

Contaminant Hydrogeology - Part 1: Physical Processes

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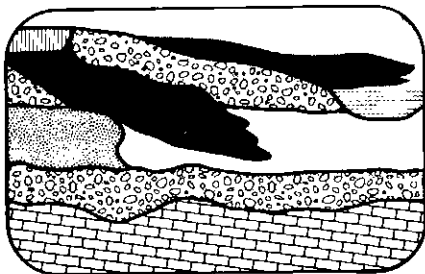
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Résumé de l'article

L hydrogéologie de l'alimentation en eau et l'hydrogéologie des polluants sont deux branches très distinctes des sciences physiques. La première se fonde sur l'hydraulique des aquifères, la mécanique des sols, la macro-stratigraphie, et l'interprétation des systèmes d'écoulement souterrain en termes du taux volumétrique de l'écoulement. Par contre, la seconde repose sur la microstratigraphie, l'hydrogéochimie et sur l'étude de la dispersion hydrodynamique et des vitesses d'écoulement interstitiel. La plupart des méthodes développées pour l'hydrogéologie de l'alimentation en eau sont peu aptes à l'hydrogéologie des polluants. La première partie de cet article a un double but. [1] d'abord de réviser les facteurs géologiques et hydrodynamiques qui contrôlent le mouvement des matières dissoutes dans les systèmes d'écoulement souterrain peu profonds. [2] ensuite de décrire quelques-uns des moyens à la disposition de l'hydrogéologue étudiant les aspects physiques de la contamination des eaux souterraines et de signaler certains des problèmes qui peuvent se produire durant leur utilisation. Jackson et Cherry discuteront des aspects géochimiques dans la deuxième partie de cet article qui paraîtra dans le prochain numéro de *Géoscience Canada*.

Articles



Contaminant Hydrogeology Part 1 Physical Processes

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Summary

Water-supply hydrogeology and contaminant hydrogeology occupy very different parts of the scientific spectrum; the former is based on aquifer hydraulics, soil mechanics, macrostratigraphy, and interpretation of groundwater flow systems in terms of volumetric flow rates. In contrast, the latter depends on microstratigraphy, pore water velocities, hydrodynamic dispersion, and hydrogeochemistry. Most of the methodology developed for water-supply hydrogeology is not well suited for contaminant hydrogeology. The purpose of Part 1 of this article is twofold: - 1) to review the geologic and hydrodynamic controls of the movement of dissolved contaminants in shallow groundwater flow systems, and 2) to outline the nature of some of the tools available to the hydro-

geologist investigating the physical aspects of groundwater contamination and to indicate some of the problems that may arise in their use. The geochemical aspects of contaminant hydrogeology will be discussed in Part 2 by Jackson and Cherry, in a future issue of *Geoscience Canada*.

Résumé.

L'hydrogéologie de l'alimentation en eau et l'hydrogéologie des polluants sont deux branches très distinctes des sciences physiques. La première se fonde sur l'hydraulique des aquifères, la mécanique des sols, la macrostratigraphie, et l'interprétation des systèmes d'écoulement souterrain en termes du taux volumétrique de l'écoulement. Par contre, la seconde repose sur la microstratigraphie, l'hydrogéochimie et sur l'étude de la dispersion hydrodynamique et des vitesses d'écoulement interstitiel. La plupart des méthodes développées pour l'hydrogéologie de l'alimentation en eaux sont peu aptes à l'hydrogéologie des polluants. La première partie de cet article a un double but. (1) d'abord de reviser les facteurs géologiques et hydrodynamiques qui contrôlent le mouvement des matières dissoutes dans les systèmes d'écoulement souterrain peu profonds. (2) ensuite de décrire quelques-uns des moyens à la disposition de l'hydrogéologue étudiant les aspects physiques de la contamination des eaux souterraines et de signaler certains des problèmes qui peuvent se produire durant leur utilisation. Jackson et Cherry discuteront des aspects géochimiques dans la deuxième partie de cet article qui paraîtra dans le prochain numéro de *Géoscience Canada*.

Introduction

During the past 10 to 15 years the emphasis in hydrogeology has been gradually shifting from aquifer exploration and groundwater resources development to problems of subsurface contamination. Three factors have contributed to this change. First, without the public alarm over environmental degradation and the subsequent governmental response, financial resources would not have been made available for subsurface contamination studies. Second, the remarkable advances in instrumentation for chemical analysis made in the last two decades have allowed accurate determinations to be made of many trace contaminants in the environment. Finally, during this period scientists have created a body of theory and practice which has begun to permit the analysis of the dispersive and sorptive properties of subsurface-flow systems.

Having introduced the term, we shall now define the meaning of contaminant hydrogeology as the application of hydrogeological and geochemical theory and practice to the protection of aquifers from contamination to the protection of surface water environments from contamination transmitted through subsurface flow systems, and to the design and monitoring of subsurface waste management facilities. Furthermore we shall designate a dissolved species as a contaminant if it is present at concentrations above the concentration levels that would occur under natural conditions.

This review will only be concerned with the transport of solutes in the saturated groundwater zone. It will further be assumed that the contaminated water has a density and viscosity similar to uncontaminated water in the same system. Problems of

contamination from the insoluble components of petroleum products, sea-water intrusion, gas migration and contaminant transport in the unsaturated zone will not be considered. By this, we do not imply that these problems are not important. On the contrary, for anything meaningful to be said, they would require their own reviews.

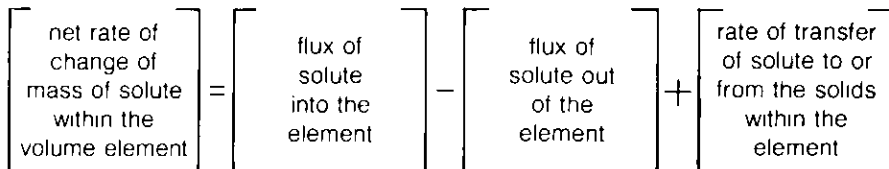
Contamination problems for which the following discussion is appropriate would include the migration of the soluble components of leachate from sanitary landfills, septic fields, waste lagoons, feedlots, road salts, surface applied chemicals such as fertilizers, pesticides, buried radioactive wastes and many others. The specific contaminants would include heavy metals, dissolved fraction from petroleum products, other soluble organic materials including pesticides, nutrients such as nitrogen and phosphorous, radionuclides, and a wide range of salt solutions.

In these problems groundwater is the transporting vehicle and sorption of the contaminant in the porous medium is the retarding mechanism. We will not deal specifically with biochemical mechanisms that cause concentration changes of some types of contaminants. Attenuation of a solute in a groundwater flow system refers to the reduction in concentration that occurs as a result of the combined effects of mechanical mixing, molecular diffusion, and sorption due to chemical processes such as ion exchange, precipitation, and co-precipitation

The Transport Equation

The purpose of the following discussion is to show the principles involved (Bear, 1972) in developing the fundamental differential equation that describes the movement of contaminants in groundwater flow systems, and then to give an indication of the physical significance of the various terms in the equation. As such, this discussion is not completely rigorous mathematically.

This equation is known as the transport equation. Applying the law of conservation of mass to the convection of a contaminant in a dispersive porous medium in which chemical sorption occurs yields, for an arbitrary volume of porous medium:



Mathematically this can be stated as:

$$1) \quad n \frac{\partial C}{\partial t} = - \text{div } F + \frac{\partial q^*}{\partial t}$$

where C is the solute concentration (mass/unit volume of solution), F is the solute flux (mass per unit area/unit time), div is the vector operator divergence, n is the porosity (volume voids/total elemental volume), and q* is the mass of solute transferred to or from the solid phase in the elemental volume. The solute flux F includes two terms: flux resulting from the average bulk movement of the fluid, referred to as convection, and which can be represented by

$$2) \quad F_C = nVC$$

and flux resulting from dispersive effects which can be represented by

$$3) \quad F_D = -nD\nabla C$$

where V is the vector of the average linear pore water velocity, D is the dispersion coefficient and ∇ is the vector operator gradient. The negative sign before the dispersive term indicates that the contaminant moves towards the zone of lower concentration. The nature of the dispersion process is discussed later.

Since the total solute flux across the sides of the elemental volume of porous medium is the sum of equations (2) and (3), substitution into equation (1) and assuming steady one-dimensional flow and solute transport in the positive X direction results in

$$4) \quad \frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) - V \frac{\partial C}{\partial x} + \frac{1}{n} \frac{\partial q^*}{\partial t}$$

In this form D is assumed to be independent of concentration. The first term on the right hand side of equation (4) describes the movement of the solute resulting from dispersive effects, the second term describes the movement resulting from convective or bulk flow of the fluid, while the last term accounts for the losses and additions of the solute due to chemical processes.

In contaminant hydrogeology the problem is to obtain quantitative or at least semi-quantitative estimates for each of the terms in this equation.

Hydrogeologists who wish to simulate real contaminant migration patterns using mathematical models must use some form of this equation extended in two or three dimensions in a very formal sense. Field hydrogeologists faced with the direct field problem of mapping contaminant plumes using test drilling, piezometers or observation wells are dealing with the combined result of the processes described in this equation. We will now briefly discuss the velocity and dispersive terms in equation (1). The sorption term will be discussed in part 2. In essence these three terms are the foundation of contaminant hydrogeology.

Determination of Groundwater Velocities

The groundwater velocity referred to in equation (1) is the average linear pore water velocity, which means that it is the velocity that one would obtain if one knew the linear distance between two points along the actual flow path of the water and divided it by the time required for travel due to convection between the two points. On a microscopic scale, the real average water velocity in the pore spaces is larger than the average linear velocity because the interstitial flow paths have considerable tortuosity, particularly in granular deposits (Fig. 1). The average linear pore water velocity, hereafter referred to simply as the groundwater velocity, is related to the specific

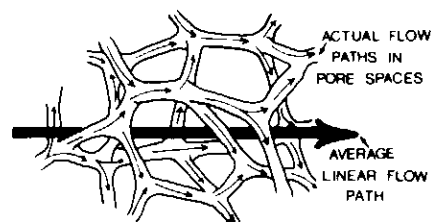


Figure 1
Schematic representation of the conceptual flow paths of the average linear groundwater velocity.

discharge u described by the Darcy equation, by

$$5) \quad v = \frac{u}{n\epsilon} = -\frac{K}{n\epsilon} \nabla h$$

where u is the volume flux defined as the volume flow per cross sectional area orthogonal to the flow vector per unit time, K is the hydraulic conductivity, often called the coefficient of permeability, h is the hydraulic head, and ϵ is an empirical constant dependent on the characteristics of the porous medium. Grisak and Jackson (1975) have pointed out that the data of Ellis *et al.* (1968) indicates values of ϵ between 0.98 and 1.18 for the homogeneous sands used in their experiments. Grisak and Jackson state that to their knowledge there are no published data on ϵ determinations for non-uniform or heterogeneous materials. It is normally assumed that $\epsilon = 1$ and therefore $v = u/n$. This is sometimes called the Dupuit-Forchheimer assumption.

Methods for determining the velocity in groundwater flow systems can be grouped into three main categories: (1) artificial tracers, (2) environmental isotopes, and (3) the Darcy equation with the Dupuit-Forchheimer assumption. The tracer method is the most direct and the most accurate. Tracers commonly used are salts such as NaCl or CaCl₂, dyes such as rhodamine or fluorescein, and artificial radioisotopes such as tritium, sulphur-35, and others. The method usually involves injection of the tracer at one or more wells with subsequent monitoring along the predicted flow paths. This type of tracer study is usually quite expensive and time consuming because numerous observation wells or piezometers are required to map the migration patterns in heterogeneous geologic materials and because natural groundwater velocities are commonly very low. Long periods of observation may be required to obtain representative results. Also, the rate of change of the tracer concentration at the observation wells can be very difficult to interpret in a heterogeneous geologic environment. To date very few tracer injection experiments have been conducted in Canada, which may to some extent reflect a general lack of familiarity by Canadian hydrogeologists with artificial tracers, rather than their relative

degree of usefulness in contamination studies in this country.

Another approach to the use of artificial tracers is the single-well dilution technique, sometimes called the point-dilution method. This involves placing a tracer in the slotted zone of a well bore while maintaining the natural water level and measuring the change in concentration in the well bore as the tracer is transported into the groundwater flow system. The tracer concentration is then related to the natural groundwater velocity in the undisturbed geologic materials exterior to the borehole zone (Brown *et al.*, 1972). The method can also be used in some situations to determine the direction of flow in the borehole. Point dilution tests require little field time and are relatively inexpensive compared to most other methods of groundwater velocity determination. However the value of groundwater velocity obtained from this method is applicable only to a local volume of geological materials in the vicinity of the well bore. A comprehensive review of point-dilution techniques is presented by Halevy *et al.* (1967). The only published Canadian example of its use is by Barry and Merritt (1970) and Merritt (1975). There is a need for evaluation of this technique in a variety of Canadian hydrogeological environments.

The main environmental isotopes suitable for groundwater velocity estimates are tritium and carbon-14. These two radioactive constituents can be used to obtain approximate "ages" of groundwater in many subsurface environments. Tritium is a radioisotope of hydrogen having a mass of three and a half-life of 12.3 years. It occurs in the environment as a result of both natural and artificial processes. Cosmic radiation established a concentration of about 10 Tritium Units (T.U.) in temperate zone continental meteoric waters (Brown *et al.*, 1972). One Tritium Unit corresponds to a concentration of one tritium atom per 10¹⁸ hydrogen atoms. After 1953 the tritium content of precipitation increased as a result of thermonuclear testing (Brown, 1961), with values as high as 10,000 T.U. occurring in the northern hemisphere in 1963 following extensive weapons testings in 1961-2. From this time the tritium concentrations in rain and snow

have decreased. During the past few years the average annual value has been about 80 to 120 T.U. at Ottawa (R. M. Brown, pers. comm., 1975). Once tritium enters the groundwater zone, the concentrations are affected only by radioactive decay and mixing (dispersion). Assuming that mixing is not a major influence, R. M. Brown (*in* R. H. Brown *et al.*, 1972) has indicated that the following cases can occur, for a northern hemisphere continental site in 1972:

- 1) "The water has a concentration of < 3 T.U. This means that no water younger than 20 years is present. That is, more than 20 years are required for water to reach the sampling point from the recharge area. This is the case of most confined aquifers. Phreatic aquifers can have low tritium content due to (a) very slight infiltration (arid and semi-arid regions), (b) long percolation time (low transmissivity, great depth of water table), (c) age stratification of water below the water table.
- 2) The tritium content is 3-20 T.U. A small amount of thermonuclear tritium is present, indicating most probably water of the first test period, 1954-61.
- 3) The tritium content is > 20 T.U. The water of high tritium content is obviously of recent origin. If variations occur through the year and are related to the variations in precipitation over the recharge area, the flow-through is rapid and direct and the transit time may be evaluated from the time-lag in appearance of the annual peaks. The variability may also be caused by a seasonal change in the source of the water or the relative proportions of water from different sources, e.g. a tritium-free water of deep circulation and a young water of high tritium content, generally of a more superficial circulation."

Although there is need for quantitative data on the dispersive properties of groundwater flow systems in a variety of Canadian hydrogeologic settings, tritium serves at the present time as a useful indicator of relatively young groundwaters. We anticipate that it will soon become a rather routine tool in contaminant hydrogeology. Tritium does not require special sampling or handling methods.

Carbon-14 has a half-life of 5,730 years and, like tritium, occurs as a result of both natural and man-made processes. It can be used to detect relatively old groundwaters and is useful in the age range of about 1000 years to about 30,000 years. The ^{14}C content of groundwater decreases by radioactive decay. If the effects of mixing are negligible the fraction of the original ^{14}C remaining at any point along the flow path is a measure of the time since the water entered the groundwater zone from the soil zone. Since the ^{14}C is measured relative to the total inorganic carbon content of the sample, the origin of both the ^{14}C and the stable carbon must be taken into account in the calculation of the groundwater age. This problem is discussed by Brown (1972), Wigley (1975) and others. Payne (1972) has concluded:

"The present status of knowledge is such that individual ^{14}C measurements in the form of estimated ages should be treated with caution. Differences in age at different points in an aquifer, thus arriving at estimated groundwater velocities, are to be preferred. In any case, the isotope data should be examined together with the overall chemistry to give added confidence in the interpretation."

If the general directions of groundwater flow are known in a regional groundwater flow system, the differences in ^{14}C ages of samples along the flow paths can be used to calculate average groundwater velocities. This technique enables many of the uncertainties associated with true age estimates from raw ^{14}C sample radioactivity levels to be avoided. The identification and delineation of segments of groundwater flow systems in which there is old, low-velocity water can be very useful in studies for subsurface waste management. Because of very low hydraulic conductivities in areas of unfractured clayey deposits, it is quite feasible for shallow groundwater to be many thousands of years old.

Tritium and ^{14}C data are most useful if the general directions of groundwater flow are known from water-level observations in wells or piezometers. In Canada active research on the use of tritium and ^{14}C in groundwater studies has recently been initiated at the Chalk

River Nuclear Laboratories (AECL) and at the University of Waterloo. These techniques are more widely used in Europe.

The most common approach to estimating groundwater velocities in contaminant studies is the use of pumping tests and single-well water-level response tests for estimating hydraulic conductivities (K) along with water-level measurements in piezometers and wells to determine the hydraulic gradients. This information can be used with porosity estimates to calculate velocities using the Darcy equation with the Dupuit-Forchheimer assumption as indicated in equation (5). In their application to subsurface contamination problems hydrogeologists with a base of experience in the water supply field are often unduly confident.

Pumping test methods are described in detail by Walton (1970), Kruseman and De Ridder (1970) and many others. These tests yield bulk average values of K for relatively large segments of the groundwater regime. In contaminant hydrogeology these values are only marginally useful at best. In stratified hydrogeologic settings they can be seriously misleading because the hydraulic conductivities of the layers in which most of the contaminant movement occurs are often much larger than the bulk average values calculated from pumping test data. If pumping tests have a role to play in contaminant hydrogeology, it is probably in the area of continuity testing of permeable beds in stratified deposits, rather than for determination of useful K values.

Methods for single well response tests are described by Hvorslev (1951), Ferris and Knowles (1954) and Cooper *et al.* (1967). The apparent K values that can be calculated from this type of test data depend on: 1) the true K value of the geologic materials near the slotted zone of the well or piezometer, and 2) the degree of clogging or borehole disturbance. These K values often seriously underestimate the K value of the undisturbed geologic materials and must be used with great caution.

For the Darcy equation with the Dupuit-Forchheimer relation to be useful in contaminant hydrogeology, it will be necessary to develop means of determining reliable K distributions on

a micro-stratigraphic scale. In other words, we will have to determine K values for critical beds or lenses that may only be a fraction of a metre in thickness. In most hydrogeologic settings in granular deposits this will require detailed and careful coring to obtain relatively undisturbed samples for permeameter testing in the laboratory. One of the rare Canadian examples of this approach is the study of Parsons (1960). It is difficult to avoid the uncertainties inherent in the application of K values determined on cores from the vertical direction to velocity estimates in the horizontal direction.

Use of the Darcy equation with the Dupuit-Forchheimer relation for groundwater velocity determination in fractured rock or fractured cohesive deposits such as some glacial tills or lacustrine clays may yield very misleading results because not only is a representative K value difficult to determine within an uncertainty of less than plus or minus one order of magnitude but porosity also may have an order of magnitude or more of uncertainty associated with it (Grisak *et al.*, 1975). In granular non-indurated deposits such as the Quaternary deposits of Canada, porosity is almost invariably in the relatively narrow range of 0.2 to 0.45. In these materials the main source of uncertainty is the K estimate. As hydrogeologists gain experience in the field of contaminant studies, there will probably be a shift from obtaining velocity estimates using the Darcy-Dupuit-Forchheimer approach to increased usage of artificial tracers and environmental isotopes.

Dispersion and Complex Flow Paths

As a solute is transported in a groundwater flow system it gradually spreads and occupies an ever-increasing portion of the flow domain beyond the region it is expected to occupy according to the average ground-water velocities. This spreading phenomenon that causes dilution of the contaminant is called hydrodynamic dispersion. It occurs due to: 1) the thermal-kinetic energy of the particles (diffusion) and 2) mechanical mixing due to fluid convection. The results of the dispersive processes in homogeneous granular deposits are shown schematically in Figure 2.

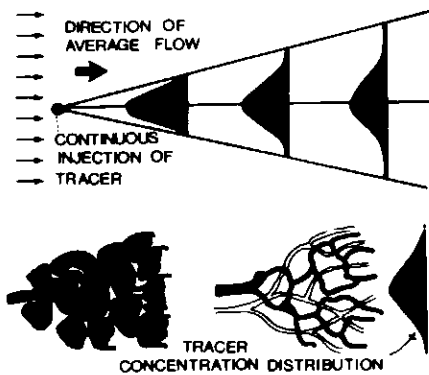


Figure 2
Schematic representation of the dilution process caused by the mechanical dispersion in granular porous media (adapted from Danel 1952 and Bear, 1972)

In the convective component, contaminated and uncontaminated water are mixed therefore causing contaminant dilution as a result of the velocity distribution within single pores, and the velocity distribution resulting from the pore size distribution. Since this velocity distribution is random and cannot be described on a molecular level, the dispersion coefficient D must be considered as an empirical number. Dispersion is the net result of two processes, which in the direction of flow can be expressed as

$$6) \quad D_L = D_L^* + D_D$$

where D_L is the longitudinal dispersion coefficient, D_L^* is the longitudinal coefficient of mechanical dispersion due to convective mixing, and D_D is the effective coefficient of molecular diffusion in the porous medium.

In contaminant movement in aquifers the contribution of D_D to the dispersion term is usually negligible because the groundwater velocities are not small, resulting in the D_L^* term being relatively large. In finer grained beds such as unfractured clays, clayey silts, and shales the groundwater velocities are normally very low and molecular diffusion can be significant.

In laboratory experiments the coefficient of dispersion in the direction of flow is normally found to be much larger than the coefficients in the two transverse directions. The coefficient of dispersion is assigned values in these three orthogonal directions. The directional nature of the dispersion coefficients is generally considered to relate to the directional nature of the

hydrodynamic processes with respect to flow rather than to directional geometric properties of the porous medium. In other words, granular deposits that are geometrically isotropic, and consequently have isotropic hydraulic conductivities, are still directional with respect to dispersion. In laboratory experiments using homogeneous porous materials D_L is normally found to be larger than the transverse dispersion coefficient, D_T , by a factor of 5 to 20. Although geometric properties of the medium may affect dispersion independent of the directional effect of flow, it does not appear that suitable experiments have been performed to evaluate this possibility. The mathematical complexity that would result is considerable.

From laboratory experiments using cylinders or boxes filled with granular media such as sand or glass beads it has been established that

$$7) \quad D_L = \alpha_L v^m$$

where α is a characteristic property (length units) of the porous medium known as dispersivity and m is an exponent which is commonly close to unity and depends upon the amount of mixing that occurs due to molecular diffusion normal to the direction of flow (Bear, 1972, p. 606). In laboratory experiments on homogeneous granular materials values for α_L are of the order of 10^{-1} to one cm, which in effect indicated that dispersion is a relatively minor process under laboratory conditions that involve granular homogeneous materials or materials assembled in simple layered arrangements (Greenkorn, 1970). The dispersivities associated with the migration patterns of contaminants or artificial tracers in the field can be estimated using mathematical models, either analytical or numerical, based on equation (1) or its expansion in 2 or 3 dimensions. To reduce the uncertainties in the dispersivity estimates when calibrating these models, it is desirable to analyse the migration patterns of non-sorptive solutes, that is, solutes that do not interact chemically with the solid porous medium as transport occurs. Examples of relatively non-sorptive contaminants or tracers are Cl^- , NO_3^- , tritium and the stable isotopes, oxygen-

18 and deuterium. Approximate numerical solutions to equation (4) in two dimensions and without the sorption term are generally used in digital-computer simulation studies of the observed migration patterns of these constituents. From field studies the distribution of values for the following parameters are estimated: (1) hydraulic conductivity, 2) porosity, 3) hydraulic head, and 4) contaminant concentration. The first step in the modelling procedure is to simulate the hydraulic head distribution. This usually involves considerable adjustment of the K distribution until the simulated head pattern adequately resembles the field pattern. The next step is to simulate the contaminant concentration distribution using the simulated flow pattern and a trial-and-error adjustment of the values of the dispersivities, α_L and α_T , until the simulated contaminant migration pattern closely resembles the pattern observed in the field. In fractured rock, it is usually necessary also to treat porosity as a trial-and-error adjustment parameter.

This approach using two-dimensional digital models has been used by Konikow and Bredehoeft (1974), Robson (1974) and Pinder (1973) for contamination patterns in granular deposits, and it has been used in fractured rock by Robertson and Barraclough (1973) and Bredehoeft and Pinder (1973). Longitudinal and transverse dispersivities obtained from the above simulation studies are generally in the range of 10^1 to 10^4 cm, which is as much as five orders of magnitude larger than typical laboratory dispersivities. If the above field values are truly representative of dispersive capabilities of natural geologic materials, we would be left with no alternative but to conclude that contaminant plumes in active groundwater flow systems spread extensively both longitudinally and laterally. If this is the case, detection of the migration paths of contaminated groundwaters in heterogeneous materials should be a relatively simple task not requiring large numbers of monitoring points. An alternative explanation for the excessively large dispersivities obtained in the simulation studies is that the fitting procedure makes use of excessive dispersive fluxes to account for part of the

transport component that is really convective. This error could be difficult to identify, particularly in situations where the distribution of water-level and contaminant concentration data is rather sparse, as in the case of the investigations cited above. None of the above studies included an extensive analysis of parameter sensitivity. The above studies involved apparent contaminant migration patterns obtained from samples collected from boreholes either uncased or slotted over large vertical intervals; for example, hundreds of metres in the study area of Robertson and Barraclough (1973). Contaminants moving with little or no attenuation within narrow horizons would normally be detected at greatly diluted concentrations when sampled in the open boreholes. Using the trial-and-error simulation procedure to explain the dilution on the basis of a two-dimensional model of the three-dimensional system, one would probably resort to a strong dispersive flux and a weaker convective flux. It is our conclusion that dispersivities obtained by parameter adjustment procedures based on simulation models of poorly monitored field situations probably have little physical significance in terms of the actual dispersive capabilities of the hydrogeologic system.

Another problem encountered in the two-dimensional digital simulation approach to studies of regional contaminant migration patterns is that some simulation results are found relatively insensitive to dispersivity as an input parameter (Konikow and Bredehoeft, 1974; Robson, 1974). Robson concluded that the larger the numerical grid interval used in the model, the less sensitive the model is to dispersivity within a given simulation period.

Determination of useful values of dispersivity in field problems of contaminant migration is rather crucial in contaminant hydrogeology. If dispersivity values of the order of magnitude typical of laboratory tests on simple granular materials are appropriate, contaminant dilution by dispersion is very weak. If the values commonly reported in the literature as a result of digital simulation studies have real physical significance, we can

expect both granular and fractured geological materials to be capable of causing great dilution of contaminants in groundwater flow systems. An example of the difference in the dispersive capabilities of a low dispersivity groundwater regime and a high dispersivity groundwater regime is shown in Figure 3.

The question arises as to how can useful dispersivity values be obtained for field situations. This problem is far from being resolved. One approach is the two-well tracer injection test as described by Grove and Beetem (1971) and Grove (1971). However the mathematical models used to calculate dispersivities from these tests are based on the assumption that the tracer transport regime can be represented adequately in two dimensions and that the geologic materials at the test sites are homogeneous.

We expect that the dispersivities of natural geologic materials which are inherently heterogeneous compared to the materials normally used in laboratory dispersivity experiments are somewhat larger than the laboratory values. Theis (as quoted in Grove and Beetem, 1971) suggested that field values may be two orders of magnitude larger. A major effect of heterogeneities of different hydraulic conductivities is to cause abrupt changes in the groundwater flow paths. This is illustrated for two simple cases in Figure 4. Using sand-box experiments, Skibitzke and Robertson (1963) showed that the presence of small discrete lenses of high hydraulic

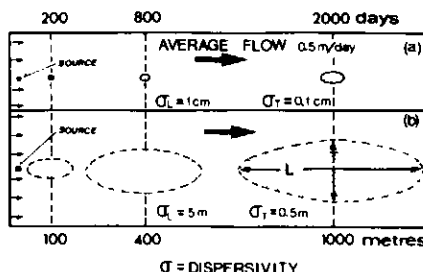


Figure 3
Changes in the areal extent of a contaminant zone as a result of dispersion in a steady, uniform flow system. Contaminant enters the system as a small slug at the source point. Patterns are shown for (a) low dispersivities, typical of laboratory results, and (b) dispersivities two and one-half orders of magnitude larger. Calculation procedures from Baetsle (1969).

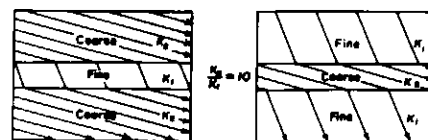


Figure 4
Refraction of groundwater flow lines across strata of different hydraulic conductivities (K_1, K_2) (from Hubbert, 1940).

conductivity within a matrix of lower conductivity sandstone can cause much stronger dispersion than occurred when the lenses were not present (Figure 5). Hillier (1975) using a box of similar design, showed that the presence of discrete lenses of lower conductivity can cause flow pattern distortions that produce even less transverse dispersion than occurred when the lenses were not present. In other words, heterogeneities can cause spreading or channelling or fingering of contaminant migration plumes. These effects are shown schematically in Figure 5. Because of heterogeneities caused by stratigraphic variations of different scales in geologic materials, the number and spacing of piezometers or wells necessary to adequately monitor migrating zones of subsurface contamination or zones of potential contamination cannot be determined without detailed drilling programs. The nature and density of drilling required in contaminant hydrogeology is much different than in water-supply hydrogeology.

In one of the few very detailed three-dimensional monitoring studies of contaminant migration reported in the literature, Childs *et al.* (1974) reported the following conclusions based on investigations of waste-migration patterns from septic field systems in sandy deposits near Houghton Lake, Michigan:

"The waste-migration plumes at Houghton Lake range from simple, multichemical plumes that move with regional flow to complex plumes that bifurcate, that show different migration patterns for different chemicals, and that move up the regional gradient for short distances. The complexity of these patterns is attributed to a combination of the following system properties: loading rate and recharge at the waste source, local hydrology, chemical-

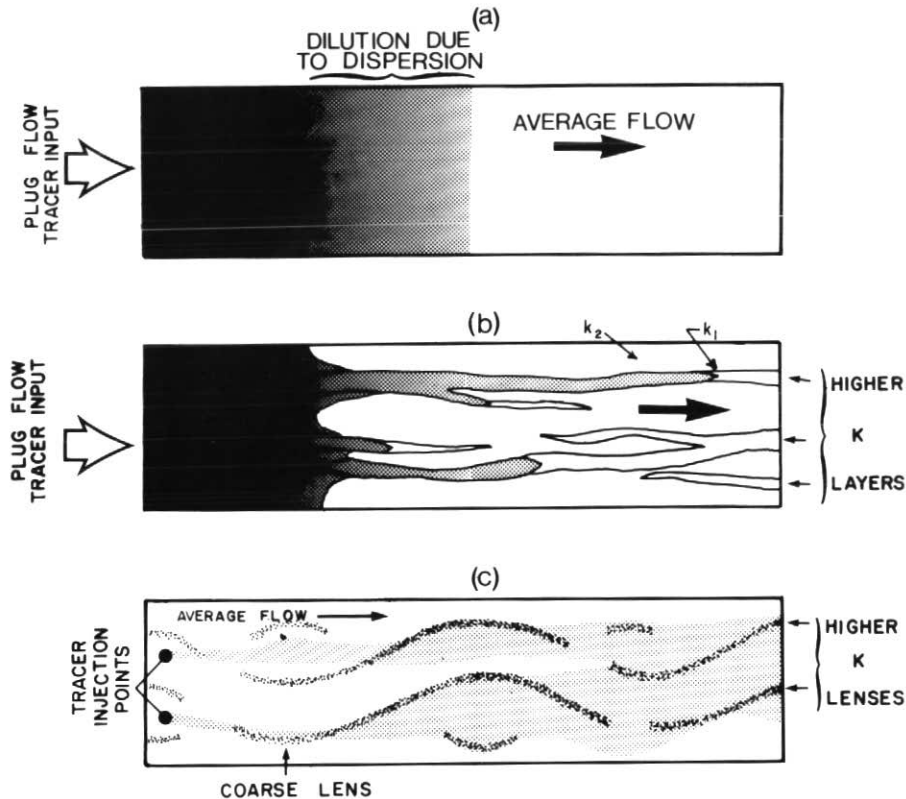


Figure 5
Dispersion in granular materials (a) simple dilution front in homogenous material (b) lingering of tracer front caused by layered

heterogeneities (adapted from de Josselin Jong, 1961) (c) strong lateral spreading caused by irregular high K lenses (adapted from Skibitzke and Robertson, 1963).

adsorption capacity of the soil, soil microbiology, regolith texture and fabric, and proximity to other waste sources. Based on the observed patterns, it is suggested that observation wells be placed so that an in-depth, 3-dimensional array of samples can be obtained."

These conclusions are especially noteworthy considering the fact that Childs *et al.* concluded that the deposits in the study area are "homogeneous to the eye". They also noted that:

"the plumes migrate along zones in the regolith that, although they are texturally similar, show subtle differences in fabric that result in slight variations in permeability. These bifurcations indicate that detection of a shallow plume does not negate the existence of other plumes of the same constituent at depth."

In the field it is difficult to recognize the degree of influence of micro-stratigraphic variations on flow line irregularities and velocity variations

using hydraulic head data from wells or piezometers. The hydraulic head distributions can be relatively smooth within the range of water-level measurement error, but because the velocity vector is proportional to the first derivative of the hydraulic head function in space (Eq. 5), variations of V can be large. This has been demonstrated by Hiller (1972) using digital simulations of hypothetical two-dimensional flow in porous materials with random heterogeneities of permeability. He concluded that the influence of permeability variations on the fluid pressure distribution is small compared to the irregularities in the front of a tracer moving through the system.

In regard to dispersion in fractured geologic materials the statement by Castillo *et al.* (1972) is a reasonable indication of the current status of investigations:

"Although the basic theoretical aspects of . . . (dispersion) . . . have been treated at length for the case where the permeable stratum is

composed of granular materials, the classical concept of flow through a porous medium is generally inadequate to describe the flow behaviour in jointed rock, and it becomes increasingly unsuitable for the analysis of dispersion. Despite these limitations, little work has been directed toward extending these ideas to handle flow through jointed rock formations . . ."

Using a simulation model verified by laboratory experiments described in a separate paper by Krizek *et al.* (1972), Castillo *et al.* show that very irregular dispersion patterns can be produced by relatively simple joint patterns. In nature, most joint or fracture systems are complex and in many situations could produce contaminant migration patterns that would be very difficult or impossible to monitor.

In Canada nearly all bedrock that has significant permeability is fractured. This includes such diverse materials as shale, sandstone, limestone, dolomite, and igneous and metamorphic rocks of the Precambrian Shield. The prediction of flow paths and dispersion in these materials may, in many situations, not be a practical endeavour.

In the Interior Plains Region and locally in other regions, clayey Quaternary deposits such as glacial tills and glaciolacustrine clays are commonly fractured. Grisak and Cherry (1975) and Grisak *et al.* (1975) have shown that the fracture networks represent a hydraulic continuum through which groundwater flows at velocities many orders of magnitude larger than in unfractured clayey deposits. The reason for the extreme velocity differences is evident from the Dupuit-Forchheimer relation. The effective bulk fracture porosity of the fractured tills and clays is in the order of 10^{-4} whereas the porosity of the unfractured materials is in the range of 0.2 to 0.4. The influence of fractures on the sorption term in equation (1) is discussed in Part 2 of this paper.

Conclusion

The differential equation that describes the migration of dissolved contaminants in groundwater flow systems has been established for more than a decade. For the movement of conservative constituents it includes two main physical parameters (1) groundwater velocity and (2) dispersivity. The problem facing hydrogeologists in the following decade is to determine the most reliable and efficient methods of determining these parameters under field conditions and to develop a more quantitative understanding of the uncertainties associated with the field determinations.

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