly, the hydraulic conductivity along fractures oriented radially to the drift should decrease by no more than 40% at the drift perimeter and by no more than 7% as appropriately averaged over a 5-m distance from the drift. Changes in the absolute magnitude of the normal stress parallel to the drift are small ($< 15\%$), averaging to zero around the perimeter of the drift. There should be little direct effect on the inflow along drift-perpendicular fractures (i.e., the longest H-zone fractures).

A 3-D simulation of the stress field around the drift was made by Tinucci and Israelsson (1991) using the discrete fracture code 3-DEC. The result of their work essentially confirms the conclusions based on the 2-D plane strain analysis presented above. In a two-dimensional simulation with a fully coupled model, Monsen et al. (1991) show no significant differences with the continuum model results. It is difficult to see how changes in normal stress across fractures could decrease the overall permeability of the first 5 m of rock by a factor of 40. On the other hand, shear displacements may result from excavation. These may lead either to increases or to decreases in permeability, depending on the amount of shear and the accompanying normal stress acting on the fracture. Although shear deformation cannot be ruled out as a contributor to flow reduction, the fact that pressure heads began to rise before the main conductor was excavated does not support this theory.

Two-phase flow caused by differential drying during ventilation has been suggested as a possible reason for a decrease in flow (K. Pruess, personal communication, 1991). Drying could be caused by the ventilation procedure. As the ventilation rate is increased, either by raising the temperature in the drift or increasing the air flow rate, the measured inflow of water will change. At first, an increased ventilation rate will increase the measured flow as more water is essentially sucked out of the rock. The rock will then start to dry out, and air invasion could decrease the effective permeability of the rock near the wall. During one stage of the drift inflow measurements, the plastic sheets were removed, thus effectively increasing the ventilation rate. When the sheets were removed, the measured flow rate increased. This indicates that the ventilation was not producing any significant two-phase flow effects.

Blasting can damage the rock through the creation of new fractures (i.e., increase permeability) or cause gas to be intruded into the rock mass and shake loose fine particles, which then block flow paths (i.e., decrease permeability). The effect of fracture formation may explain some of the difference between the Macropermeability Drift (MD) and the VD because the MD was excavated with a smooth blasting technique and the VD was excavated with a pilot and slash technique that caused very little blast damage to the rock. It may be that the careful blasting in the VD did not increase the permeability near the drift as much as blasting did in the MD.

The near-surface waters at Stripa are rich in carbonates, and the deeper waters are rich in sodium. Mixing of these waters occurs when both waters flow toward the same sink, i.e., the VD, resulting in a water that is oversaturated in calcite. Precipitation of calcite in the fractures would decrease the permeability, but this precipitation should be independent of whether the drain consists of a borehole or a

drift. In addition, if calcite precipitation were significant, a permeability reduction would be expected during the SDE, but this was not observed.

During the last step of the SDE, gas bubbles were observed in the outflow tubing. Gas bubbles that are constantly released as water approaches atmospheric pressure could have a very significant effect by causing two-phase flow and a significant decrease in relative permeability if the gas bubbles remain in the rock mass. Samples of the inflow water show that as much as 5 or 6% by volume of the water is nitrogen that comes out of solution at atmospheric pressure (Laaksoharju, 1990). Application of Henry's law to the measured gas content of the inflow water shows that much smaller amounts of gas should come out of solution at the 17-m pressure head used in the last step of the SDE. Thus the scenario whereby degassing causes two-phase flow is consistent with a significant flow drop between the SDE and the VD. Degassing is also consistent with the observation that pressures began to increase immediately following the start of excavation. Finsterle and Vomvoris (1991) attempted to numerically simulate degassing for the VD and found no effect on inflow rate, but they might have obtained a different result if the simulations had used different parameters or geometry, more like those of the true flow system.

In conclusion, the most plausible cause for a significant decrease in the permeability of the skin surrounding the VD is degassing as the pressure of the water is dropped to atmospheric on inflow. Excavation method, stress effects, and dynamic loading may also have some importance. It should be noted that the orientation of this tunnel with respect to the maximum principal stress and the dominant fracture orientation and its small size (< 3 m diameter) may be largely responsible for the fact that stress changes appear to be relatively unimportant. An important consequence of these observations is that hydrologic measurements in tunnels cannot be used straightforwardly for characterizing the flow system because of the unknown magnitude and cause of the skin. It is certainly inappropriate to consider inflow measurements to drifts as indicative of the undisturbed hydrologic regime. In the case of the SCV modeling effort, the VD measurements were dominated by physical effects that were not part of the modeling exercise. Hence, the VD inflow was not useful for examining the appropriateness of the modeling efforts. The combination of the SDE and VD experiments were, however, very valuable for understanding excavation effects. The process of gas dissolution is eventually reversible, and if a low-permeability skin is caused by two-phase flow effects, refilling the tunnel is likely to cause permeability to increase. This is of importance for the storage of nuclear waste in underground repositories, for water transport tunnels, and for other cases where inflow to an underground excavation needs to be understood. This phenomenon may create an

opportunity to study two-phase flow effects in fractured rock by controlling the pressure in boreholes drilled from an underground facility.

WHAT WAS LEARNED FROM MODELING THE TRACER TESTS

A series of tracer simulations were compared with results of *in situ* tracer tests. The simulations were based on two 2-D equivalent discontinuum models of the H-zone. The first, mentioned above in the section on the conceptual model, was annealed to the C1-2 test and is called the "C1 model." The second, called the co-annealed case, was simultaneously annealed to the C1-2 test and the observations made at the end of the SDE.

Both models were used to simulate the first Radar/Saline (RSI) experiment, i.e., injection of tracer in C1-2 and collection of tracer in a sink caused by opening the D-holes in the vicinity of the H-zone. The actual breakthrough curve was used to calibrate the model by changing the ratio of flow to velocity in the conductive elements of the model to match the breakthrough curve. Only advective dispersion of tracer was allowed. This calibrated model was then modified to include the low-permeability skin around the drift and used to predict the second Radar/Saline experiment (RSII), this time from C1-2 to the VD. Figure 4 shows the predicted and measured breakthrough curves for RSI and RSII, respectively, in the C1-2 configuration. Then a series of tracer tests from a variety of borehole intervals within the H-zone to the drift were simulated.

In the models, the change in boundary conditions from RSI to RSII had the effect of increasing the maximum C/Co. In the experiment, excavation left the maximum C/Co relatively unchanged. The increase in C/Co from the RSI simulation to the RSII simulation is explainable because the injected water is a greater proportion of the inflow to the drift than the inflow to the D-holes. However, the lack of a similar trend in the observed data may be due to (1) the effects of excavation and the resulting two-phase flow near the drift, (2) the influence of the remaining open D-holes in pulling tracer away from the drift, or (3) an increase in local dispersion phenomena caused by the higher injection pressures of RSII. Thus lack of knowledge of the boundary conditions prevents a

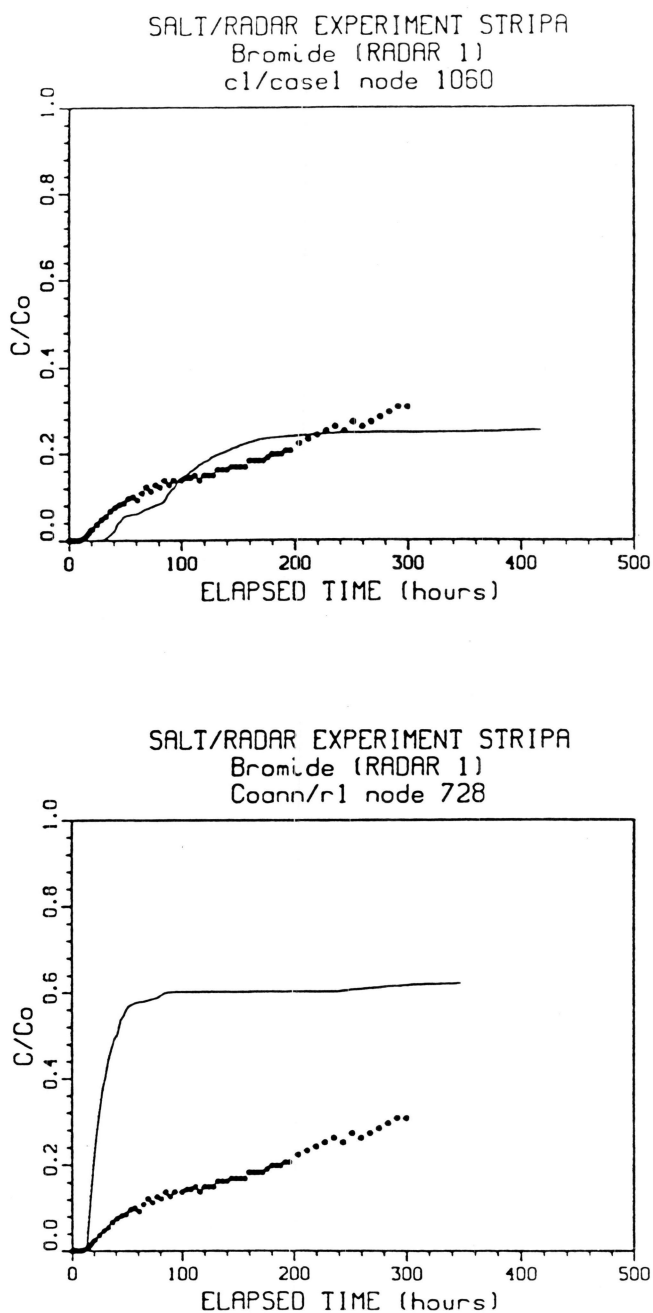


Figure 4. Predicted and measured breakthrough curves for RSI (top) and RSII (bottom). [XBL 935-796]

Table 1. Estimates of first arrival and maximum concentration for the tracer tests.

Case	Source	First arrival (hr)		Maximum C/Co	
		Predicted	Data	Predicted	Data
1	T1:2	800 to 2800	400	0.0001 to 0.0005	
2	T2:1	200 to 1400	200	0.0001 to 0.0004	0.002
3	C2	200 to never	300	0 to 0.002	0.002

good estimate of the maximum concentration. Both the C1 and the co-annealed configurations match the arrival time of the RSII data fairly well.

The tracer tests were simulated twice: once with the C1-2 configuration and once with the co-annealed configuration as described above. No dispersion coefficient was used. The breakthrough curves are all much steeper than that observed. As can be seen in Table 1, the models do extremely well in predicting the breakthrough times. It seems as if these hydraulically based models do reasonably well in predicting arrival times. However, more physical reality, e.g., more channel conductance variability, may be needed to capture more of the transport behavior. Knowledge of boundary conditions is critical to predicting tracer transport in a way that prediction of flow is not anywhere near as sensitive to.

CONCLUSIONS

Some of what was gained from the Stripa Project was not planned: as in most earth science research, the results may not exactly match the original goals. Nevertheless, the actual results are significant. The stated aims of the project included "validation" of fluid flow and transport codes. I would argue that this is not a possible achievement in a strict sense. Simply changing the definition of validation in such a way that validation somehow becomes achievable trivializes and obfuscates an accurate assessment of the modeling effort. What we have learned is that the codes are a mathematical formalization of the exceedingly more important effort of "conceptual modeling." Stripa is by far the best example of conceptual modeling done to date.

Although only the modeling efforts done by LBL are discussed here, all of the modeling efforts that have been done show that the key to good modeling is good characterization. Each of the codes has advantages and disadvantages, and each could be applied with flexibility in meeting the challenge of predicting behavior. None of the codes would have come anywhere near making good predictions without a good understanding of the fracture system.

A recommendation for future work is that future studies of tracer transport in fracture networks should not be confounded with excavation effects. There are many things that we do not fully understand about the physics of the transport phenomenon in fractures. It may be possible to match breakthrough curves, but we do not yet know the best way to build predictive models. The SCV project has shown clearly that we do not understand the hydrology of excavations. Coupling these two problems makes it very difficult to interpret the experiments.

It may be very productive to conduct a series of inter-reference tests as the basis for an iterative model development process. The idea would be to optimize the model to one test and predict the second, then optimize the model to

the first two tests and predict the third, etc. In this way it may be possible to see how the ability to predict improves with additional data. It will be very important to study the effects of excavation in such a way that the various physical phenomena can be deconvolved. Much of the inferences about a rock mass being considered for a nuclear waste repository will be made from observations in underground excavations. We will consequently need to know how to condition our inferences to reflect the excavation effects. Finally, in formations rich in dissolved gases, underground excavations in otherwise saturated rock may provide an excellent opportunity to perform controlled studies of two-phase flow in fractures.

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Evaluating the Degradation of Chlorinated Hydrocarbons in Contaminated Groundwater

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Since 1983, it has become known that groundwater beneath the site of the Lawrence Livermore National Laboratory (LLNL) has been contaminated with volatile organic compounds (VOCs), notably PCE, TCE, 1,1- and 1,2-DCE, 1,1,1-TCA, and 1,1- and 1,2-DCA. The Environmental Restoration Division (ERD) of LLNL is exploring many alternatives to remove the VOCs from groundwater so as to comply with the regulations of the Environmental Protection Agency (EPA). In evaluating the relative merits of these strategies, an important issue concerns whether the dissolved organic compounds undergo degradation into

daughter products and, if so, determining the half-lives of such degradation reactions.

The purpose of this study is to analyze the water quality data already collected from the site by the ERD for evidence of degradation. This work is based on the premise that dissolved organic compounds may follow a variety of degradation pathways, determined largely by the overall groundwater geochemistry, notably redox conditions. Therefore, it is rational to commence the evaluation effort with a study of the thermodynamic state of groundwater at the site. A detailed report of this study is presented in McNab and Narasimhan (1992).