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Key Points:

- Subsurface Precambrian rock with fractures is not well characterized
- Permeability data was compiled from decades of research by Atomic Energy of Canada Limited
- Permeability-depth relationships for equivalent porous media rock mass and fracture zones were determined

Supporting Information:

Supporting Information may be found in the online version of this article.

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Analysis of Crystalline Rock Permeability Versus Depth in a Canadian Precambrian Rock Setting

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Abstract Over the last 50 years, there has been an increased interest in characterizing Precambrian crystalline rock, such as the Canadian Shield, to investigate the feasibility of deep geologic repositories for isolating used nuclear fuel from the biosphere. Extensive work has been conducted in Canada with a large amount of that work undertaken by Atomic Energy of Canada Limited. Few peer-reviewed journal articles were published based on these data, so a large amount of the data, specifically on fracture zones, are unavailable for modelers and analysts. By collecting and analyzing over one-hundred technical reports, journal articles, and conference proceedings, written between 1975 and 1996, it was possible to characterize plutonic Precambrian crystalline rock and separate the data into (1) equivalent porous media (EPM) for rock mass and (2) fracture zones (FZs). A third category, aggregate media (AM), was used herein to represent the entire data set (EPM + FZs). Using the data from these studies, a novel logistic function was fit to represent the mean permeability, with respect to depth, of crystalline rock for EPMs and FZs in plutons. Understanding rock permeability is critical for the long-term isolation of used nuclear fuel so that accurate predictions of fluid flow and mass transport can be evaluated in the area of the proposed storage location.

1. Introduction

Multiple countries (e.g., Canada, Finland, Sweden, and USA) around the world have undertaken studies regarding the management of used nuclear fuel. In Canada as well as globally, a solution for managing the long-term disposal of used nuclear fuel has been sought for several decades. Canada's management plans include the construction of a Deep Geologic Repository (DGR) to store the used nuclear fuel deep underground in stable rock settings. A DGR, according to Canada and Sweden, is a disposal area located deep underground (500–1,000 meters below the ground surface [mBGS]) in a suitable rock formation where used nuclear fuel could be isolated to minimize its impact on the environment and human health (Dixon & Rosinger, 1981; King et al., 2001; McMurry et al., 2004). The feasibility of the DGR concept for Canada was presented in 1994 by Atomic Energy of Canada Limited (1994) and Davison, Chan, and Brown (1994). In 2005, this was also the recommendation of the Nuclear Waste Management Organization (NWMO) as part of their Adaptive Phased Management (APM) program (NWMO, 2005).

Investigations into crystalline and sedimentary rock settings have been ongoing since the 1970s. Early work was led in Canada by Atomic Energy of Canada Limited (AECL). For over 20 years, AECL conducted detailed field investigations at multiple sites on the Canadian Shield to characterize crystalline rock in an effort to determine if the Canadian Shield would be a suitable location for the construction of a DGR for storing used nuclear fuel. This research was not conducted at locations that were being considered as potential candidate sites for a DGR. Rather, these sites were chosen because all were plutons and were considered representative of the Shield; these sites were for research and information gathering purposes. Between 1973 and 1996, seven research areas (RAs) were operated to investigate hydraulic properties, rock properties, geologic profiles, and to conduct hydraulic and geochemical testing. Aside from characterizing the RAs, extensive research was conducted to develop and validate methods for characterizing crystalline rock.

If a DGR is to be built within the Canadian Shield, a vast amount of data need to be assimilated, understood, and incorporated into the models that aid in the design and safety analysis of a DGR. There is a need to understand both the geological and tectonic history of a potential used nuclear fuel disposal site as well as the movement of groundwater through the host rocks (Kamineni & Stone, 1983; Stone, 1982). Because crystalline rock is commonly fractured, the movement of groundwater (and potential contaminants) through the rock mass and fracture zones is difficult to discern (Stone & Kamineni, 1982). Groundwater flow through a fractured medium is typically controlled by the fracture properties (e.g., location, orientation, aperture size, and continuity; Davison, 1980). Fractures can vary hydraulic properties greatly and attempts to characterize them is an ongoing and important research area (Brown & Kamineni, 1989; Domenico et al., 1995; Frost et al., 1995; Gascoyne et al., 1997; Hillary, 1982a; Hillary et al., 1985; Hillary & Hayles, 1985; Jensen, 2001; Ohta & Chandler, 1997; Peterman et al., 2016; Read, 1990a, 1990b; Stone, 1985; Thompson et al., 2011; Tian, 2016).

For this study, the authors have reviewed the available research from the seven RAs operated by AECL to compile a record of in situ borehole hydraulic testing permeability values with a specific interest in understanding how encountered fractures affect permeability over the entire depth of the areas of interest. Three categories of interest include: the equivalent porous media (EPM) rock mass, fracture zones (FZs), and aggregate media (AM). The EPM rock mass is not only considered intact rock, but also a composite of intact rock, sealed/infilled fractures, and limited hydraulic connectivity fractures (Long et al., 1982). EPM rock mass in this study does not include identified conducting fracture zones. In general, for a fracture to be included in the EPM rock mass, it needs to be infilled/nonconductive or it does not intersect a conductive fracture. Fracture Zones are considered a distinct domain from the EPM rock mass as they are areas of enhanced permeability created by extensive hydraulically connected fractures. The AM uses the complete data set including both the EPM rock mass and FZ data. When using the AM approach, it is not possible to represent fractures with separate physics to improve modeling, as can be done with some models such as FRAC3DVS (Therrien et al., 2001) and Hydrogeosphere (HGS) (Therrien et al., 2010). The end goal is to develop an understanding of permeability with respect to depth in these three categories (EPM, FZs, and AM) and provide a method of calculating reliable mean permeability values for Precambrian rock in the Canadian Shield. This research focuses on permeability as it has a significant influence on fluid flow and mass transport which will impact the movement of contaminants through the geosphere. For example, the geosphere attenuates the migration of radionuclides from a DGR to the biosphere. As permeability decreases, attenuation increases, making a comprehensive understanding of permeability for Precambrian rock in the Canadian Shield essential.

In order to develop permeability versus depth relationships, it is necessary to first understand how permeability varies spatially and how it is affected by the other properties of the rock. Many studies have been conducted to determine general permeability values for both consolidated and unconsolidated geologic materials (Achtziger-Zupančič et al., 2017; Brace, 1980; Gleeson et al., 2011; Huenges et al., 1997; Ingebritsen & Gleeson, 2015; Pepin et al., 2015; Ranjram et al., 2015; W. Sanford, 2017; Zharikov et al., 2014). Several of these studies are interested in horizontal variations or a single permeability value to represent an entire domain. However, it is expected that permeability values will vary in space, both horizontally and vertically (Ingebritsen & Gleeson, 2015; Ranjram et al., 2015; W. Sanford, 2017; Zharikov et al., 2014). Horizontal permeability values can vary by orders-of-magnitude over short distances due to fracture interactions, while mean vertical permeability values are assumed to generally follow a decreasing trend with respect to depth (Achtziger-Zupančič et al., 2017; Brace, 1980; Park et al., 2008; Pepin et al., 2015; Ranjram et al., 2015; Sykes et al., 2009). It has been noted by W. Sanford (2017) that while the decreasing trend in permeability is recognized and has been estimated, it has not been well quantified. In the case of the Precambrian rock of the Canadian Shield, this variation in permeability with depth is likely attributed to the amount of fracturing that is present in the rock with more hydraulically connected fractures near the surface and less connectivity or nonconductive fractures at depth (Park et al., 2008; Ranjram et al., 2015; Sykes et al., 2009). While this is important when looking at the rock mass as a whole, it does not allow for research or models which distinguish between the rock matrix and fracture zones separately. As stated by Tsang et al. (2015), the predominant pathway for fluid flow is through the fracture network. At the scale of our work, discrete fractures and intact rock mass are characterized as an equivalent porous medium, whereas fracture zones are characterized separately. Understanding the physics of these distinct domains and how they interact can improve predictions on fluid flow and mass transport in fractured rock settings.

2. Background

2.1. Atomic Energy of Canada

To understand the importance of AECL's work and its significance to current research, it is necessary to understand what prompted the research and its need in Canada. Canada built its first nuclear reactor in 1944–1945 at Chalk River (Atomic Energy of Canada Limited, 1997). In 1952, Atomic Energy of Canada Limited took over managing and advancing the nuclear reactor program. This led to the development of the heavy water moderated power reactor CANDU (CANadian Deuterium Uranium) (Brooks, 1993) and the construction of reactors in Rolphton (near Chalk River Laboratories), Pinawa (near Whiteshell Laboratories), and Douglas Point (near Lake Huron) (Atomic Energy of Canada Limited, 1997). In the early 1970s, the Pickering Nuclear Power Plant in Ontario came online using the first commercial CANDU reactor and by the end of the 1970s, the Bruce Nuclear Power Plant on Lake Huron was also operational.

Expansion in the nuclear energy programs meant safely storing the used nuclear fuel. While the nuclear plants had dry storage locations on site, these would eventually fill so alternative solutions were needed. It was proposed that the used nuclear fuel could be stored in DGRs, but finding a good site would require a comprehensive (and long-term) research program to both identify an ideal candidate site and prove that the DGR concept was safe (Atomic Energy of Canada Limited, 1997).

Research on the geological and hydrogeological properties of the Canadian Shield began in 1975 and continued through to the 1990s (Dixon & Rosinger, 1981). It was assumed that Ontario would be the main location of nuclear power in Canada so preliminary research into igneous rocks began in 1975 by AECL. Following this, in 1976, geoscience research in Ontario was expanded (Thomas & Dixon, 1989). In 1978, the Canadian Government started the Nuclear Fuel Waste Management Program (NFWMP) and the job of researching and dealing with the long-term disposal of used nuclear fuel became AECL's responsibility (Dixon & Rosinger, 1981; Milnes, 2002; Minister of Energy, Mines and Resources Canada and the Ontario Energy, 1978).

2.2. AECL Research Program

AECL began a broad research program to identify multiple plutonic rock sites that were thought to be representative of plutons in Ontario (Brown et al., 1982b; Gale et al., 1981). They quickly narrowed the number of sites from the 1,365 originally identified to 55. However, most of these sites only had surface studies performed (e.g., airborne surveys, outcrop sampling, lineament mapping) with no drilling or subsurface investigations. Eventually, the initial proposed site list was reduced to fewer than 10 sites, which became Reasearch Areas, thought to be representative of the Canadian Shield plutons, and the main research program began. The plutons, mostly in Ontario, were each located in different structural subprovinces of the Canadian Shield to investigate the suitability of each rock formation (Whitaker et al., 1994). The end goal, however, was not to pick one of these research areas as a disposal site, but to investigate and develop site characterization techniques for subsurface conditions which would make characterizing a potential disposal site more accurate and help confirm the safety of a DGR (Minister of Energy, Mines and Resources Canada and the Ontario Energy Minister, 1981; Thomas & Dixon, 1989; Whitaker et al., 1994).

AECL conducted research using geological surveys, borehole drilling and logging, hydrogeological testing, and the modeling of five research areas on the Canadian Shield (Whitaker et al., 1994). Because fractures are a common feature in Canadian Shield rock settings, assessing the nature of FZs and the long-term stability of the geosphere eventually became an important aspect of this work (Gascoyne et al., 1988). In 1984, construction began on an underground research facility, the Underground Research Laboratory, near Pinawa, Manitoba, to conduct subsurface experiments (Kozak & Davison, 1992; Milnes, 2002). In total, AECL conducted research at seven research areas (Figure 1) but only five of those areas produced reports with quantitative data. Chalk River, East Bull Lake, Atikokan, Whiteshell, and the Underground Research Laboratory (URL) each had significant research programs that were undertaken (Dixon & Rosinger, 1981). The White Lake and Overflow Bay research areas were either operated only briefly or did not become fully operational research areas (Milnes, 2002).

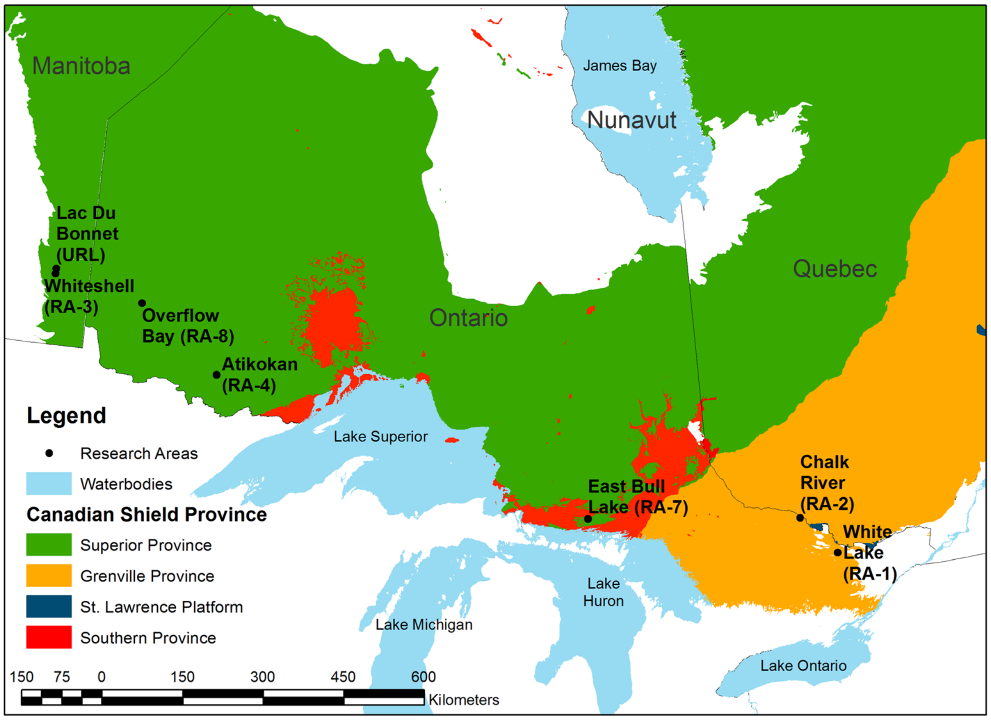

Figure 1. Atomic Energy of Canada Limited Research Areas (RAs) on the Canadian Shield.

Vast amounts of data were collected during the AECL research programs. Surface and geophysical surveys, geological stratigraphy and borehole logs, hydrogeological samples and analysis, and fracture characterization were some of the key studies in the research programs. Most of the reports that encapsulate these data were hard copy prints that now only exist spread out across libraries in Canada. This makes it extremely difficult to assimilate this important information and put it to use. The surveys, logs, samples, and characterizations from these reports are summarized by research areas in the following sections with additional information on each researh areas (and their respective boreholes) available in the supplemental information section.

2.3. AECL Research Areas

All of the RAs chosen by AECL are located on plutons within the Canadian Shield. These areas were chosen, in part, due to their geological stability (Atomic Energy of Canada Limited, 1994; Brown et al., 1982c; Dixon & Rosinger, 1981; Katsube & Kamineni, 1983; Rummery & Rosinger, 1983; Thomas & Dixon, 1989). The entire Canadian Shield has not had any major orogenic activity in the last 600 million years with some parts of the Shield having no activity for two billion years (Davison et al., 1994). In Ontario, the Superior province is to the west and the Grenville province is to the east with part of the Southern province between the two. The Canadian Shield ranges in age from 0.99 to 3.6 billion years (Percival & Easton, 2007). The Superior province is older than the Grenville province and has been inactive longer. Figure 1 shows the location of the AECL research areas. Whiteshell, the URL, Overflow Bay, and Atikokan are located in the Superior province of the Canadian Shield. East Bull Lake is on the border of the Superior and Southern province. Chalk River and White Lake are in the Grenville province.

2.3.1. Chalk River

The Chalk River Research Area (RA-2) and Chalk River Laboratories are located in Chalk River, Ontario (~180 km northwest of Ottawa, Ontario). It is located in the Grenville province with rocks ranging in age from 0.99 to 2.69 Ga (Percival & Easton, 2007). The RA is located on folded quartz monzonitic orthogneisses and paragneisses (Brown et al., 1982c; Stone, 1984). The RA began used nuclear fuel disposal related research in 1977 and was continued off and on over multiple periods by different groups; AECL (1977–1983), the Siting Task Force (1992–1995), and Chalk River Laboratories (2006-present) (Peterman et al., 2016; Thompson et al., 2011; Whitaker et al., 1994).

When research started in 1977, the focus was on developing and testing methods to characterize plutonic rock, both physically and chemically (Stone, 1984). Specifically, they were interested in assessing crystalline rock characteristics at small scales in boreholes (Stone, 1984). As research progressed, the scale of interest expanded to regional levels with depths up to 1 km (Brown et al., 1982a). Four main projects were conducted: (1) to characterize and validate a model of groundwater flow; (2) a radioactive tracer experiment to trace flow between two boreholes at a depth of 100 mBGS; (3) development of groundwater sampling and in situ monitoring in a borehole; and (4) examining groundwater discharge to Precambrian Shield lakes to understand the effects of these lakes on groundwater movement (Pearson & Davison, 1985).

2.3.2. East Bull Lake

The East Bull Lake Research Area (RA-7) was located ~25 km north of Massey, Ontario in the Algoma District (Bottomley et al., 1986; McCrank et al., 1985). It was located in the Superior province near the Southern province (Pearson, 1984). The rock ranges in age from 2.6 to 3.6 Ga (Percival & Easton, 2007). The East Bull Lake pluton is 23 km^2 and is composed of gabbro-anorthosite (Brown & Kamineni, 1989; Ermanovics et al., 1982). Research began at this site in 1980 and was conducted until 1992 (Whitaker et al., 1994). The research at this site was focused on mapping the shape of the pluton, the distribution of rock types, and the characteristics of faults and fractures (McCrank et al., 1985). Later on, the research was expanded to study the hydrogeological characteristics, hydrogeochemical characteristics, and the evolutionary processes of groundwater (Bottomley et al., 1986). During the 1980s, 4 deep boreholes (EBL-series) and 14 shallow boreholes (P-series) were drilled. Cores for the four deep boreholes were recovered (Bottomley et al., 1990; Ermanovics et al., 1984). Hydrogeological sampling, via production injection packers (PIPS), was performed in the 14 shallow boreholes and in three of the four deep cored boreholes (Bottomley et al., 1986). On-going monitoring continued until closure of the site in 1992 (Bottomley et al., 1986).

2.3.3. Atikokan

The Atikokan Research Area (RA-4) was located 15 km north of Atikokan, Ontario in Northwestern Ontario (Brown et al., 1980). It was located in the Superior province with the age of the pluton estimated at 2.65 Ga (Pearson, 1984). The pluton in this area, named the Eye-Dashwa Lakes pluton, is composed of biotite-hornblende granite (Whitaker et al., 1994). It intrudes into a tonalitic to granitic to amphibolitic gneiss (Dugal et al., 1981). Research began here in 1979 with surface based studies (Dugal et al., 1981; Stone, 1984). The goal of the research at Atikokan was to characterize a large crystalline rock area to a depth of 1 km in order to determine groundwater flow patterns (Pearson & Davison, 1985). In the 1980s, multiple boreholes were drilled and cores for eight deep boreholes were recovered (Gibb et al., 1988; Stone, 1984). Studies into regional scale groundwater flow modeling began in 1984 (Whitaker et al., 1994). Hydrogeological monitoring continued here until 1985 (Soonawala et al., 1987; Whitaker et al., 1994).

2.3.4. Whiteshell

The Whiteshell Research Area (RA-3) was located in eastern Manitoba near Pinawa (~100 km northeast of Winnipeg, Manitoba) (Katsube & Hume, 1987b). This RA was located in the Superior province on the Lac du Bonnet Batholith, a large granite pluton (Percival & Easton, 2007; Whitaker et al., 1994). The batholith is estimated to be between 2.6 and 3.6 Ga (Percival & Easton, 2007). This RA was opened in 1977 (at the same time as the Chalk River Research Area) with extensive research undertaken, during the 1980s, on site characterization, hydrogeological modeling, and geophysical modeling (Stone, 1984). The research steps undertaken were similar to those conducted at Chalk River with a focus on developing and testing physical and chemical characterization methods of plutonic rock at small scales with an expansion to regional scales over time (Stone, 1984). Studies on regional scale groundwater flow modeling began in 1984 (Stevenson et al., 1996). Hydrogeologic measurements were conducted using single- and straddle-packer equipment (Davison, 1980).

2.3.5. Underground Research Laboratory

The Underground Research Laboratory (URL) was a large underground complex located near the Whiteshell Research Area (Stone, 1984). The URL was considered part of the overall Whiteshell RA however because of the extensive and unique work conducted at the URL, both at the surface and within the subsurface facility, it was often referenced as a separate location and will be discussed as such herein. The URL was the largest research project that AECL managed with major experiments to: (1) investigate structural and groundwater flow models; (2) model site characteristics; (3) run migration experiments; and (4) develop new research technologies (Read, 1990a; Stone, 1984). Work at the URL was broken into multiple stages. In the early 1980s, preliminary studies (Stage 1) were conducted including airborne and geological surveys as well as shallow boreholes (Ohta & Chandler, 1997; Whitaker et al., 1994). Following this, five deep boreholes were drilled (Stage 2). The cores of these five boreholes were logged and the holes were used for geophysical research and hydrogeological sampling/testing (Guvanasen et al., 1985; Ohta & Chandler, 1997). A further eight boreholes and 30 percussion holes were drilled at this site prior to the construction of the URL (Stage 3) (Guvanasen et al., 1985; Ohta & Chandler, 1997). Construction of the URL began in 1984 and was completed in 1990. The URL main shaft was 443 m deep with major experiment levels at 240 mBGS and 420 mBGS (smaller levels were placed at 130 mBGS and 300 mBGS) (Ohta & Chandler, 1997). Ten permit sites (A–J) located off-site, but associated with the URL Research Area, were chosen and four of them (A, B, D, and G) were drilled, tested, and sampled (Gascoyne, 2000). Permit area G, located 5.5 km east of the main URL site, has the most comprehensive data record of the permit sites (Ejeckam et al., 1988a). Over 130 boreholes were eventually drilled, at the URL, that ranged in-depth from 160 to 1,090 m (Ohta & Chandler, 1997).

2.3.6. Other Areas

White Lake (RA-1) was located 65 km west of Ottawa, Ontario in the Grenville Province and sat on a biotite-granite pluton in a gneissic metamorphic terrain (Dugal et al., 1979; Gale et al., 1981). Aeromagnetic surveys began in 1975 and were followed by shallow boreholes and borehole television surveys in 1976 (Dugal et al., 1979). The White Lake Research area was only operational for this period before it was shut down (Dugal et al., 1979).

Overflow Bay (RA-8) was selected in 1981 for preliminary surveys but never became an operational research area (Pearson, 1982b). It was 30 km south of Dryden, Ontario in the Superior Province. The RA was a massive, fine to medium grained hornblende gabbro with a large fault at the south end (Pearson, 1982b).

3. Methods

3.1. Data Compilation

To create an accurate and realistic characterization of Canadian Shield hydrogeologic properties, specifically permeability in EPM rock mass and FZs, a significant amount of data describing subsurface conditions were required. As was described in the previous section, these data exist but are spread out in a multitude of reports written by AECL based on their research studies. Achtziger-Zupančič et al. (2017) compiled some of these data, plus more research data from many other countries, to create a global permeability database with almost 30,000 data points. A total of 549 permeability records (that had no fracture information) for the AECL Research Areas were extracted from their global permeability database. Using this as a starting point, the authors of this study used the Canadian data and then supplemented them with additional AECL data to build a more detailed and comprehensive understanding of Precambrian rock (Canadian Shield) permeability including fracture zones. Through AECL reports, some of which are mentioned in the previous sections, additional information was added to the database. Many boreholes, that were not in the original Achtziger-Zupančič et al. (2017) database, were added to broaden its coverage and additional supporting information was added to the existing data points. New details on fracture characteristics and properties (e.g., degree of fracturing, fracture status (open, closed), fracture location) were added to all records.

In some studies, hydraulic conductivity values were determined so it was necessary to have density and dynamic viscosity in order to convert these values to permeability. However, not all AECL data sets compiled were complete. Usually, the missing data consisted of temperature, density, and dynamic viscosity. While this information does not affect the permeability data or fracture properties reported, it was essential for accurately converting permeability values to hydraulic conductivity values (and vice versa). Because density and viscosity are temperature dependent, each AECL RA was analyzed to investigate the temperature trends in the available data. The temperature gradients at Atikokan, Chalk River, East Bull Lake, the

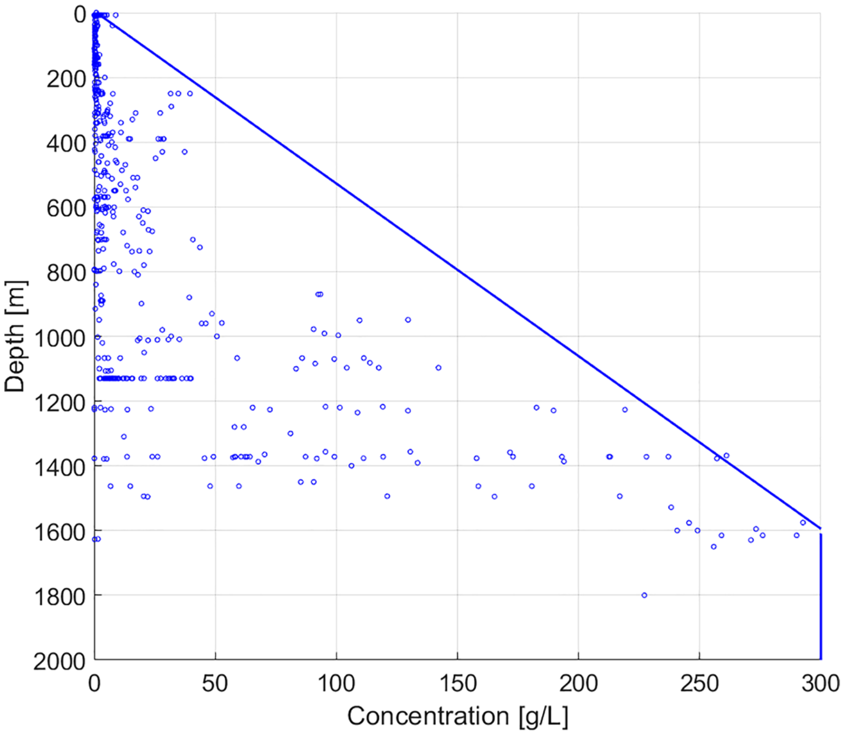

Figure 2. Plot of total dissolved solids versus depth with upper bound line.

URL, and Whiteshell were determined to be 11.24, 10.55, 25.07, 9.9, and 10.09°C/km, respectively (Atomic Energy Control Board, 1986b; Davison, 1980; Davison et al., 1994, Davison et al., 1984; Dugal et al., 1979; Ejeckam et al., 1988; Gascoyne, 2000; Hillary, 1982a; Hillary & Hayles, 1985; Kamineni & Katsube, 1982; Latham, 1987; Ophori et al., 1996; Paillet & Hess, 1986; Pearson, 1982a; Raven, 1986; Raven et al., 1985; Stone, 1984; Thomas & Dixon, 1989; Tian, 2016; Whitaker et al., 1994). This allowed depth-specific missing temperature data to be inferred, at each RA, based on the temperature trend at that RA. This linear extrapolation, while simple, is accurate in regions of low permeability.

Once the missing temperature data were resolved, it was necessary to determine density and dynamic viscosity at each RA. This part was more difficult because density and viscosity are also dependent on temperature and salinity. It was known that the Canadian Shield has high levels of salinity at depth. Bulk geochemistry data were collected for sites on the Canadian Shield. Using total dissolved solids (TDS) data from Frape et al. (1984); Frape et al. (1985); Frape and Fritz (1987); Gascoyne et al. (1987); Bottomley et al. (1994); Douglas et al. (2000); Gascoyne (2000); Bottomley et al. (2003); Gascoyne (2004); Stotler et al. (2009); Peterman et al. (2016); Tian (2016), a general understanding of the maximum TDS versus depth in the Canadian Shield was determined (Figure 2). It can be seen that the TDS concentration increases with depth. Figure 2 shows a linear trend based on 516 data points from AECL and mine field data to a depth of 1,600 mBGS and is constant at 300 g/L below that. Then, it was possible to use the methods described by Batzle and Wang (1992) to calculate the density and viscosity at any depth based on temperature, pressure, and TDS. Pressure is considered static pressure as determined by Hubbert (1940) and is based on fluid density. Note that fluid density is approximately linearly related to TDS. Batzle and Wang (1992) used the following equations to calculate the density (and viscosity (η) [cP]) of water (ρ_w) [g/cm^3] and brines (ρ_b) [g/cm^3] using temperature (T) [°C], pressure (P) [MPa], and salinity (S) [mass fraction].

$$\rho_w = 1 + 1 \times 10^{-6}(-80T - 3.3T^2 + 0.00175T^3 + 489P - 2TP + 0.016T^2P - 1.3 \times 10^{-5}T^3P - 0.333P^2 - 0.002TP^2) \quad (1)$$

$$\rho_b = \rho_w + S\{0.668 + 0.44S + 1\times10^{-6}[300P - 2400PS + T\left(80 + 3T - 3300S - 13P + 47PS\right)]\} \quad (2)$$

$$\eta = 0.1 + 0.333S + \left(1.65 + 91.9S^3\right) exp\left\{-\left[0.42\left(S^{0.8} - 0.17\right)^2 + 0.045\right]T^{0.8}\right\} \quad (3)$$

A program was written to calculate fluid density and viscosity at regular depth intervals (e.g., 10 m). Finally, by using the temperature, TDS, dynamic viscosity, and density values, it was possible to convert hydraulic conductivities to permeabilities (and vice versa) with a high degree of confidence. Some uncertainty may exist through the extrapolation of temperature values but they should be minimal given the amount of data that exists to support the temperature trends.

3.2. Data Categories

Using AECL borehole records that were collected using television and acoustic televiewer borehole logging, fractures and fault zones that were identified as open and hydraulically connected were categorized as fracture zones. The remaining data were considered part of the equivalent porous medium (EPM) rock mass. As stated previously, the EPM rock mass consists of the intact rock and discrete fractures that are considered either closed, not hydraulically connected, or of small scale. It was assumed that the finite nonconductive fractures affect the hydrological properties of the EPM rock mass to some degree. In the few cases where no borehole log or report explicitly stated that an open flowing fracture was observed at a specific depth in a borehole, but the permeability value at that depth strongly implied that it should be classified as a flowing conductive fracture (i.e., higher permeability than found at shallower depth), the data point was labeled with reduced confidence. This allowed for filtering based on a confidence rating if desired or warranted. The confidence label is not critical to this work and was not used to remove values from the data sets, but may be a useful metric at a later date. The final category for the data was AM, which used all the data from both the EPM rock mass data set and FZ data set assuming an EPM approach.

3.3. Data Analysis

Separating the data into meaningful and insightful groups continued by first looking for trends based on rock type and geographical location. Permeability versus depth plots for both EPM rock mass and FZs were produced. In previous studies, it has been found that power law functions were appropriate to represent many hydrological processes (Cardenas, 2008; Harman et al., 2009; Rupp & Selker, 2005; Selker et al., 1999; Snowdon & Craig, 2015) so a power law function (Equation 4) was used.

$$\log_{10}(k) = a \times d^b \quad (4)$$

where k is permeability [m^2], d is depth [m], a is a fitting parameter, and b is a fitting parameter.

Prior work conducted by Manning and Ingebritsen (1999), Ingebritsen and Manning (2010), and Achtziger-Zupančič et al. (2017) used a logarithmic function to fit permeability data versus depth. Their function (Equation 5) has its shape defined by two fitting parameters. Part of the analysis in this study involves assessing this function to see how it fits the AECL data for the Canadian Shield.

$$\log_{10}(k) = a \times \log(d) + b \quad (5)$$

where k is permeability [m^2], d is depth [m], a is a fitting parameter, and b is a fitting parameter.

Following this, an in-depth analysis was conducted to determine better curves, using permeability measurements and their associated test depth ranges, that could define how permeabilities changed with respect to depth. For example, if a packer test was conducted over a 20 m borehole length, the measured permeability value was considered to be uniform over that entire length and not a point measurement. This increased the information coverage along the borehole and prevented assumptions about the position of the measurement during the packer test.

To determine what function could better describe the permeability versus depth relationship, a new approach was defined. A 200 m moving average window method was used starting at the surface and moving down through the media in 10 m intervals. During this, the data for the EPM rock mass and FZs were statistically analyzed to identify and remove extreme outliers using the Interquartile Method (Barbato et al., 2011; Tukey, 1977). This method involved determining the interquartile range (IQR), the distance between the 1st and 3rd quartile of the data for a specific depth interval, and then classifying any values, that were either below the 1st or above the 3rd quartile by 3 times the IQR, as extreme outliers. Only extreme outliers were excluded during the analysis. This was done to remove values that were statistically not following the trend of the data. The result of this is that a single outlying value does not dramatically skew the data trend.

After excluding the outliers, the remaining data points were used to find generalized relationships between permeability and depth for the EPM rock mass, FZs, and AM. The mean of the $\log_{10}$-transformed permeability values is determined for each moving window within half the window length above and below the target depth (e.g., 100 m above and 100 m below). A 200 m window was chosen because it produced a mean curve with a good balance between too little and too much smoothing. When the moving window was reduced to 50 or 100 m, the mean curve was noisy and when the moving window was expanded to 500 m, the mean curve did not fit the data well. A comparison of different window lengths for the moving averages is available online in the supplementary information for this study. Any permeability measurement depth range that overlapped the window was included in the mean calculation. The calculated $\log_{10}$ mean permeability versus depth was plotted and showed a distinct S-curve trend that could be fit by a logistic growth curve (Levenbach, 1973; Nelder, 1961; Oliver, 1969; Turner et al., 1969). Modifying the logistic growth curve to a five-parameter logistic equation (Equation 6) yielded a new relationship for mean permeability versus depth in the EPM rock mass, the FZs, and the AM in Precambrian rock settings.

$$\log_{10}(k) = \beta + \frac{\alpha - \beta}{\left(1 + \left[\frac{d}{\gamma}\right]^{\delta}\right)^{\epsilon}} \tag{6}$$

where α is the $\log_{10}$ mean permeability at the surface $[\mathrm{m}^2]$, β is the $\log_{10}$ mean permeability at infinite depth $[\mathrm{m}^2]$, γ is the depth where the curve inflects between α and β [m], δ is rate of permeability decrease, ϵ shifts the symmetry of the curve laterally, d is depth [m], and k is permeability $[\mathrm{m}^2]$.

Once the five-parameter logistic curve was determined, an evaluation of the function and its parameters was undertaken to check its statistical significance. First, the p-values for each parameter and the overall function were calculated. Given that p-values are generally only useful for indicating whether or not a parameter is significant, but not to what degree, a sensitivity analysis was used to determine the importance of the independent variables for the five-parameter logistic function for the EPM and FZ mean permeability fitting functions. Given the logistic function in Equation 6, a normalized sensitivity (S_k) can be calculated for each fitting parameter (ω). It was assumed that $k' = \log_{10}(k)$ in the sensitivity analysis. The normalized sensitivity allows for a relative comparison of the importance of each fitting parameter as the scale of the parameter is taken into account (McCuen, 1974). The normalized sensitivity is computed as the product of the derivative of the function with respect to the parameter and the ratio of the parameter to the function value (Equation 7). Equations for the derivatives of each parameter can be found in the supplemental information section.

$$S_k(\omega) = \frac{\partial k'}{\partial \omega}\frac{\omega}{k'} \tag{7}$$

4. Results and Discussion

Assessing the raw permeability data, for EPM rock mass and FZs, shows a clear decreasing trend of permeability with depth (Figure 3). The available permeability data appears to have a lower limit at $10^{-21}[\mathrm{m}^2]$ for the EPM rock mass and at $10^{-19}[\mathrm{m}^2]$ for FZs. This lower limit appears to be in line with the findings of INTERA Environmental Consultants, Inc. (1983). It is not clear from the data if the EPM rock mass

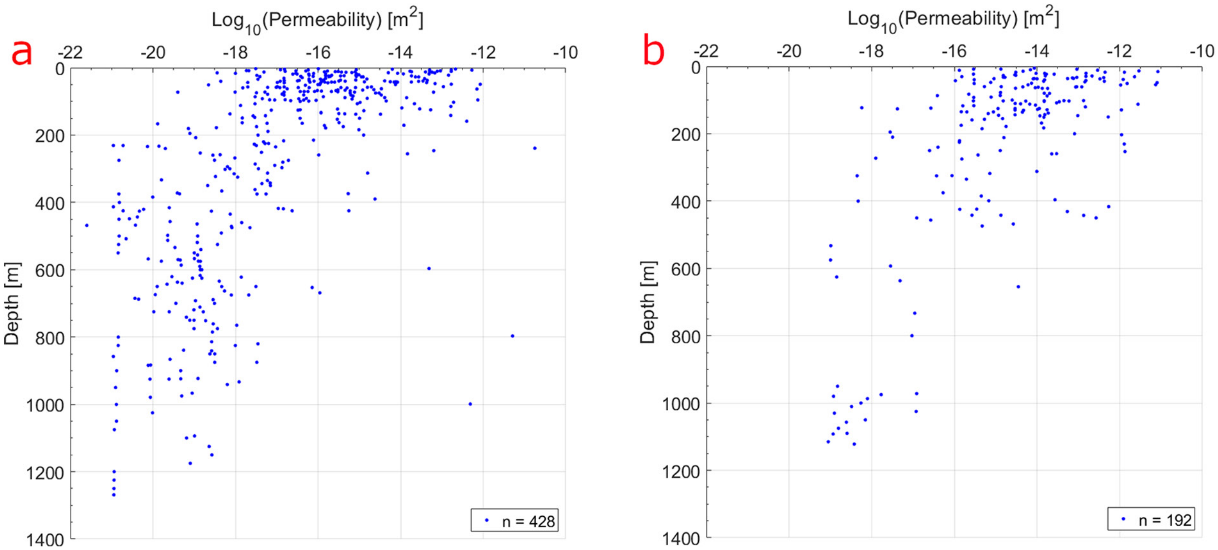

Figure 3. Permeability versus Depth for (a) EPM rock mass and (b) FZs in the Canadian Shield from AECL RAs. EPM, equivalent porous media.

permeability lower limit is a property of the media or a limitation of the measurement equipment. Manfredini (1983) commented that values of 10^{-21}[m^2] were at the extreme low end of the field testing equipment used which may imply that rock permeability is lower than testing could determine. An upper limit on the permeability data for both the EPM rock mass and FZs appears to be 10^{-12}[m^2] and 10^{-11}[m^2] respectively. This upper limit is usually in shallow measurements (<200 mBGS). From Figure 3, it can be seen that there are substantially more data in the top 200 m than there are below and that some of the plotted EPM rock mass data points look like they should belong to the FZ data set (i.e., data points that are distinctly apart from the main cloud of data). These points were not explicitly referenced in an AECL report as fracture zones, so they may have been incorrectly classified (by AECL) or they may simply be outliers. This could also be the case for some near-surface values where the EPM rock mass permeability values are higher than FZ permeabilities or it could be because the EPM rock mass is being influenced by nearby fractures that are not captured in the EPM rock mass data. No data were excluded from these analyses based on the raw data, the major rock types, or locations.

A comprehensive understanding of the rock types in the Canadian Shield and the RAs previously studied could improve characterization of crystalline rock sites. To better understand these, the data were parsed according to major rock type and by location. Figure 4 shows the EPM rock mass and FZ data separated by the three primary rock types that comprise the plutons at the AECL Research Areas; granite, gneiss, and gabbro. It is clear in the plots that the majority of the gneiss measurements are in the upper 200 m, there are more granitic measurements than the other two rock types combined, and the granitic rock measurements are the only ones that were taken at depths below 800 mBGS. Few gabbroic measurements were taken in general. The EPM rock mass data, regardless of rock type, appear to follow the expected trend of decreasing permeability with increasing depth. This is best shown by the granitic measurements because there are data from the surface to below 1,200 mBGS. The same pattern is apparent in the gneiss and gabbroic rock but the pattern is truncated by the limited number of measurements at depth. The gneissic rock trend, due to the sparsity of the data, may appear to be constant, but is decreasing with depth even though there is not enough data to only use the gneissic rock measurements to do an analysis beyond the shallow subsurface. Fitting a simple power law relationship through the following sets: (1) all the data, (2) just the gneiss and granitic data, and through (3) only the granitic data shows how permeability changes with depth by rock type groupings (Figures 4a and 4b). These categories were chosen due to the abundance of data. When the first two sets are evaluated for trends, it can be seen that permeability decreases faster at depths above 400 mBGS than the third set that is just the granitic data and that permeability decreases at a slower rate below 400 mBGS than the third set that is just the granitic data. It should be noted that the power law curves for cases (1) and (2) are coincident. Removing the gabbroic data has minimal impact on the trend which is

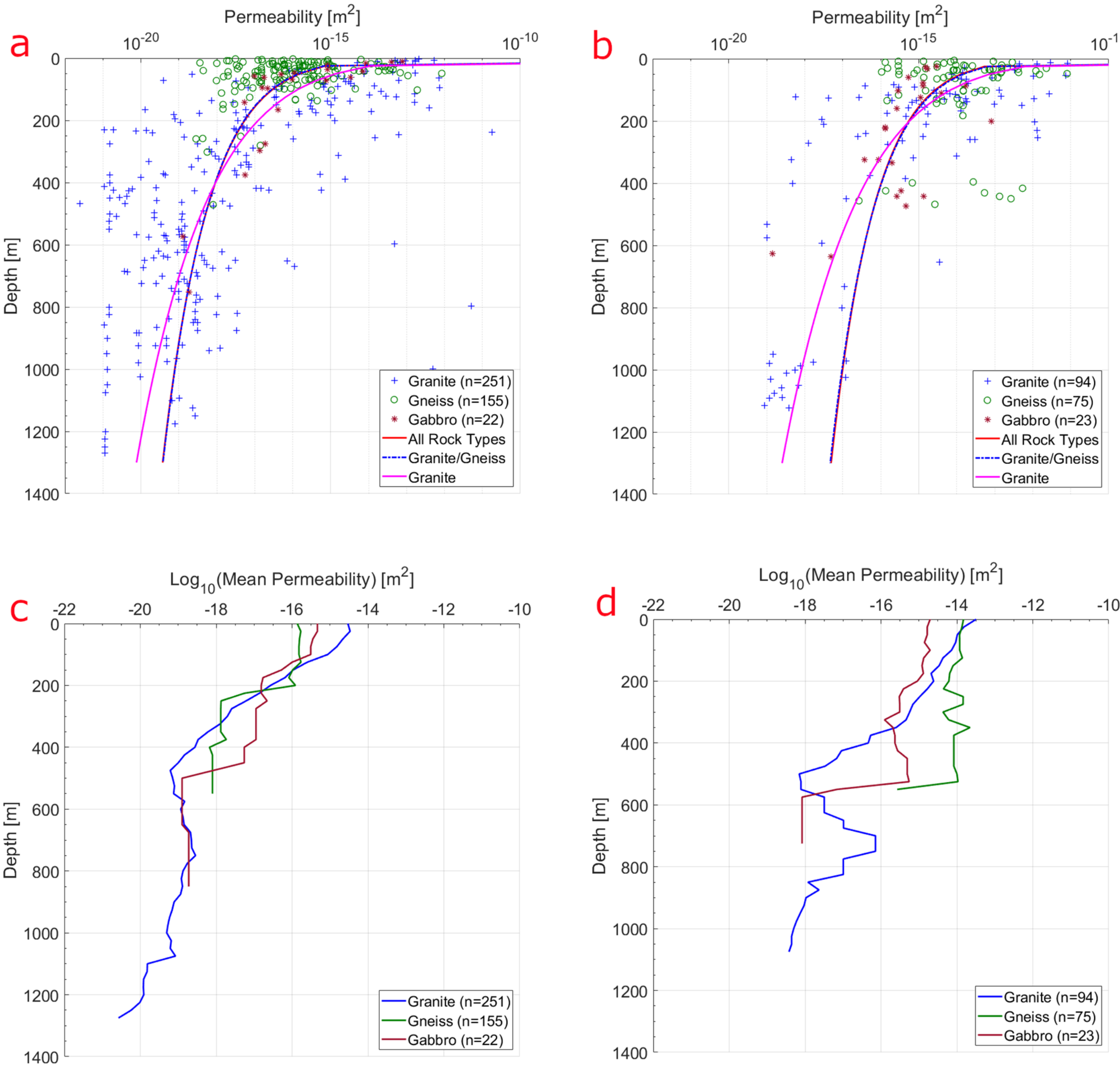

Figure 4. Permeability versus Depth for (a) EPM rock mass and (b) FZ; and Mean Permeability (200 m Moving Average) versus Depth for (c) EPM rock mass and (d) FZ for each rock type in the Canadian Shield from AECL RAs. Note that in (a and b), the curves for "All Rock Types" and "Granite/Gneiss" are coincident. EPM, equivalent porous media; FZ, fracture zones.

likely due to the gabbroic data comprising only 6.3% of the total data set. This implies that the abundance of near-surface measurements in gneiss rock is skewing the trend and may or may not be representative of deep rock conditions. Without additional gneiss data at greater depths, it is not known if conditions are being properly represented.

Another analysis of the data was undertaken to look at each AECL Research Area. The data were parsed by RA and plotted in Figure 5. First, the only RAs with deep measurements are granitic rock locations, Atikokan and the URL. Second, East Bull Lake is composed of gabbroic rock, and third, Chalk River and Whiteshell are composed of gneiss rock for the zones investigated. This information is merely a comparison between Figures 4 and 5 with no quantitative analysis. It is interesting that the previously mentioned data points, that could be outliers, are all from the same research area, the URL. With the exception of Chalk River, which is predominantly shallow measurements, each RA appears to have the same decreasing permeability trend with depth that was seen in the raw data (Figure 3) and in the rock type (Figure 4) analysis.

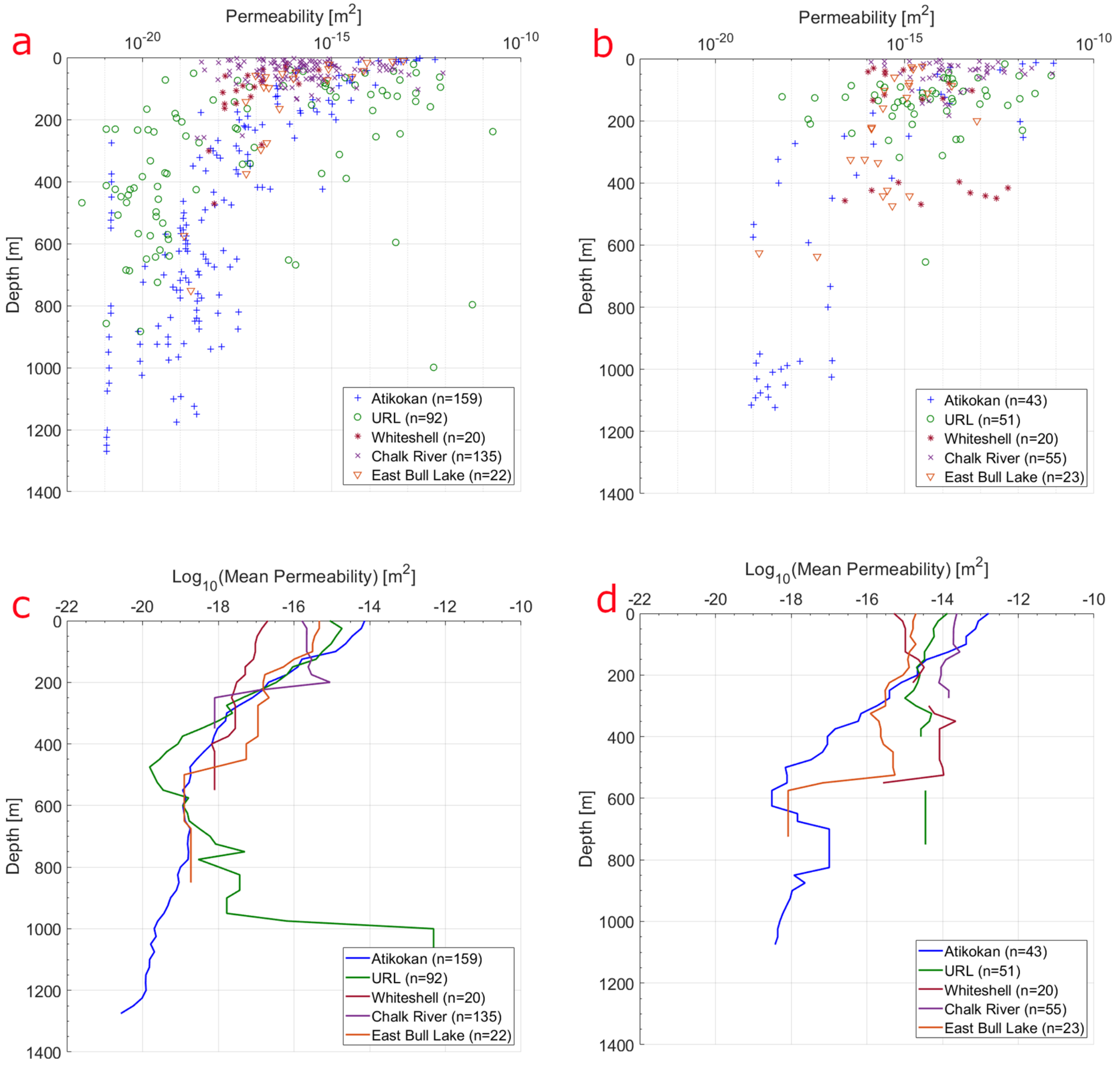

Figure 5. Permeability versus depth for (a) EPM rock mass and (b) FZ; and Mean Permeability (200 m Moving Average) versus Depth for (c) EPM rock mass and (d) FZ for each AECL RA on the Canadian Shield. EPM, equivalent porous media; FZ, fracture zones.

Because each RA appears to follow the same decreasing permeability trend with depth, there was confidence that it was possible to find generalized rules to define how mean permeability varies with depth in crystalline rocks for both EPM rock mass and fracture zones. This can be clearly seen in Figure 5c between 0 and 1,000 m. In this figure, at depths greater than 1,000 mBGS, there is an increase in permeability that arises from data that are classified as "less certain" because the permeability values are in the range of the fracture zone permeability, but no reports explicitly identified a fracture zone at these depths. This does not demonstrate that they are not fracture zones, just that they can not be confidently identified as such. Due to the limited data at some depths, the 200 m moving average lines are discontinuous (Figure 5d).

As mentioned in the rock type analysis, it was found that the use of a power law relationship results in a severe mismatch at shallow depths (Figures 4a and 4b). Following the basic analysis of the data characteristics based on rock type and location for each of the three data categories, the data were fit using the logarithmic function (Equation 5) previously mentioned. This fit shows a decreasing trend for the permeability versus

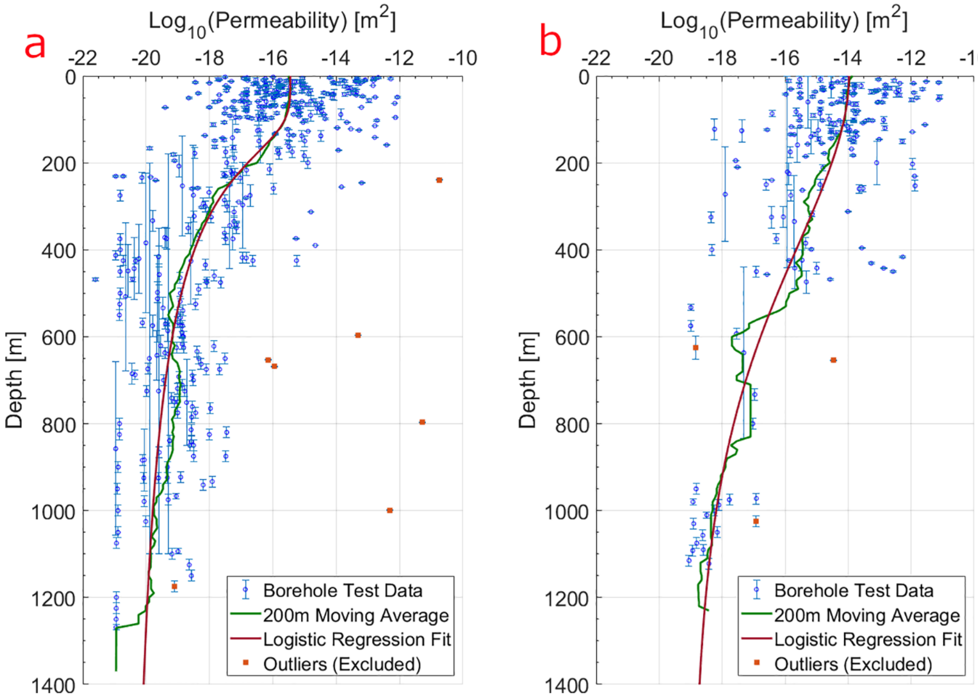

Figure 6. Ranged permeability measurements, extreme outliers, 200 m sliding window mean Permeability versus Depth, and fitted relationship for (a) EPM rock mass and (b) fracture zones in the Canadian Shield from AECL RAs. EPM, equivalent porous media.

depth relationship similar to a power law relationship. However, like the power law function, the logarithmic function is not capable of representing permeabilities at shallow depths appropriately. At shallow depths, these functions approach the surface as an asymptote which leads to either infinitely high permeability at the surface or the need to shift the function which alters the curve to not fit the data well overall. It was thought that another function could be introduced which would result in a more representative permeability versus depth relationship for Canadian Shield settings.

In order to calculate this general relationship to define permeability versus depth in Canadian Shield settings appropriately, the data for EPM rock mass and FZs were first statistically analyzed for outliers. It was found that seven extreme outliers, based on the IQR method, existed in the EPM rock mass data set and three in the FZ data set. These data points were excluded from further analysis. Using a 200 m moving average window, the mean permeability in 10 m intervals was calculated (Figure 6). The permeability values from in situ hydraulic testing with their test depth ranges, the 200 m moving average, and a smooth fitted five-parameter logistics function (Equation 6 and Table 1) are shown on this plot. Excluded extreme outliers are also marked. The permeability lower limits, discussed previously, were used during calibration of the logistic function fits.

Table 1
Curve Fitting Parameters and Confidence for Permeability Versus Depth Relationships

Category	α	β	γ	δ	ϵ	R^2	RMSE
EPM	−15.45	−21	151.4	4.2	0.1919	0.9465	0.345
AM	−14.95	−21	205	3.16	0.279	0.9424	0.397
FZ	−13.97	−19	1,200	1.878	3.397	0.9631	0.302

Abbreviations: AM, aggregate media; EPM, equivalent porous media; FZ, fracture zones. RMSE, root mean squared error.

The use of the five-parameter logistic function (Equation 6) minimizes errors at the tails of the curves and has the same general shape as the moving average. The logistic function also adequately matches the trend visible in the data allowing for maximum and minimum mean permeability values to be approached from surface to depth. The 5-parameter logistic function, as mentioned previously, uses the mean permeability at the surface as an upper bound and the mean permeability at an infinite depth as a lower bound. The remaining fitting parameters are defined by the path between the surface and depth. γ denotes the inflection point of the curve, while δ controls the slope or speed of descent, and ϵ shifts the symmetry of the curve laterally to adjust for a nonsymmetrical shape. While it may be fairly straightforward to determine the maximum and

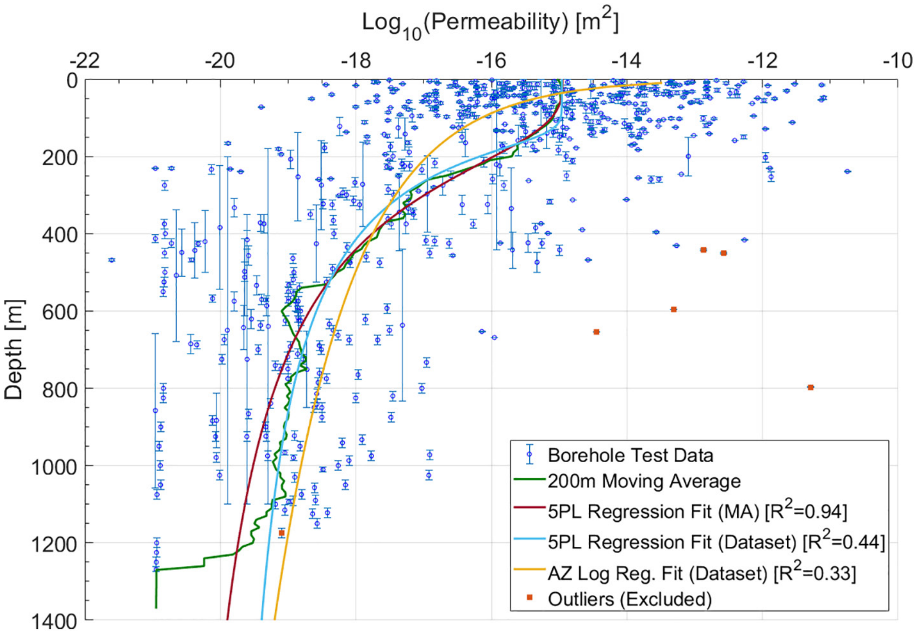

Figure 7. Permeability versus depth for the AM data set along with the moving average. Data are fit to a 200 m moving average with the five-parameter logistic function and to the entire data set with both the five-parameter logistic function (Equation 6) and the logarithmic function (Equation 5). AM, aggregate media.

minimum permeability, the remaining parameters are more difficult to determine without fitting. γ can vary widely based on the rate of descent to the minimum which is determined in part by δ. Currently, this function must be fit to data to determine the curve, however it may be possible to predict permeability at any depth given the maximum and minimum mean permeability along with a thorough understanding of how quickly permeability approaches the minimum.

A comparison of the fits for the AM using Equations 5 and 6 can be seen in Figure 7. Curve fitting is done to the moving average and to the entire data set. As can be seen, the five-parameter logistic function yields a higher R^2 value (0.94 using the moving average, 0.44 using the data points) than Equation 5 (0.33 using the data points). The R^2 values and root mean squared error (RMSE) values can be found in Table 1. An analysis of the fit is provided for each fitting parameter and the overall fit in Table 2. Each parameter and the overall fit is considered significant ($p < 0.05$). The normalized sensitivities (Equation 7) for the EPM rock mass and FZ, plotted as a function of depth, are shown in Figures 8a and 8b, respectively. The normalized sensitivity represents the percentage change in the $\log_{10}$ mean permeability value due to a 1% change in a fitting parameter. As shown in the figures, the normalized sensitivity for a given fitting parameter varies with depth. This is expected as, for example, α specifies the upper limit and β specifies the lower limit of the logistic function. As such, α is the dominant parameter for the portion of the logistic curve at shallow depths in the EPM and FZ normalized sensitivity plots, with $S_k(\alpha) = 1$ and all other parameters $S_k(\beta, \gamma, \delta, \epsilon) = 0$ for $d = 0$. The greater the depth (d), the more dominant (β) becomes as $S_k \rightarrow 1$. At intermediate depths, where the logistic curve transitions between the upper and lower bounds, parameters such as γ, δ, and ϵ become more

Table 2
P-Values for 5-Parameter Logistic Function Parameters for Mean Permeability Versus Depth Relationships

Category	α	β	γ	δ	ϵ	Fit
EPM	1.56e-146	4.98e-28	2.4e-34	0.027	0.038	7.01e-232
AM	9.86e-128	0.040	3.08e-11	2.15e-05	0.002	1.9e-222
FZ	1.44e-144	1.53e-09	1.07e-127	7.51e-45	0.027	1.12e-211

Abbreviations: AM, aggregate media; EPM, equivalent porous media; FZ, fracture zones.

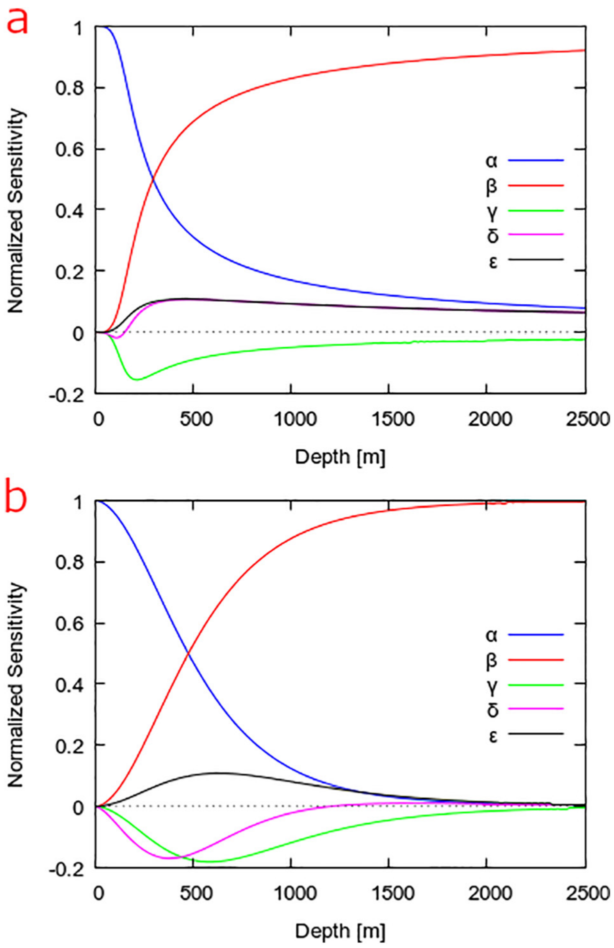

Figure 8. Normalized sensitivity of logistic function for (a) EPM and (b) FZ curve fitting parameters. EPM, equivalent porous media; FZ, fracture zones.

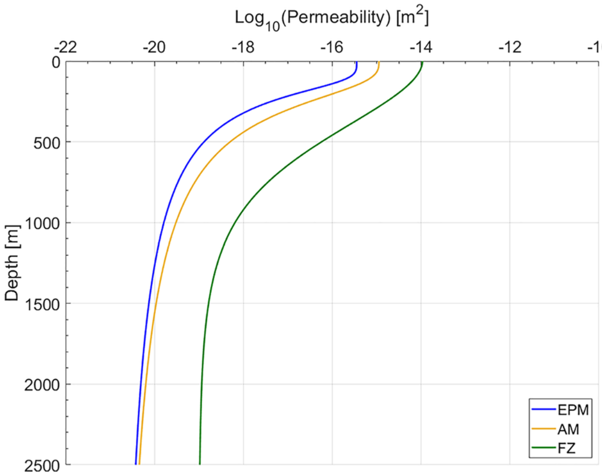

Figure 9. Mean permeability versus depth for EPM rock mass, AM, and FZs for the Canadian Shield AECL RAs. AM, aggregate media; EPM, equivalent porous media; FZ, fracture zones.

significant. Based on the normalized sensitivity analysis, all five fitting parameters meaningfully contribute to the logistic function.

Additionally, of the three functions investigated, the five-parameter logistic function is the only one capable of fitting the shape of the curve indicated by the moving average for both the moving average and entire data set. A further comparison of the five-parameter logistic function and the logarithmic function can be found in the supplementary information section using the Achtziger-Zupančič et al. (2017) global data set. Figure S2 shows that when using the global data from Achtziger-Zupančič et al. (2017), the five-parameter logistic function can fit the data with a higher R^2. The logarithmic function (Equation 5) used in Achtziger-Zupančič et al. (2017) had a data set R^2 of 0.20 whereas the five-parameter logistic function (for the same data set) produced an R^2 of 0.69, and an R^2 of 0.99 when using the moving average mean permeability.

In Figure 6, it can be seen that the moving average for the EPM rock mass is smoother than the moving average for the fracture zones. This is likely because there are less data in the FZ data set. The fitted curve produced a smoothed relationship that defines permeability versus depth in the EPM rock mass and fracture zones. The parameters, R^2 values, and RMSE values for the fitted logistic curves are provided in Table 1; both curves are a good fit of the data with high R^2 values. Plotting the two relationships together (Figure 9) more clearly shows how different the EPM rock mass permeability and the fracture zone permeability are and how they change with depth. EPMs have a sharp decrease in permeability above 500 mBGS and then continue to relatively slowly decrease with depth whereas FZ permeability more gradually decreases over 1,000 m of depth before reaching its lower limit. This figure clearly shows that fracture zone permeability is generally at least two orders-of-magnitude higher than EPM permeability. While this is expected, there is a lack of quantitative data on this comparison in the literature. A third fit was added to Figure 9 which shows the AM data. The AM fit included all the data for both the EPM rock mass and FZs. It shows that when all the data are used, the permeability versus depth relationship falls between the EPM rock mass and FZ with a bias toward the EPM rock mass curve due to the amount of data points in the EPM rock mass data set. This relationship could be used if insufficient data were available to separate FZs from the EPM rock mass data, however because the AM lacks discrete fracture zones, it cannot fully represent a dual continuum.

5. Conclusion

The collection, compilation, and analysis of this database on Canadian Shield (Precambrian) plutonic crystalline rock properties for EPM rock mass and fracture zones is extremely important for characterizing site properties. Even though much of the testing and research was conducted many decades ago, a compilation and analysis of the data has not been published and therefore the scientific community has been unable to readily use the data. The data compiled and analyzed in this study will benefit many research projects on crystalline rock that are ongoing in Canada and other countries.

It has generally been assumed that fracture zones represent enhanced permeability zones in crystalline rock settings, and they have been treated as a second continuum or domain in models and studies for decades. However, the mean permeability versus depth curves for the rock have not been available. By using fracture zones and fault zones identified in AECL research studies, it was possible to differentiate the EPM rock mass from FZs in order to analyze permeability versus depth relationships. This analysis resulted in general mean permeability versus depth relationships showing how fracture zone permeability differs from EPM and AM scenarios. As seen in these mean relationships, fracture zone permeability is higher than the EPM rock mass permeability by two or more orders-of-magnitude and even at depth, they do not overlap. This clearly implies that even at depth, some fractures exist and have a pronounced impact of the hydraulic properties of Precambrian crystalline rock.

With the use of the 5-parameter logistic function (Equation 6), it is possible to determine mean permeability in EPM, FZs, and AM at any depth such that the characterization of Precambrian rock is enhanced and modeling of these settings can be more representative of actual physical locations. This function can also be used to determine mean permeability from the data in Achtziger-Zupančič et al. (2017). This novel logistic function fits the permeability versus depth relationship better than a power law function or simple logarithmic fit and can be used to estimate mean permeability for both near-surface and deep rock locations for EPM rock mass and for FZs. If fracture data is available for a site, differentiating between EPM rock mass and FZs would improve model studies, however when no fracture data is available, it is still possible to estimate permeability values through the use of an AM. Additionally, this function serves as a useful means for assessing data from new site investigation programs in Canadian Shield settings.

Appendix A: Data and Source Overview

For a complete list of AECL RA data sources separated by borehole, please see Tables S7 and S8.

Data Availability Statement

Supporting data for this research can be found at Snowdon et al. (2020).

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