Investigating Contaminated Sites On Fractured Rock Using The DFN Approach

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Abstract

This presentation provides an overview of a major field - focused program of studies aimed at improved investigation methods and understanding organic contaminant source zones and plumes in fractured porous sedimentary rock. This research began in 1997, when intensive field studies were initiated at a TCE contaminated site on steeply dipping and faulted sandstone in California. Now, with collaborations involving several disciplines (analytical chemistry, mathematical modelling, geophysics, microbiology), the program includes three other sites contaminated with chlorinated solvents in addition to the California site: a Wisconsin site on flat-lying sandstone and two sites in Ontario on flat-lying dolostone. These four sites have important differences so that they are broadly representative of sedimentary rock but they have several aspects in common, including: much site data from earlier conventional investigations, contamination initially caused decades ago by DNAPL flow into the rock, sufficient matrix porosity (2-20 %) to allow diffusion-driven chemical mass transfer between fractures and the rock matrix causing strong influence on contaminant behaviour, deep contaminant occurrence (greater than 350 m below ground surface at one site), and each site receives much regulatory attention. Also, the plume fronts advance at rates much slower than the average linear groundwater velocity in the fracture networks. Based on the field results obtained to date, a general conceptual model for the formation and long-term evolution of source zones and plumes in fractured porous sedimentary rock is proposed. This conceptual framework is being tested and the various processes quantified through field investigations using a suite of high-resolution techniques that I refer to as the **d**iscrete-fracture **n**etwork (DFN) investigation approach. This then allows application of DFN numerical models, such as FRACTRAN and HydroGeoSphere, to simulate flow and contaminant transport at these sites. Conventional field methods used in fractured rock studies are poorly suited for plume delineation or characterization and therefore, new methods are being developed and used at all of the sites. In the DFN approach, emphasis for data acquisition is on data specific to individual fractures and the fracture network as well as the rock matrix blocks between fractures so that the characteristics and interactions between these two domains can be discerned. Hence, the spatial scale of measurements on continuous rock core and also in the core holes must be exceptionally detailed. Rock core contaminant analyses at each site confirm that nearly all of the contaminant mass now resides in the low-permeability rock matrix although the down-gradient transport occurs in numerous, well-connected fractures. Therefore, quantifying the interactions between these domains is essential for improving the understanding of individual site conditions regarding the prediction of plume behavior and/or response to site remediation. The investigations at the field sites will continue for several years.

Introduction and Background

The behaviour of contaminants in fractured rock is now one of the few remaining scientific frontiers in physical hydrogeology. The status of knowledge concerning groundwater flow and contaminant migration in fractured rock has been reviewed by the U.S. National Research Council (NRC, 1996), Lapcevic et al. (1999), Berkowitz (2002) and Neuman (2005). These reviews detail considerable published literature concerning the conceptual nature of fractures and hydraulic conditions in fracture networks based on borehole investigations in uncontaminated fractured rock (primarily based on work by the petroleum industry, USGS studies of the Mirror Lake granitic system in New Hampshire and investigations of prospective radioactive waste repositories). Furthermore, many publications concern mathematical models representing hypothetical or idealized fracture networks for contaminant behaviour in fractured rock systems (e.g., Smith and Schwartz, 1984; 1993; Sudicky and McLaren, 1992; Therrien and Sudicky, 1996; and many others). However, these modelling endeavours generally do not represent actual field sites or any particular type of rock, and field data of actual contaminant distributions and contaminant behaviour in fractured rock, particularly sedimentary rock, are almost non-existent.

Current concepts for the nature of contaminant plumes in fractured rock are quite speculative and parameterization of model inputs is inadequately supported by field data. Although many techniques for borehole logging and hydraulic testing exist (e.g. review by Sara, 2003), general agreement in the literature indicates these techniques are severely limited in their prospects for providing quantitative information about the length and interconnectivity of the fractures in fracture networks (NRC, 1996; Berkowitz, 2002). Unlike behaviour in igneous rock, contaminants in sedimentary rock can reside predominately in the porous rock matrix while downgradient transport occurs in the fractures. Therefore, determination of the contaminant distribution in sedimentary rock requires measurement of contaminant concentrations in both the fracture network and the rock matrix. Most literature pertaining to groundwater flow and solute behaviour in fractured rock concerns igneous rock such as granite. Several countries have proposed creation of deep repositories for radioactive waste in granitic rock and the search for and assessment of prospective sites has involved intensive field studies. However, these studies have not involved existing contaminant plumes as such plumes do not (yet) exist in these environments (i.e., no radioactive waste has been disposed of in this type of rock). The research has included tracer experiments but their spatial scale is small in relation to the relevant plume scale. The literature contains no well-documented cases of industrial contaminant plumes in any type of fractured rock.

In essence, the state of knowledge at this time concerning actual contaminant plumes in fractured rock is where the understanding of contaminant plumes in granular porous media (sand & gravel aquifers) was in the 1950's. Back then, vague concepts existed for plumes but no plumes had been delineated / characterized in any detail to show what reality was really like. However, the difficulty of the challenge posed by fractured rock is much greater than that posed then by granular media because the scale of variability and complexity imposed by fracture networks is so much greater, as well as increased costs per borehole given greater depths and need for comprehensive monitoring is so much greater. Also, an important contribution to the understanding of contaminant behaviour in granular aquifers has been large-scale, natural-flow tracer experiments with detailed 3-D monitoring to examine effects of heterogeneity on dispersion (e.g. Sudicky 1986, Garabedian et al. 1991).

Such natural-gradient experiments at relevant spatial scales have not been conducted in fractured rock and are generally cost-prohibitive. Therefore, for fractured rock there is no alternative but to rely on intensive studies of actual contaminated sites to gain insights concerning plume formation and evolution and quantify the influences of the various processes such as advection, dispersion and degradation. In essence, the plumes represent long-term, large-scale tracer experiments, and is the thrust of my research program in fractured sedimentary rock at the University of Guelph based in Ontario, Canada.

Origin and Nature of the DFN Approach

Ten years ago I initiated use of chemical analyses (rock core VOC analyses) done at very closely spaced vertical intervals on contaminated sandstone core in the style presented in Figure 1 to determine the nature of the contaminant distribution at a location in California where TCE had entered sandstone decades earlier and this has led to a systematic way for investigating contaminated bedrock following what I now refer to as the discrete - fracture network (DFN) approach represented in the Figure 2 flow chart. This core-focused field study grew out of conceptual modelling supported by analytical modelling concerning dissolution and diffusion effects on chlorinated solvent DNAPL in fractured porous geologic media represented by fractured clay and fractured sandstone with literature derived parameters (Parker et al., 1994; 1997). From the rock core analyses done at the California sandstone site mentioned above, it was evident that the DNAPL had initially flowed primarily downward through a network of many interconnected fractures, spaced 1-5 m apart, and that over the subsequent years or decades, all or nearly all of the immiscible phase liquid has been transferred by dissolution and diffusion into the rock matrix blocks between the fractures where the mass now resides in the dissolved and sorbed phases. Comparison of the rock core contaminant profiles with groundwater analyses done on samples from conventional monitoring wells and multilevel systems (MLSs) showed that these water analyses gave misleading results because of effects of vertical flow in the holes when the holes were open, allowing cross contamination between fractures with different initial concentrations (Sterling et al., 2005). Conventional methods of borehole geophysics and hydrophysics also gave misleading results about flow in the sense that the aim is to understand the flow in the fracture network during ambient conditions not the disturbed flow imposed by the open borehole. From this initial experience a decade ago and subsequent experience at other sites where the rock core VOC analyses method has been applied, the DFN approach was designed to determine the distribution, transport and fate of contaminants in sedimentary rock and it has now been applied to some degree at more than 18 sites with chlorinated solvent contamination, from which four were selected as focus of a long-term intensive field studies. Two of these are in the USA (California and Wisconsin) and two in Canada (Cambridge and Guelph in the Province of Ontario). Table 1 provides a summary of the hydrogeologic conditions.

Chlorinated solvents have been in the subsurface beneath many industrial properties for several decades allowing plumes to migrate down-gradient several hundreds to thousands of metres or more. These contaminants can now serve as tracers to study contaminant migration over the relevant large space and time scales most relevant in contaminant hydrogeology. Chlorinated solvent compounds are not naturally occurring in the environment, hence, even extremely low level detects (possible due to exceptional measurement sensitivity) serve as reliable evidence of contamination over several orders of magnitude. The physical and chemical properties of the common chlorinated solvents make them good indicators of the physical hydrogeologic system characteristics, including the fracture network connectivity and distribution of groundwater flow.

Table 1: Summary of contaminant types, site hydrogeology and causes of the contamination at the four field research sites.

Field Site/ Owner	Rock Type	Major Parent Chemicals	Degradation Products (in order of abundance)	Entered ground water (main period)	Water table depth and Max. cont. depth (meters bgs)	Overburden Thickness and Type (meters)	Cause of Contamination/ Comments
Cambridge Ontario	Dolostone aquife on shale aquitard; flat lying	Metolachlor, TCE	None	1978-1990	20m 150 m into shale	25-35 Glacial; sand and silt, and thin basal till	Agricultural chemical packaging; no DNAPL found; metolachlor plume goes to a municipal well; below MCLs;
Guelph, Ontario	Dolostone aquife on shale aquitard; flat lying	TCE, minor PCE	cis-DCE, VC	1990s	3-4 m 50 m but may be deeper	3-5 Till	Auto-parts manufacturing; small lateral plume extent expected; no DNAPL found
Simi, California	Sandstone with siltstone, shale nterbeds; 30° di	TCE, minor TCA	cis-DCE, 1,1-DCE, t-DCE, VC	1950s-1960s	15- 100 m >300 m	0-5 Alluvium	Rocket engine testing, research; many plumes from many different source areas; no DNAPL found NE area focus
Wisconsin	Sandstone and minor dolostone with minor siltstone; flat lying	PCE, TCE, TCA, Ketones	cis-DCE, 1,1-DCA, 1,1-DCE, VC	1950s-1960s	above grade-25 m Nearly all mass shallower than 60 m	7-40 Glacial sand, silt and clay layers	Solvent recycling; plume extends ~3km from source zone; 35,000L DNAPL pumped out and residual DNAPL remains

The research based on the DFN approach applied at the four study sites has two general goals:

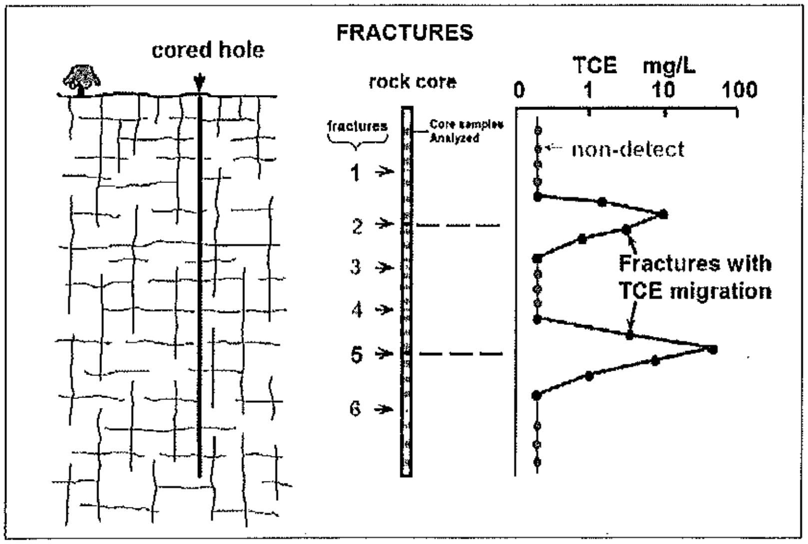
(1) to develop and demonstrate the effectiveness of an approach that relies on several new field methods for determining the nature, extent and controls on the transport and fate of organic contaminants in fractured sedimentary rock; and

(2) to develop a field-verified general conceptual model for contaminant migration and fate in fractured sedimentary rock with emphasis on chlorinated solvents.

The overall approach is to perform 3-D high resolution characterization and associated process studies based on the DFN framework where both the fracture network and matrix properties are studied in appropriate detail at the four study sites. Organic contaminants of industrial origin have existed in the rock at these sites for decades while migrating primarily under natural groundwater flow conditions. The sites offer appropriate diversity in characteristics (Table 1) to provide a strong framework for assessing the general conceptual model.

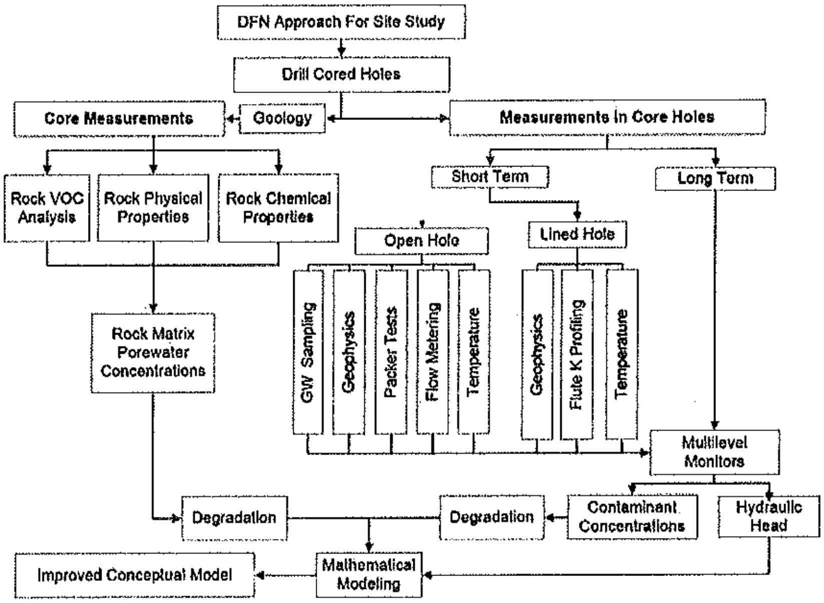
The research goal is to understand the formation and evolution of existing relatively extensive contaminant plumes and investigations of the groundwater flow governing the plumes must be directed at the flow conditions causing contaminant transport. This flow is referred to here as the natural or ambient flow regime, even though there may be influences caused by pumping of water supply wells. This emphasis on natural flow conditions is an important distinction in the DFN approach because it means that flow conditions created by open boreholes or imposed during hydraulic testing are only minimally relevant. The challenge, therefore, is to develop methods for borehole data acquisition that pertain most directly to the ambient flow in the fracture network. Essentially all conventional fractured-rock borehole test methods relevant to the hydraulic conditions and properties, except for depth-discrete multilevel monitoring, (see comprehensive review by Sara, 2003), are done in open holes into which data acquisition equipment is inserted downhole. Flow metering, fluid resistivity and conventional downhole temperature logging and full-hole borehole dilution tests pertain to imposed (forced advection) hydraulic conditions, by applied fluid pressure as in the case of packer tests or vertical flow in the open hole caused by the hole itself (borehole cross connection between fractures). Therefore, in this research program, emphasis is on identifying and /or developing new methods aimed at understanding the borehole properties and flow regime under the ambient flow conditions. Price and Williams (1993), Sterling et al. (2005) and others have demonstrated that open holes in fractured rock commonly have borehole cross connection that disturbs the hydrochemical conditions. Hence, minimizing borehole cross connection is necessary while data are being acquired from the holes, a particularly important caution when investigating contaminated zones. Immediately after drilling each hole, the hole is sealed, usually using a FLUTe liner but sometimes using packer strings or the Solinst continuous modular packer system. In addition to the prevention of cross connection, FLUTe lined holes provide two other advantages: measurements of hydraulic conductivity continuous down the hole when the liner is first installed and temperature profiling in the water column inside the installed liner.

Figure 1: Schematic diagram illustrating use of rock core contaminant analyses to identify migration pathways by identification of diffusion haloes associated with active fractures.



The studies are directed at understanding the behaviour and fate of contaminants, primarily common volatile organic contaminants (i.e. chlorinated solvents), in fractured sedimentary rock with emphasis on the formation and evolution of plumes (spatial scales of 100s to 1000s of meters in longitudinal extent), and therefore, the research seeks to conduct those field and laboratory measurements needed for this particular scale of understanding. Although several numerical discrete-fracture-network (DFN) models exist for simulating contaminant transport and fate at the plume scale, no actual plumes at fractured rock field sites have been monitored at the range of scales necessary for both the fracture network and the matrix conditions needed to calibrate or verify any of these models.

Figure 2: DFN approach for site study



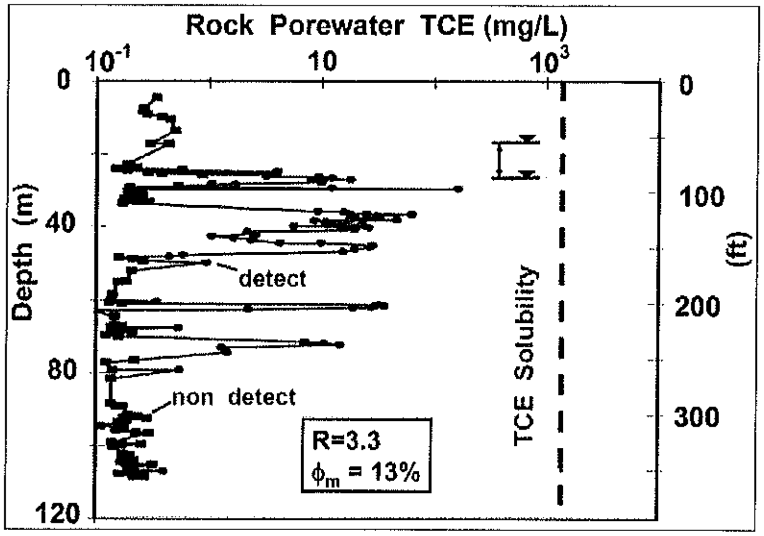
Role of Rock Core Contaminant Analyses

The distribution of contaminants within chlorinated solvent plumes in fractured sedimentary rock has strong spatial variability due to heterogeneity in source zone contaminant mass distributions, fracture network and matrix characteristics accompanied by temporal variability in groundwater flow. To measure the scale of these variabilities requires application of a specific combination of unconventional and conventional field and laboratory methods. The research activities involve development and testing of several methods recently developed to complement the existing array of tools and techniques to advance the depth-discrete data sets to support the DFN field approach (Figure 2).

One major reason why so little is known about contaminant migration and fate in fractured sedimentary rock is that traditional research approaches involve only sampling water from the fractures. However, field studies using the rock core VOC analysis method show contaminant mass storage is dominated by the rock matrix rather than the fractures, and the contaminant concentrations in the fractures and the matrix are not in equilibrium (Hurley and Parker, 2002; Sterling et al., 2005; Parker et al., in review). This disequilibrium between fracture and matrix zones is evident in the rock core concentration profile from the California site shown in Figure 3. Therefore, sampling only the groundwater from the fractures cannot provide the overall mass distribution. Furthermore, when conventional boreholes are drilled, the water from a fracture in one section of the borehole migrates to another section of the borehole due to differences in head between the two sections. This creates an un-natural flow and contaminant transport condition within the system known as borehole cross-connection. This condition will also persist across the screened interval of a conventional monitoring well, and as a result, results from sampling the well do not reflect the natural system (Price and Williams, 1993; Sterling et al., 2005).

Rock core analyses provide contaminant mass and phase distributions more relevant to contaminant behaviour than those obtained from monitoring wells or other types of borehole water sampling alone. The determination of the nature and extent of the contamination, with emphasis on elucidating the internal anatomy of contaminant plumes (including contaminant distribution in the rock matrix where groundwater is nearly immobile due to low permeability), is the foundation for understanding the processes governing the contaminant distribution.

Figure 3: Example of rock core analysis results for TCE in sandstone at a location near TCE DNAPL source zone at the California site. All analyses are much below TCE solubility indicating lack of DNAPL presence. (modified from Sterling et al. 2005)



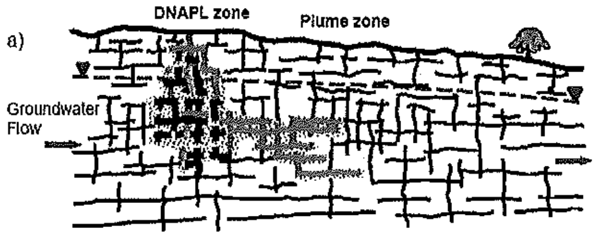
The rock-core based approach has several advantages over conventional methods for contaminant investigations in fractured sedimentary rock. For example, it provides a time-integrated finger print of plume behaviour. In the rock matrix block, the extent of the halo evolving outward from each fracture can increase over several decades, depending on the duration of the dense, non-aqueous phase liquid (DNAPL) source. This allows the halo extent to be used as an indicator of the age of contamination (time since contaminant arrival) on a fracture by fracture basis. In contrast to analyses pertaining to the rock matrix, which generally has low permeability, groundwater sampling in the borehole using depth-discrete multi-level groundwater monitoring systems allows the current chemical concentrations in the hydraulically active factures to be determined and permits evaluation of plume variability over time. However, drilling and related borehole cross connection effects can influence the results of groundwater sampling. The rock core analysis method avoids this problem because the low permeability matrix is not easily cross connected during drilling and core retrieval prior to sample collection (Sterling et al., 2005). In addition, the rock core contaminant analyses provide a direct measure of contaminant mass storage because the pore space in the rock matrix constitutes nearly the entire contaminant mass storage volume; the exception is the potentially large contaminant mass percentage stored in the fractures if DNAPL persists. However for the rock core analyses to show the actual mass distribution with useful accuracy, the samples must be collected from the core at closely spaced interval (Lawrence et al., 2006).

General Conceptual Model

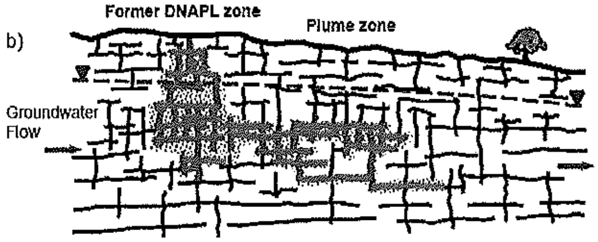
Parker et al. (1994; 1997) proposed a new conceptual model for chlorinated solvent DNAPL source zones, supported using analytical models for DNAPL behaviour in water-saturated fractured porous media such as clay and sedimentary rock. In this model, the immobile DNAPL film in the fracture dissolves into the contiguous water film in the fracture, establishing an aqueous concentration gradient driving mass into the porous matrix by diffusion. This mass transfer can cause complete dissolution of the DNAPL phase after some period of time that depends on the thickness of the DNAPL film (i.e., fracture aperture and initial fracture DNAPL saturation) and the diffusion driven mass transfer rate into the matrix; however, this time is short relative to the time elapsed since contamination of these sites (decades ago). Building on the work of Parker et al. (1994; 1997), VanderKwaak and Sudicky (1996) developed a numerical model to show the dissolution time is dramatically shortened when active groundwater flow is present in the fracture containing the DNAPL. In this model, the 'source zone' evolves relatively rapidly (i.e., DNAPL dissolution followed by continued changes in concentration distribution and contaminant flux from the source to the plume) and has a strong influence on plume development and internal concentration behaviour. The lack of DNAPL persistence in all or major parts of the source zone represents a major difference between typical source zones in fractured porous sedimentary rock and those of granular aquifers where DNAPL as free product and / or residual can persist for extremely long times (Pankow and Cherry, 1996). The conceptual model for complete loss of the DNAPL phase from chlorinated solvent source zones has been assessed at the field sites using closely spaced sampling of continuous rock core at each of the four field sites. These results support the conclusion that the DNAPL phase has completely dissolved away (Hurley and Parker, 2002; Sterling et al., 2005; Parker et al., in review) and all or nearly all of the mass is stored in the matrix (Goldstein et al., 2004). Complete dissolution of the DNAPL phase may not occur when the DNAPL is of low effective solubility as complex mixture of compounds, such as at the Wisconsin site and sites with creosote, coal tars and PCBs.

Another major conclusion from applications of the rock core VOC method in zones where DNAPL contamination had occurred is that the concentration profiles (concentration vs. depth) indicate the occurrence of numerous pathways for contaminant migration in each hole, consistent with observations of fracture occurrence in the cores. However, the existence of numerous active fractures is not consistent with results of conventional borehole fluid resistivity and temperature logging and borehole flow metering that typically indicate only two or three active fractures in each hole (Sterling et al., 2005; Pehme et al, 2007). Therefore, the rock core VOC results support the conceptual model for fractured sedimentary rock in which the DNAPL initially occupied many, mostly small to intermediate aperture fractures, and then dissolved away allowing the mass to be transferred by diffusion into the nearby matrix. Groundwater flow through the DNAPL zone in the fractured rock causes a down-gradient dissolved-phase plume to form. In this conceptual model, the plume forms in a network of many interconnected fractures of variable aperture and length without dominance over long distances of any large-aperture fractures. The evolution of a chlorinated solvent source zone and plume in fractured sedimentary rock is illustrated in cross-section at three stages in Figure 4, illustrating the strong influence of diffusive mass transfer into the low permeability matrix blocks both in the source zone and plume.

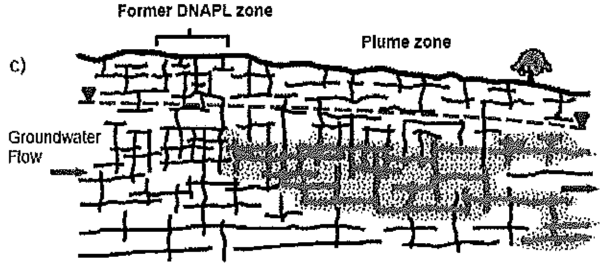
In the past few years, the conceptual model for chlorinated solvent DNAPL behaviour in fractured porous media outlined above has been combined with a conceptual model for the formation and evolution of contaminant plumes from the source zone, referred to here as *the general conceptual model for source zones and plumes*. This model, which includes DNAPL disappearance after several years or a couple of decades and plume formation in networks of many interconnected fractures within a porous medium, has been represented stylistically with simulations using 2-D discrete fracture models (e.g., FRACTRAN by Sudicky and McLaren, 1992) with assignment of fracture and matrix parameters consistent with borehole measurements in the field and laboratory measurements on core samples (see Figure 5).



Early: DNAPL in fractures dissolves and diffuses into rock matrix



Intermediate: No DNAPL remains, diffusion of aqueous-phase out of matrix in source area



Late: Contaminant mass has diffused out of former source area, plume continues to grow and attenuate

Figure 4: The discrete fracture network (DFN) approach for investigating contaminated sites on fractured sedimentary rock, includes intensive data acquisition from contaminated cores and from the corehole. Open hole conditions are minimized. Illustration of conceptual stages in the time evolution of source zone and plume at chlorinated solvent DNAPL sites on fractured porous sedimentary rock: a) DNAPL flows in fracture network and begins to dissolve and diffuse into rock matrix. DNAPL flow ceases soon after DNAPL input to the rock ceases. b) All DNAPL mass has dissolved completely and the contaminant mass now exists almost entirely in the rock matrix as dissolved and sorbed mass due to diffusion driven mass transfer. Therefore, the source zone no longer has DNAPL and there is not distinct difference in contaminant state between the zone initially referred to as the source zone and the plume. c) Groundwater flow through the initial DNAPL source zone has caused complete mass translocation from much of the initial source zone into the downgradient plume ; the plume front is migrating only slowly or is stable or shrinking due to the combined effects of matrix diffusion and degradation.

In studies of contaminant migration in granular media (i.e. non-indurated geologic deposits), the plug flow advance of plume fronts is estimated using the average linear groundwater velocity ($\bar{v}$) which is the Darcy flux divided by the effective porosity relevant to transport. This porosity is commonly between 0.2 – 0.4 (Freeze and Cherry, 1979).

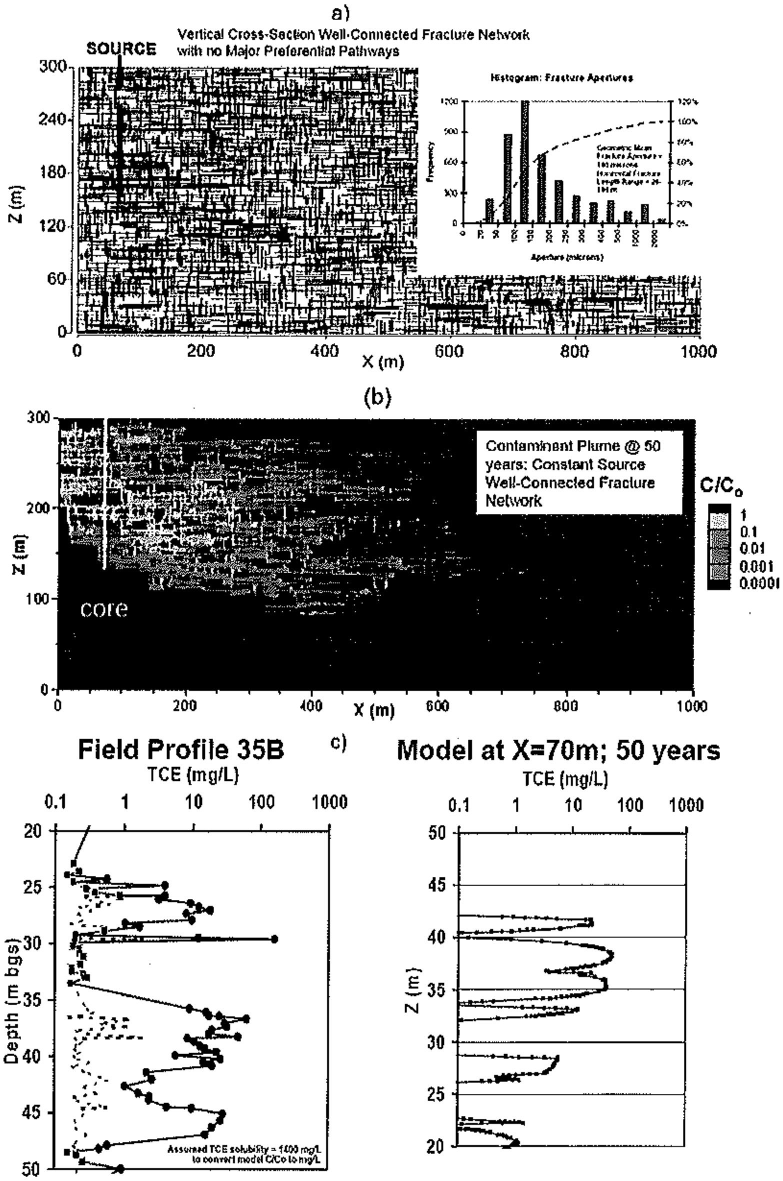
The $\bar{v}$ concept is also applicable to fractured rock in which many interconnected fractures exist, in which case the $\bar{v}$ is the Darcy flux divided by the bulk fracture porosity (q/ϕ_{fb}). For intact fractured rock, typical values of ϕ_{fb} are 10^{-3} to 10^{-5}. The overall magnitude of Darcy flux variations in fractured rock terrain are generally in the same general range as in granular media terrain and therefore the calculated $\bar{v}$ range typical of fractured rock is orders of magnitude larger than that of granular media. For example, $\bar{v}$ in fractured sedimentary rock is generally on the order of a kilometre to tens of kilometres per year. The potential consequences of such high $\bar{v}$ values to plume expansion and arrival at receptors are large and therefore there is emphasis in the research program on acquiring field data that more reliably determine $\bar{v}$.

Although existing evidence indicates that $\bar{v}$ in the fractured rock aquifers at the four field sites is very large (in the range indicated above typical of fractured rock), the results of the plume investigations conducted to date indicate that the actual plume fronts over decades have advanced at rates which are orders of magnitude smaller than the respective $\bar{v}$'s. Therefore, studies are aimed at quantifying the processes responsible this apparent strong plume front retardation relative to groundwater advection. These studies then have two thrusts: i) improved estimates of $\bar{v}$ based on better measurements of Darcy flux and bulk fracture porosity and ii) more detailed examinations of plume front travel. Plume front retardation is a concept initially established by Foster (1975), further illucidated by Freeze and Cherry (1979) and represented in several DFN modelling papers (e.g Grisak and Pickens, 1980; Lipson et al., 2005) but it has not previously been demonstrated. Greatest confidence in $\bar{v}$ values must come from comparisons of $\bar{v}$ results obtained from independent methods. Therefore, effort is being directed at determining $\bar{v}$ using methods based on temperature, chemical, dilution (borehole dilution) or environmental isotopes (atmospheric tritium and/ or carbon-14). Although the groundwater flow is governed by Darcian flow, the methods in this latter group do not involve measurements of the parameters used in Darcy Law (i.e. K, head gradient) and therefore the results are independent of Darcy-based calculations for $\bar{v}$.

Temperature Measurement in Sealed Boreholes for Identification of Active Fractures

The detection of all fractures in which significant flow occurs is a critical data requirement for the DFN approach. Furthermore, the capability of quantifying the amount of fracture flow in individual fractures over a range of several orders of magnitude is necessary. Various possibilities to acquire such data down-hole have been assessed and the most insightful method proved to be high-resolution temperature logging inside lined holes. The power of this approach is gained from two independent advances: 1) improved sensitivity to monitor temperature variability to 0.0001 °C (probe capability) under ambient temperature conditions and when heat is added (active line source) and its dissipation is monitored, as realized (Pehme et al., accepted 2006; Pehme et al., 2007a; 2007b); and 2) utilization of FLUTe liners to temporarily seal the borehole but provide access to static water column inside the liner, allowing measurement of ambient temperature distributions. When temperature logging is done in open bore holes (i.e., holes without liners), as is conventional practice, the vertical flow in the open hole typically swamps the minor but important, temperature signals and therefore larger number of hydraulically active fractures that likely occur in many holes are not identified. The temperature profiling research provides substantial supporting data concerning hydraulically active fractures at each of the four field sites (Pehme et al., submitted). Most recently, an important advance in this temperature logging technology has been initiated involving a prototype for identifying hydraulically active fractures in lined boreholes to resolve flow direction and flow rate under natural flow conditions.

Figure 5: Example of DFN simulations using FRACTRAN (2-D numerical model; cross section display) of TCE plume in fractured sandstone with fracture and matrix properties consistent with those of the California site: a) source location on fracture network domain; aperture distribution shown, b) TCE plume (no degradation) after 50 years, and c) stylistic comparison of rock core TCE profiles 75m from source at 50 years.



Contaminant Degradation

The behaviour and fate of organic contaminants in fractured sedimentary rock are influenced by physical processes (advection, dispersion and diffusion), sorption and in some cases biotic and abiotic degradation. Little peer-reviewed literature exists about chlorinated solvent degradation in fractured sedimentary rock and none examines abiotic versus biotic degradation pathways or evaluates where this degradation is occurring (fractures versus rock matrix). Long term groundwater sampling at all of the field sites shows occurrences of compounds typical of biotic TCE degradation (cis- and trans- 1,2-dichloroethene and in some cases vinyl chloride). Pierce et al. (in prep) examined TCE degradation at the California site and concluded both biotic and abiotic degradation occurs in these sandstones. However, whether this degradation occurs solely in the fractures or in the rock matrix was not determined. Based on a study at the Wisconsin site source zone, Austin (2005) showed abundant chlorinated solvent degradation products in monitoring wells; if this degradation occurred prior to entry of the mixed organic wastes into the subsurface (either in the overburden soils or bedrock) or during storage prior to their release to the subsurface was not determined. The two Canadian sites have less abundant transformation products compared to the US sites, which may be due to the different rock types (differences in mineralogy and pore structure/connectivity) and/or the length of time since contaminants entered the subsurface (15-20 years ago for the Canadian sites versus 40-50 years at the US sites).

Simulating Plumes Using DFN Numerical Models

Although the research is focused on the field studies, mathematical models play an important role in the interpretation of field information and testing and validating components of the general conceptual model. Existing models will be used with emphasis on discrete-fracture network (DFN) numerical models (e.g., FRACTRAN, FEFLOW, FRACMAN, HEATFLOW and HydroGeoSphere) for contaminant behaviour and fate. Both DFN and equivalent porous media (EPM) models will be used to represent groundwater flow. In the DFN models, the fracture networks are generated with many discrete fracture elements and each fracture is usually assigned statistically-derived parameters including length, spacing, orientation, and aperture. The DFN models most relevant to this research are those in which the fractures are superimposed onto a porous rock matrix allowing advection, diffusion, sorption and degradation of contaminants in both the matrix and fractures. The numerical models selected for this part of the IRC research are those that also include rigorous representation of the diffusion-driven contaminant mass transfer between fractures and the rock matrix.

The main objective of the DFN modelling of contaminant transport is to achieve good similarities between contaminant distributions at the field sites and the simulated distributions while maintaining consistency/reasonableness between the field information and the model boundary conditions and model parameter assignments. The contaminant plume characteristics and plume geometry over time (temporal evolution) for both the fractures and the rock matrix represented by DFN numerical simulations of the plumes must show reasonable similarities to the field information constrained by the appropriate boundary conditions and parameter values in order to field verify the general DFN conceptual model. For the DFN plume simulations using numerical models to serve their purpose, the 3-D plume shapes must be mapped and show similarities to the model results for both the fractures and the matrix. Also, the fracture network responsible for the contaminant transport must have large numbers of interconnected, hydraulically active fractures. This task is particularly challenging for fractured rock because some of the model input parameters, such as fracture interconnectiveness, cannot be measured directly (Berkowitz, 2002). Fracture connectivity is, in effect, a result of statistical assignments in the model but it cannot be determined explicitly in the field. Also, uncertainty is associated with the timing and mass of DNAPL inputs into the rock decades ago that eventually resulted in today's contaminant distributions. Nevertheless, application of detailed spatial resolution, field techniques for both the fractures and the rock matrix, and comparisons with distributions from model simulations can narrow the knowledge gap.

When the DFN models are used to simulate groundwater flow and contaminant transport, the hydraulic head, water velocity, and water flux distributions in each of the many thousands of fractures in the network are displayed. In the field, such measurements cannot be made in thousands of fractures but 1-D profiles at selected locations (i.e., boreholes) can be made to the degree necessary for model versus field comparisons at useful spatial scales. This is shown in Figure 5, with 2-D FRACTRAN simulations of the California site and comparison of a field TCE concentration profile derived from rock core compared to a vertical profile through the model output. The extremely detailed profiles of head (Meyer et al., submitted) and groundwater contaminant concentrations from particular boreholes (i.e., exceptionally small spacing between monitoring points particularly in the multilevel monitoring systems) and the extremely detailed contaminant concentrations (concentration versus depth profiles) obtained from the rock matrix (e.g., Sterling et al., 2005; Goldstein et al., 2004) will provide information with unprecedented detail supporting the DFN approach. The high-resolution ambient temperature profiling described by Pehme et al. (in press) provides another independent avenue for comparison between DFN model simulations and the field. Molson et al. (2007) indicate the nature of this modelling approach.

A key input parameter for DFN modelling of contaminant migration is fracture aperture and fracture network geometry, which is difficult to quantify appropriately. There is no alternative but to rely on use of the Cubic Law in conjunction with borehole hydraulic tests to obtain depth discrete hydraulic conductivity values from which values for hydraulic aperture are derived. For this, two types of tests are primarily used: straddle packer injection tests and FLUTe hydraulic conductivity profiling. The straddle packer tests are conventional in their general design however the equipment and procedures have been find-tuned to maximize potential for acquiring more accurate hydraulic apertures. The FLUTe profiling is done in the same holes as the packer testing and the types of data sets taken together provide much stronger bases for deriving information about fracture aperture and the nature of the fracture network local to the borehole. Information about the larger-scale nature of the fracture network is derived from pumping tests, cross-hole hydraulic tomography and plume behaviour over decades.

The patterns of fractures in sedimentary rock are much different than those in igneous rock, which have been the emphasis of most of the hydrologic research pertaining to DFN issues in the context of groundwater flow. However, interest concerning insights from geological observations of fractures in sedimentary rock is increasing (NRC, 1996). For example, Graham Wall (2006) used sedimentological and structural geology principles in field studies of outcrops of peritidal and basinal carbonate sequences in fold-thrust settings to examine the development of fractures in these rocks. Cooke et al. (2006) summarize recent structural geology and fracture mechanics studies on relatively undeformed carbonate rock sequences to provide important insight into the major controls on groundwater flow paths in these rocks. Efforts are being made at the four field sites to incorporate such geological approaches into the development of concepts for the geometry of the fracture networks. For the Cambridge and Guelph sites, quarries excavated into the dolostone formations situated nearby are being examined for fracture network geometry (style). One of the difficulties inherent in quarry observations is the separation of the effects of blasting from natural characteristics. Nevertheless, quarries can provide useful information. At the California site, many natural outcrops on site and in areas adjacent to the site are being used for fracture network observations.

Concluding Remarks

This research program based on intensive field studies at the four sites has show that, even though there are substantial hydrogeologic complexities attributed to fracture networks in rock, the source zones and plumes are readily amenable to insightful investigations relying on intensive data acquisition (i.e. multiple, independent and high-resolution data sets) from continuous core and from the coreholes. In the early years of this research, there was concern that contaminant migration would occur almost exclusively along a few, major pathways (i.e. "superhighways") resulting in sparse random and/or chaotic contaminant pathways that would prove to be difficult to locate, hence not easy to delineate or monitor (i.e. non-plumes) using a reasonable number of boreholes or wells for the search. This 'old' conceptual model leaves one with considerable uncertainty and may lead to overly conservative decision-making, such as excessive or inappropriate characterization and/or remediation. Although the plumes found at the four field sites are not yet fully delineated, enough information has been acquired to conclude that very large numbers of fractures are involved in the contaminant migration, and hence plume formation, causing strong transverse horizontal and vertical dispersion of the plume. Therefore, the plumes in sedimentary rock are relatively large targets and easy to detect. This likely derives from the fracture networks being quite systematic, which is a reasonable expectation given the propensity for bedding plane partings and joints in sedimentary rocks to be systematic and orderly. However, plume characterization sufficient for understanding and predicting plume behavior is more challenging given internal variability of contaminant concentrations and flow distributions. The hydrogeologically favorable attributes of many sedimentary rock types may not be common in other rock types such as crystalline rock.

Contaminant plumes in granular media (i.e. sand and gravel aquifers) generally show only minimal attenuation when degradation is slow or non existent because dispersion alone is incapable of strong overall attenuation influence. In fractured sedimentary rock, however, strong transverse dispersion in the fracture network combined with matrix diffusion can result in very strong plume attenuation. Although the average linear groundwater velocity in fractured networks is much larger than in granular aquifers, the plume fronts in fractured sedimentary rock can advance much slower due to the matrix diffusion effects and sorption in the rock matrix. Thus, there are large dissimilarities between plume behavior in fractured sedimentary rocks and granular aquifers.

It would be unreasonable to claim that a general conceptual model for source zones and plumes in sedimentary rock can be founded on model testing / verification at as few as four field sites. Therefore, data from many other sites are also being examined. For example, the same rock core VOC analysis method used at the four intensive study sites has been applied to more than two dozen other sites where chlorinated solvents occur in fractured sedimentary rock. Also, other components of the DFN field approach are being applied at other sites, such as the high-resolution temperature profiling inside lined holes. Although the number of holes analyzed at each of these other sites using the DFN methods is smaller than at each of the four intensive study sites, the data are valuable for comparing the style of the information to that predicted by the general conceptual model.

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