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A COMPARISON OF LABORATORY AND FIELD TECHNIQUES FOR CHARACTERIZING DIFFUSION IN SPARSELY FRACTURED GRANITE

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ABSTRACT

The in-situ diffusion experiment intended to improve the understanding of diffusive solute transport in SFR was conducted at AECL's Underground Research Laboratory (URL) using a comparative series of laboratory and in-situ field experiments. The work was intended to explore issues surrounding the influence of stress relaxation in rock samples, stress redistribution about underground openings, rock texture, porosity, pore geometry, and anisotropy on derived effective diffusion coefficients (D_e).

The in-situ diffusion experiments were conducted within 10 m long sub-horizontal NQ boreholes situated to intersect a range of rock stresses and textures on three levels of the URL. Following efforts to minimize the effects of well bore pressure histories and hydraulic gradients, tracers (I, Br, Li, Rb, uranine, lissamine) were injected into two test intervals within each borehole. After 15 months, one experiment from each URL level was over-cored to determine the extent of tracer diffusion into the rock. In-situ diffusivities were estimated from these tracer profiles using the finite-element code MOTIF. In-situ permeabilities were estimated from the analysis of shut-in hydraulic tests using the code nSIGHTS. The laboratory efforts were principally focused on the completion of 44 steady-state diffusion cell experiments using replicate granodiorite, granite and pegmatite rock coupons with a length of 0.03-m. Tracers included ^{3}H, I, Li, Rb, lissamine and uranine. Proof of concept laboratory work included radial diffusion experiments with 0.20 m diameter cores and steady-state experiments to investigate diffusion across fracture surfaces and at elevated temperatures (50^{o}C). Estimates of rock permeability at different orientations were determined by use of a high-pressure permeameter. Porosity estimates were determined by water immersion and diffusion experiments.

Experimental results show that rock samples removed from high stress conditions are altered as a result of the combination of in-situ stress relaxation and stresses created by drilling, resulting in laboratory-estimated D_e and permeability values that were higher than those determined in-situ. However, laboratory and in-situ D_e values determined for the 240-m Level were similar implying that samples removed from stress condition less than 30 MPa are subject to only minor alteration. In-situ experiments in SFR are also subject to uncertainty created by stress redistribution around borehole openings that could be responsible for the presence of a radially symmetric interface or resistance effect. This resistance may influence in-situ measurements of diffusion and permeability. Despite the agreement between laboratory and in-situ De values at

the 240 m Level, laboratory and in-situ experiments still possess uncertainties associated with sample alteration, scaling, in-situ stress redistribution effects, and hydrogeology.

I. INTRODUCTION

An understanding of diffusive mass transport in sparsely fractured or intact granitic rock (SFR) is important for assessing the safety a deep geologic repository located in the Canadian Shield. Although diffusion is likely to be the principle process contributing to mass transport in SFR, it is useful to develop a knowledge of the interrelationships between diffusivity, permeability, porosity and pore geometry. As is typical with many problems in geoscience, the characterization of mass transport properties in SFR contains inherent uncertainty associated with questions of sample alteration, sample scale, hydraulic gradients, rock heterogeneities and difficulties in working with very low permeability (k) and highly stressed rock. A useful approach to dealing with uncertainty in geoscience is to tackle a problem using a variety of different approaches. Therefore, the in-situ diffusion experiment [1] intended to improve the understanding of diffusive solute transport in SFR was conducted at AECL's Underground Research Laboratory (URL) using a comparative series of laboratory and in-situ field experiments. The work was intended to explore issues surrounding the influence of stress relaxation [2, 3], rock texture, porosity, pore geometry, and anisotropy on derived effective diffusion coefficients (D_e).

The locations of the in-situ experiments at the URL were chosen to capture the maximum possible variability in rock composition, mineral size, and in-situ stress magnitude and orientation. The maximum principal stress varies from 31 MPa at the 240 m Level to 54 MPa at the 300 m Level and 60 MPa at the 420 m Level. The rock types available at the URL include gneissic grey granite, leucocratic granite, xenolithic-leucocratic granite, granodiorite, pegmatite dykes and quartz veins. The grey granite is medium-grained and relatively homogeneous with up to 10% biotite and magnetite. The leucocratic granite is coarser grained and has less than 5% mafics. While the grain size of granite (1 – 5 mm) is larger than that of granodiorite (≤ 1 mm), both rocks contain similar mineral assemblages, consisting of quartz, K-feldspar, plagioclase, biotite, chlorite and sericite-muscovite as major minerals, and apatite, allanite, zircon, epidote, sphene and opaques as minor and accessory phases. The pegmatite dykes crosscut all other rock types, and are quartzo-feldspathic with euhedral or subhedral biotite and magnetite. The experimental work program began with the drilling of a total of 10 boreholes for the in-situ diffusion experiments on the 240, 300 and 420 m Levels of the URL, which contained sections of sparsely fractured rock which appear to be free of open fractures. Rock core samples from this drilling program were used to begin the laboratory experiments, which were completed before the results of the field-scale experiments became available.

II. LABORATORY EXPERIMENTS

The purpose of the laboratory studies was to estimate the porosity, effective diffusion coefficients and permeability of core samples taken from variably stressed SFR settings. The estimates of effective diffusion coefficients and permeabilities can be compared to values derived from in-situ experiments to determine whether laboratory measurements can be applied to in-situ conditions.

II.A. Porosity

Diffusivity and mass transport in a porous medium is contingent on there being a continuous path for the movement of solutes through the rock, and is related to the presence of a connected pore space filled with groundwater. Therefore, calculation of diffusive flux through a body of rock should include porosity. The effective or empirical diffusion coefficient (D_e) has been commonly used to describe diffusive fluxes and is related to the free-water diffusion coefficient (D_w) by the following equation that considers the through-transport porosity (ε_t), the constrictivity (δ) within connected pores, and the tortuosity (τ).

$$D_e = \frac{D_w \delta \varepsilon_t}{\tau^2}$$

All of the methods developed for estimating porosity involve filling the connected voids with a quantifiable substance or tracer. The usefulness of a given method depends on the ability of the tracer to penetrate all relevant pore space and on the ability to quantify the tracer. The water immersion technique, refined by Melnyk and Skeet [4] for rocks with porosities less than 5%, has been widely used in many studies [5,6,7]. The water immersion technique consists of saturating a rock sample with distilled de-aerated water under vacuum and then determining the weight of water in pore spaces by monitoring the weight of the rock sample while drying it. Connected porosity in rock samples was also estimated from the rock capacity factor derived from laboratory diffusion experiments, as described in the next section. Porosity measurements using the water immersion method were performed on freshly cut, 3 cm thick, NQ core slices and included all samples to be used in diffusion experiments. Results showed that the average immersion porosity is lowest for samples from the 240 m Level, $(2.4 \pm 0.1) \times 10^{-3}$, compared to porosities from the 300 m Level, $(3.0 \pm 0.2) \times 10^{-3}$, and the 420 m Level, $(2.8 \pm 0.2) \times 10^{-3}$. In general, there appeared to be a trend of decreasing porosity with increasing mineral size.

II.B. Diffusion Cell Experiments

The purpose of the diffusion cell experiments was to estimate effective diffusion coefficients and rock capacity factors of core samples from the diffusion holes. The basic strategy in these experiments is to position a rock sample between two solution reservoirs of equal hydraulic head (Figure 1). A concentration gradient is then established across the rock sample. Once the system has reached a steady-state, the flux of tracer across the sample is measured and the effective diffusion coefficient of the tracer in the rock sample is determined. Initial experiments established that the length of the rock core sample (Figure 1) should be 3 cm, the minimum thickness to achieve a Representative Elementary Volume (REV). During the diffusion experiment, one end of the rock coupon is in contact with a tracer solution (with ^{3}H, I, Li, Rb, lissamine or uranine) contained in a 1 L reservoir open to the atmosphere. The other side of the rock sample is in contact with an elution reservoir, which is continuously sampled by a fraction collector. The volume of sampled solution is replaced by tracer-free eluant (KNO_3 solution formulated to match the density and ionic strength of tracer solution), supplied from the eluant reservoir, which also maintains the height of solution in the elution reservoir at the same level as in the tracer reservoir. The tracer concentration in the eluant reservoir is kept low because of the continuous flushing with tracer-free eluant. As tracers diffuse through the rock sample, eventually a steady-state concentration is reached in the elution reservoir, representing the steady-state diffusion through the rock sample. The mass of tracer (M_t) diffusing through the sample under steady-state conditions at time (t) is described by the following equation:

$$M_t = De(C_oA/L)\, t - \alpha(ALC_o/6)$$

where De is the effective diffusion coefficient for a given tracer in the rock sample, A is the surface area through which the tracer diffuses, L is the diffusion path length (i.e., thickness of rock sample), C_o is the concentration of a given tracer in the tracer reservoir, and α is the rock capacity factor.

Thus, when steady-state has been achieved a plot of M_t versus time will produce a straight line with a slope:

$$\text{Slope} = De(C_oA/L)$$

and an intercept:

$$\text{Intercept} = -\alpha(ALC_o/6)$$

Since C_o, A and L are known, the slope can be used to calculate De. The intercept of the straight line can be used to calculate the dimensionless rock capacity factor (α), which represents the amount of tracer held up in the rock sample before steady-state is achieved. In the case of non-sorbing tracers the magnitude of α depends upon the total connected porosity accessed by the tracer (ε_c). While the transport porosity (ε_t) includes only the connected porosity that is contributing to the diffusion process, the total connected porosity (ε_c) also includes dead end pore space that does not contribute to the effective diffusion coefficient and only adds storage capacity. The values of De and α are the basic parameters that can be estimated from the diffusion cell data, without additional assumptions.

The laboratory efforts were principally focused on the completion of 44 steady-state diffusion cell experiments using replicate granodiorite, granite and pegmatite rock coupons to investigate the effects of rock texture and in-situ stress conditions. The steady-state diffusion experiments were also to investigate diffusion across fracture surfaces and at elevated temperatures (50^{o}C). The experimental durations of 35 to 70 days were sufficient to produce well-defined diffusion data for iodide and tritium. Laboratory estimated iodide D_e values varied from 2.0×10^{-13} to 2.2×10^{-12} m^2/s, and tritium D_e values varied from 1.7×10^{-13} to 2.8×10^{-12} m^2/s. However, the duration of these experiments was generally not sufficient to produce accurate diffusion data for lithium, rubidium and fluorescent dyes. The extension of four steady-state diffusion tests to 94 days was able to obtain reliable diffusion data for uranine, giving De values ranging between 2.9×10^{-13} and 3.7×10^{-13} m^2/sec.

A comparison of core samples with and without fractures showed that diffusivity across fracture surfaces may be lower than in the rock matrix. The increase in D_e values at 50^{o}C by factors of 2.5 and 3.1 for iodide and tritium, respectively, could be accounted for by the predicted increase in the free-water diffusion coefficient (D_w), as well as, an increase in rock sample porosity.

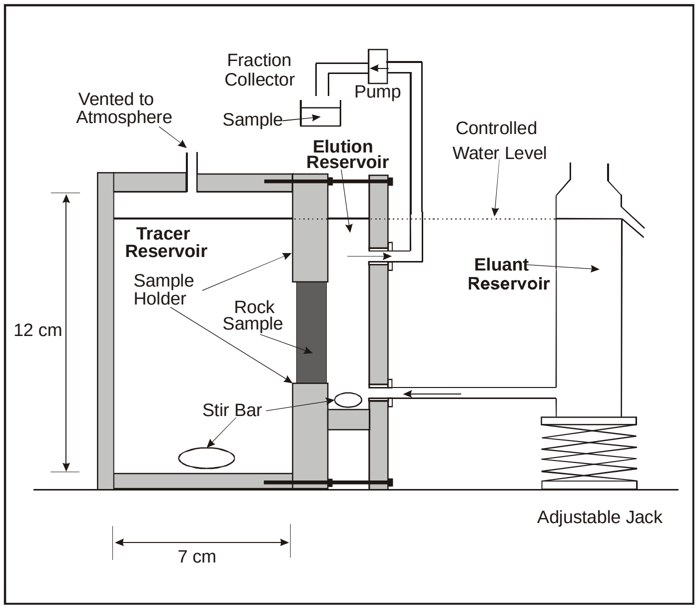

Figure 1: Schematic diagram of a laboratory diffusion cell.

II.C. Radial Diffusion Experiments

Proof-of-concept experiments were also performed with radial geometry diffusion cells (Figure 2) to evaluate the effects of sample geometry and to obtain diffusion profiles that could be directly compared to in-situ results. The radial diffusion cells contained a 190 mm diameter rock core with an internal 71 mm diameter tracer reservoir to simulate the geometry of the in-situ experiments. During the test tracer elution was monitored in an outer elution reservoir to estimate De values. The total duration of radial geometry diffusion experiments ranged from 128 to 440 days. Once each experiment was terminated the rock matrix adjacent to the tracer reservoir was sampled at six locations by drilling 2 cm diameter cores orientated perpendicular to the central tracer reservoir. These cores were cut into 0.5 cm slices, which were leached in deionised water for 33 days to extract tracers. The extracted tracers were converted to pore water concentrations to obtain diffusion profiles.

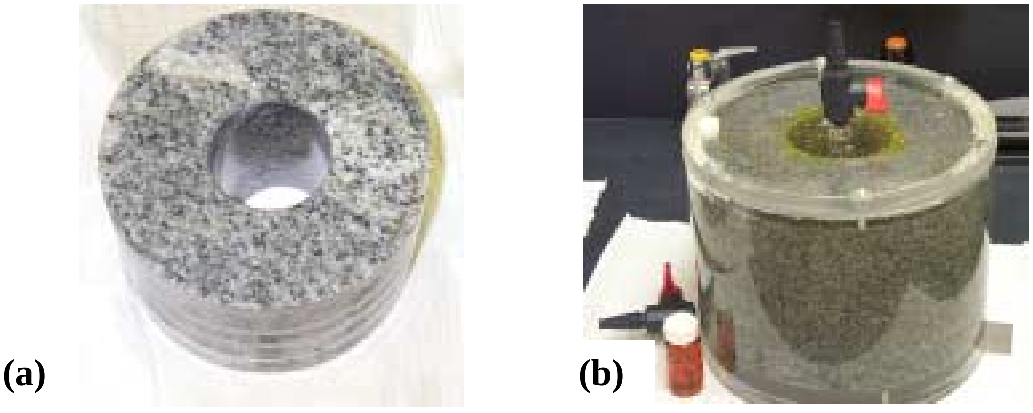

Figure 2: Radial diffusion experiment using (a) a 190 mm diameter rock core contained in a (b) radial diffusion cell.

The iodide De values estimated from the flux of iodide through the rock cores in the radial diffusion experiments ranged from 6.5 x 10^{-13} to 3 x 10^{-12} m^2/s. These results are consistent with the steady-state diffusion cell tests, indicating that sample geometry did not affect the diffusion results. The duration of the radial diffusion experiments was sufficient to produce estimates of effective diffusion coefficients for uranine (1.1 x 10^{-13} to 7.5 x 10^{-13} m^2/s), lithium (2.9 x 10^{-13} to 1.2 x 10^{-12} m^2/s), and rubidium (2 x 10^{-15} to 1.5 x 10^{-12} m^2/s).

II.D. Permeability Estimation

Laboratory permeability estimates were made on rock samples from the diffusion holes, using a hollow core permeameter[1], and the High Pressure Radionuclide Migration (HPRM) apparatus[8], which was used as a permeameter with a tri-axial confining pressure for the rock sample. The triaxial confining pressure was able to simulate lithostatic pressures of up to 17 MPa. Radial permeability values estimated in the laboratory by the hollow core permeameter technique varied between 2 x 10^{-18} and 1 x 10^{-17} m^2. When triaxial confining pressures of up to 17 MPa were applied to rock samples in the HPRM apparatus, the estimated axial permeability values dropped to between 9 x 10^{-20} and 5 x 10^{-18} m^2. In both types of tests the highest permeabilities were observed from samples taken from the highest stress conditions. It was also noted that the effect of confining pressure on permeability is not fully reversible. Once a sample has been exposed to a maximum confining pressure, a subsequent reduction in confining pressure will not return the permeability to values observed before the application of high confining pressures.

III. IN-SITU EXPERIMENTS

All boreholes were emplaced in sections of SFR, which appeared to be free of any open fractures. At the 420 m Level four test boreholes were located in Rooms 413 and 420. At the 300 m Level three holes were emplaced in Room 301, through which the URL shaft passes. The remaining three holes were positioned in the west wall of Room 214. The minimum separation distance between any two holes was 5 m.

The test boreholes were drilled into the walls of the URL tunnels at a dip of 8 to 11 degrees down from horizontal. First a 200 mm borehole was drilled to a depth of 7 m. Starting from the bottom side of this borehole, a 76 mm NQ borehole was drilled to a depth of 3 m beyond the bottom of the 200 mm borehole (Figure 3). The boreholes were completed with a multi-level packer system designed to isolate two test zones, to which tracers were added. The upper test zone (Zone 1) was defined by an upper mechanical packer, located 3 m from the borehole collar, and a lower inflatable Baski packer placed within the NQ hole. The lower test zone (Zone 2) was a 1 m long section located at the bottom of the NQ hole.

Prior to injecting tracers into the diffusion holes it was necessary to establish that diffusion hole pressures were in equilibrium with formation pore water [1]. Once the diffusion holes were filled with synthetic groundwater, the Zone 1 pressures were set to constant head values equivalent to fresh water heads at each level. The Zone 2 sections were shut in and their pressures were monitored to determine the actual formation pressure and to check whether equilibration had been achieved. After 10 months the Zone 2 pressures had stabilized to constant values, which could be reproduced after repeated pressure pulsing. This provided sufficient confidence that hydraulic equilibration with formation fluid pressures had been achieved.

Notable, however, was that observed interval pore water pressures were below estimated freshwater heads to some degree in all boreholes, possibly as a result dewatering toward the URL shaft via Fracture Zone 2 and/or radial stress redistribution within the low permeability rock adjacent the excavated tunnel[9]. During the diffusion experiments Zone 2 was shut-in to maintain hydraulic equilibrium with the formation, while the hydraulic heads in Zone 1 were maintained at constant values equivalent to the freshwater head for each level. Modelling with MOTIF[1] predicted that maintenance of the higher heads in Zone 1 would hydraulically isolate the rock mass surrounding Zone 2 from radially convergent hydraulic gradients otherwise oriented toward the tunnel.

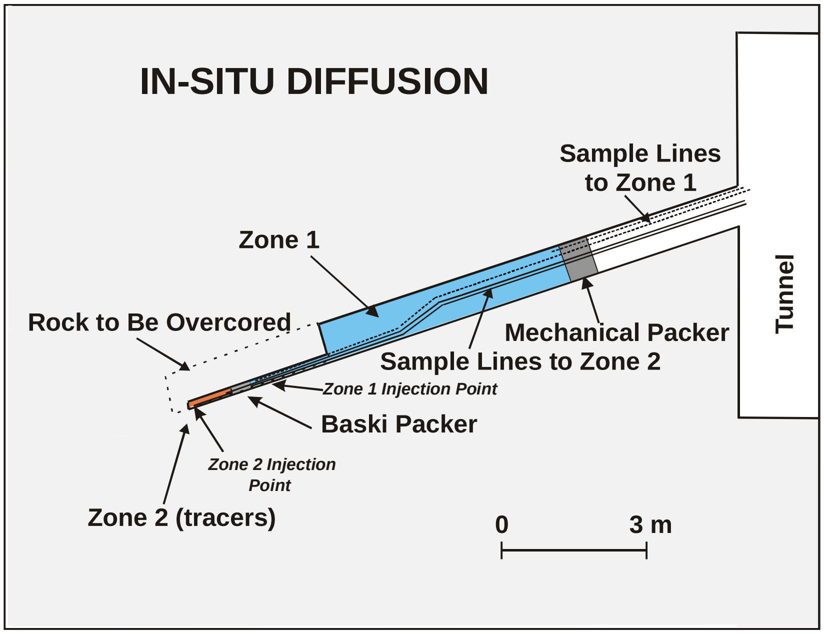

Figure 3: Schematic diagram of a diffusion borehole, showing the locations of the inflatable Baski Packer and the upper mechanical packer.

The compositions of the synthetic groundwater used as supporting electrolytes for tracer solutions were formulated to approximate as much as possible the composition of the matrix pore fluids in the surrounding rock matrix. These compositions were based on the compositions of water seeping into boreholes in close proximity to the diffusion boreholes[1]. Pore fluids at the 240 m Level were Na- Cl-SO_4-HCO_3 solutions with a TDS of 0.6 g/L. The 300 m Level had Na-Ca-Cl-SO_4 fluids with a TDS of 26 g/L, while the 420 m Level had Ca-Na-Cl-SO_4 solutions with a TDS of 90 g/L. While the TDS of tracer solutions could be matched with pore water compositions on the 300 m and 420 m Levels, the tracers had significantly higher TDS on the 240 m Level. The tracer solution used for Zone 2 contained iodide (10 g/L), lithium (1 g/L), rubidium (6.7 g/L), and lissamine or uranine (2 g/L). The Zone 1 tracers consisted of bromide (12 g/L) and uranine (2g/L). After injection into Zone 1 and Zone 2, tracer solutions were allowed to interact with the rock for a period of about 15 months.

For the purpose of this study only one borehole was terminated at each URL level. In order to determine tracer transport into the rock, at the end of the experiment the rock surrounding Zone 2 and the lower part of Zone 1 was over-cored. This was accomplished by first removing the tracers and packer systems from the diffusion holes, and then sealing the Zone 1and Zone 2 NQ borehole sections with grout to minimize tracer redistribution by drill water during the over-coring operation[1]. The diffusion holes were over-cored to a depth from 7 to 10.5 m using a 20 cm drill and using the first 7 m of the diffusion hole as a guide (Figure 3). The over-core sections were wrapped in plastic and removed to the surface, where they were photographed, measured and marked for sample drilling with a special jig for drilling 2-cm diameter sample cores orientated perpendicular to the over-core axis. Figure 4 illustrates the locations of the sample cores in a typical over-cored section. The sample 2-cm cores were cut into 5 mm thick sections, which were leached in deionised water for 35 days. This was sufficient to recover 98 to 99 percent of the iodide and bromide, and 94 to 97 percent of the fluorescent dye. Leached solutions were analyzed for iodide by ion selective electrode, bromide by ion chromatography, uranine by fluorescence, and lithium and rubidium by atomic absorption.

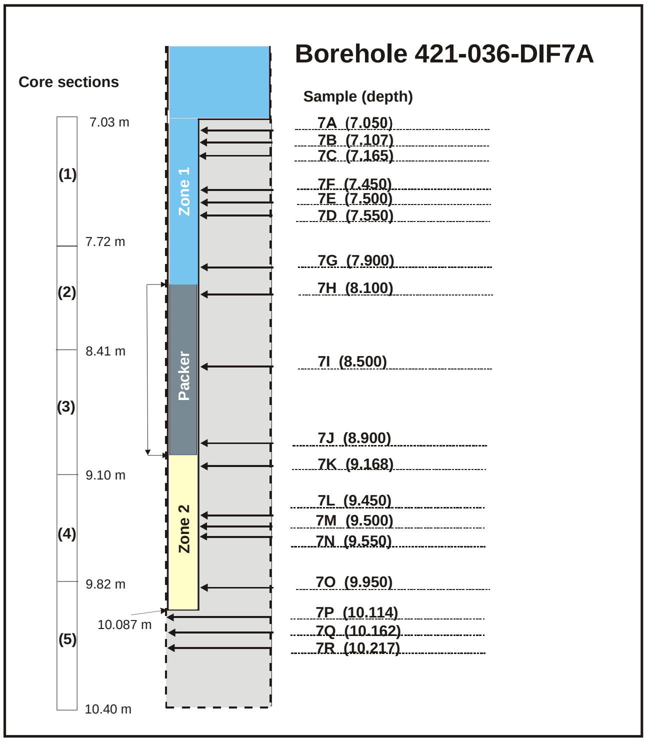

Figure 4: Schematic diagram showing the location of the sample cores cut from the over-cored section.

The total number of sample cores cut from the over-core of each borehole was 18, representing about 315 individual samples for each hole. The top 3 sample cores in Zone 1 were intended to capture tracer migration from both the wall of the NQ tracer borehole, as well as from top flat surface of the over-core (see Top – Zone 1 part of Figure 4). The 3 cores in the middles of Zone 1 and Zone 2 were set up to evaluate the effects of stress redistribution. Since the diffusion holes were drilled with a sub-horizontal orientation, the redistribution of in-situ stresses is predicted to create zones of compression above and below the hole, and zones of tension on both sides. The compressive stresses could be expected to locally increase constrictivity and reduce tracer diffusion, while the opposite would be expected in the zone of tension. While most sample cores were cut through the zone of compression, one of the middle cores (Zone 1 and Zone 2) was cut through the zone of tension while the other was cut through an intermediate direction. Several cores were positioned close to both ends of the Baski packer to assess evidence for tracer migration between the two test intervals. Three cores at the bottom of Zone 2 were intended to determine tracer diffusion profiles axially away from the test interval such that the influence of borehole geometry and stress re-distribution could be further evaluated. The tracer pore water concentrations were determined using the previously described 35 day leaching techniques. In this case leachate concentrations were converted to pore water concentrations by a factor based upon the leach volume of 10 mL and the pore volume in each sample. The sample pore volumes were determined from the weight of each sample, the rock density, and the rock porosity.

The transport of Zone 1 tracers within the rock matrix was driven by both diffusion and an outward hydraulic gradient. The hydraulic head differences between Zone 1 and the surrounding rock for the 240 m, 300 m and 420 m Levels were estimated at 84 m, 33 m, and 16 m, respectively. The transport of Zone 2 tracers was assumed to be driven by diffusion only, and therefore was the primary focus of this experiment.

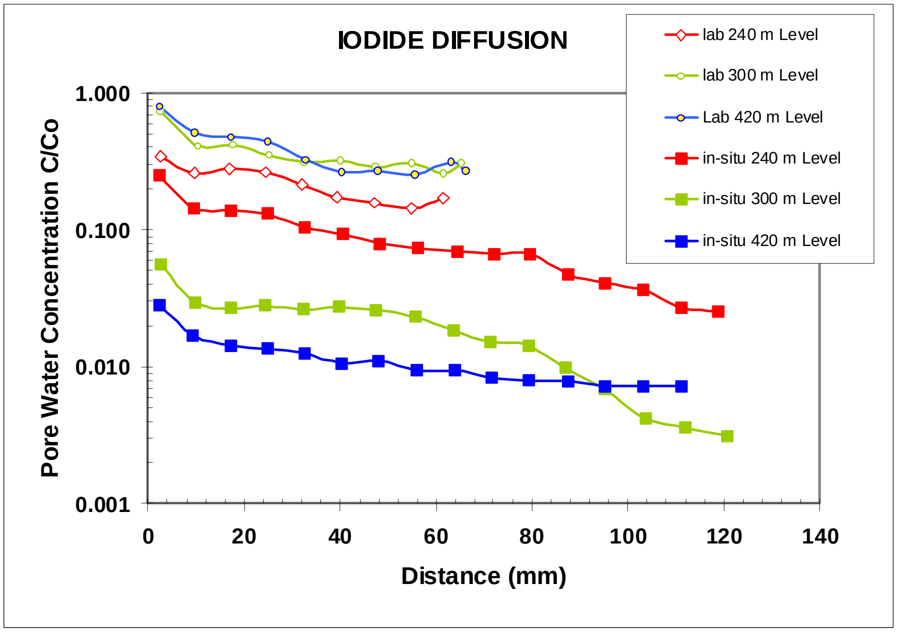

Figure 5: A comparison of laboratory diffusion profiles with average in-situ diffusion profiles (Zone 2) for different levels of the URL.

Average iodide diffusion profiles obtained from the rock surrounding Zone 2 are compared with laboratory derived diffusion profiles in Figure 5. The in-situ diffusion profiles exhibit a dog-leg pattern in which a zone of high constrictivity, within 10 mm of the borehole wall, significantly reduces tracer diffusion into the rock. This interface effect is minimal in the laboratory profiles and increases with greater depth in the in-situ profiles. In all three diffusion holes the end diffusion profile, extending downward from the bottom of Zone 2, was identical to the diffusion profiles radiating perpendicular to the test borehole axis. Tracer profiles in the zone of tension were usually not higher than in the zone of compression as one might have predicted.

In most cases the profiles in the zone of tension were lower compared to the zone of compression. Although not shown in Figure 5, it is worth mentioning that the bromide concentration profiles around Zone 1 also displayed an interface effect. Since the transport of Zone 1 tracers was also driven by hydraulic gradients their concentration profiles were higher than Zone 2 diffusion profiles by as much as a factor of 6. The core samples taken next to the packer (Figure 4) showed that Zone 1 tracer was not able to migrate past the packer toward Zone 2.

The MOTIF finite element model[10] was used to approximate a skin or zone of constrictivity at the borehole wall in order to estimate the diffusion properties of the bulk rock mass beyond this interface. An example of the MOTIF predicted average tracer diffusion profiles for the 420 m Level, which depict the radially symmetric layers gridded to vary rock properties, is shown in Figure 6. Layers 1 to 4 are assigned to the constricted zone, and have rock properties adjusted to restrict tracer diffusion into the bulk rock. Usually layers 5 to 10 are assigned bulk rock properties. However, when required, the properties of these layers can be readily manipulated to account for variation in rock properties [1]. The bulk rock De (m^2/s) values for predicted tracer distributions that best fit the observed tracer profiles are given in the legend. The in-situ results yielded iodide D_e values between 1.4 x 10^{-13} and 1.1 x 10^{-12} m^2/s. The De (m^2/s) values for the constricted layers 1 to 3 were 1 to 3 orders of magnitude less than bulk rock values.

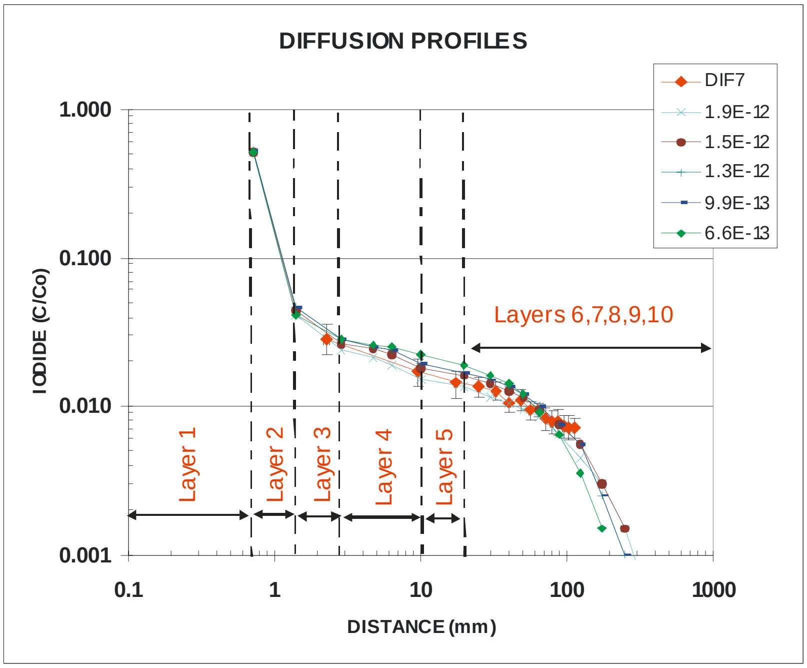

Figure 6: MOTIF Model fits to in-situ data (DIF7) from the 420 m level. The range of bulk rock de (m^2/s) values for curves fitting the data is given in the legend. Vertical dashed lines indicate the locations of MOTIF Model layers.

The hydraulic data from the pulse testing which had been performed before tracer injection were analyzed by the shut-in rising head model of Ramey et al.[11], giving estimated permeability values between 10^{-21} and 10^{-20} m^2. In an attempt to improve the interpretation of the pressure versus time data following the pulse injection, hydraulic data were assessed with the Sandia

National Laboratories well-test analysis code nSIGHTS (n-dimensional Statistical Inverse Graphical Hydraulic Test Simulator)[12]. It was also hoped that the nSIGHTS modelling would provide more insight into the presence of any skin effects in the borehole wall. Analyses of hydraulic tests performed in 4 diffusion holes using nSIGHTS indicated that permeability values did vary as a function of distance from the borehole wall. Initial relative high values decreased to a minimum within 1 to 4 cm of the borehole wall, and then rose slightly to formation values, ranging from 1.4×10^{-20} to 5.7×10^{-20} m^2.

IV. DISCUSSION AND CONCLUSIONS

Results of this study have highlighted factors to consider when planning or assessing the results of a program to define mass transport properties in low permeability SFR. Rock samples removed from high stress conditions are altered as a result of the combination of in-situ stress relaxation and stresses created during drilling [3]. Evidence for the alteration includes a progressive increase in porosity, diffusivity and permeability in laboratory samples removed from increasingly higher stress rock regimes (Table 1). Furthermore, laboratory-estimated permeability values were higher than in-situ permeabilities by a factor of 2 to 100, while laboratory-estimated D_e values for the deeper URL levels were higher than those determined in-situ by a factor as high as 15. It is noteworthy that laboratory and in-situ D_e values determined for the 240-m Level were similar (Figure 7), implying that samples removed from stress regimes less than 30 MPa are subject to only minor alteration.

Table 1: Comparison of laboratory and in-situ estimated mass transport parameters

	240 m Level (31 MPa)	300 m Level (54 MPa)	420 m Level (60 MPa)
Porosity (water immersion)	$(2.43 \pm 0.07) \times 10^{-3}$	$(2.95 \pm 0.07) \times 10^{-3}$	$(2.75 \pm 0.16) \times 10^{-3}$
Porosity (iodide rock capacity)	$(2.1 \pm 0.6) \times 10^{-3}$	$(4.8 \pm 0.8) \times 10^{-3}$	$(7.7 \pm 1.0) \times 10^{-3}$
Porosity (tritium rock capacity)	$(4.8 \pm 1.1) \times 10^{-3}$	$(6.5 \pm 0.8) \times 10^{-3}$	$(7.6 \pm 0.7) \times 10^{-3}$
Lab iodide De (m^2/s)	$(3.4 \pm 0.8) \times 10^{-13}$	$(1.1 \pm 0.2) \times 10^{-12}$	$(1.6 \pm 0.1) \times 10^{-12}$
Lab HPRM permeability (m^2)	8×10^{-20}	4×10^{-19}	1×10^{-18}
Bulk rock in-situ iodide De (m^2/s)	2.8×10^{-13} to 5.0×10^{-13}	7.1×10^{-14} to 2.8×10^{-13}	6.6×10^{-13} to 1.9×10^{-12}
Bulk rock in-situ permeability (m^2)	3.6×10^{-20}	5.7×10^{-20}	5.7×10^{-20}
Minimum in-situ permeability (m^2)	1.1×10^{-20}	3.6×10^{-21}	1.8×10^{-21}

Bulk rock and minimum permeability values estimated by nSIGHTS simulations.

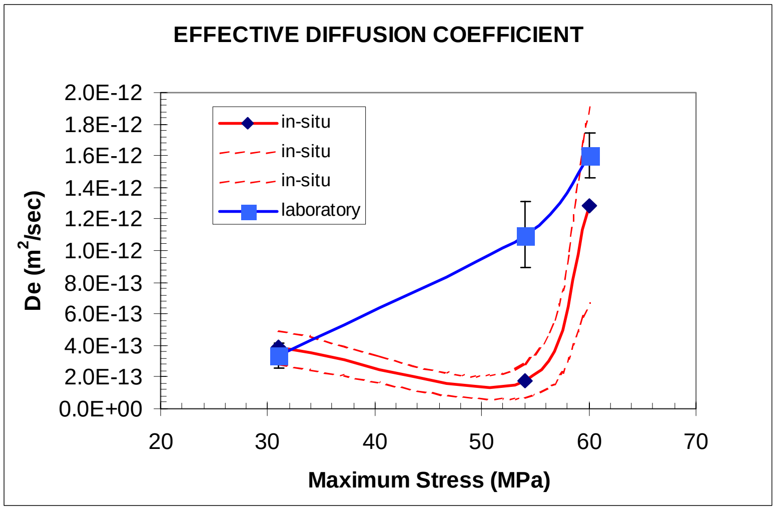

Figure 7: Laboratory and in-situ effective diffusion coefficients versus in-situ stress conditions. Dashed lines represent the range of estimated D_e values.

It is postulated that in-situ experiments in high stress environments can be affected by an interface effect, possibly created by stress redistribution, that increases constrictivity within mm of the borehole wall[1]. In theory, this explanation is consistent with rock mechanics. The results of nSIGHTS modelling indicate that changes in rock properties close to the borehole affect permeability, in addition to diffusivity. Furthermore, it is evident that the interface effect increased with higher in-situ stress, and was not apparent in laboratory experiments performed in the absence of a confining stress.

Laboratory-estimated porosity values determined by water movement in and out of pore spaces are lower than values estimated by tritium diffusion by a factor of 1.5 to 3 (Table 1). This suggests that porosity is sensitive to the method of measurement and that there may be subtle differences in the way diffusion and advection are influenced by porosity. Nevertheless, porosity does have a discernable influence on diffusivity and permeability as evidenced by a positive correlation between laboratory estimated permeability and, iodide and tritium D_e values [1].

It is evident that both rock grain size and degree of alteration exert influence on the derived rock mass diffusivity. In samples from the 240-m Level that have been subject to only minor alteration, D_e values were higher in coarse grained pegmatites compared to fine grained granites by factors of 5 for iodide and 2 for tritium. However, in the more (stress) altered rock samples from the 300-m and 420-m Levels, this trend is reversed with higher D_e values found in the finer grained granites and granodiorites. This suggests that physical rock sample alteration occurred mainly through the change in pore geometry, porosity and or connectivity at mineral grain boundaries.

The presence of alteration minerals on fracture surfaces could influence estimated diffusivities. Diffusion cell experiments using core samples with and without fractures showed that diffusivity across fracture surfaces may be lower than in the rock matrix. The design of experiments to investigate temperature effects on rock mass diffusivity required careful planning. An observed increase in D_e values at 50°C by factors of 2.5 and 3.1 for iodide and tritium, respectively, could be accounted for by the predicted increase in the free-water diffusion coefficient (D_w), as well as, an increase in rock sample porosity. The effects of a confining pressure on rock volume and porosity must be considered when planning experiments at higher temperatures.

In summary, the agreement between laboratory and in-situ estimated D_e values for the 240-m Level, where physical sample alteration was minimal, provides confidence that the methodology described in this paper has improved the understanding of diffusion and mass transport in SFR. It is recognized that laboratory and in-situ experimental results still possess uncertainties primarily associated with sample alteration, scaling, in-situ stress redistribution, and hydrogeology. Additional lines of evidence to help address this uncertainty could be obtained by comparing experimental derived D_e values to those in natural analog systems in which diffusive processes at larger space scales and time periods of geologic significance have operated. With the understanding that laboratory measurements could be affected by sample alteration, laboratory derived D_e values can be used conservatively for predicting diffusive mass transport in SFR. However, the same values may not be conservative in estimating diffusive contaminant mass exchange from fractures into the bounding rock matrix.

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