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Diffusion in Hydrogeology

John Barker

School of Civil Engineering and the Environment, University of Southampton, Highfield,
Southampton, SO17 1BJ, United Kingdom

E-Mail: J.A.Barker@soton.ac.uk

Abstract

The field of hydrogeology is primarily concerned with the flow of water below the ground surface and with transport, normally of solutes and heat, within that water. Many disciplines have contributed to this endeavor which requires skills from across the spectrum of science, engineering and beyond. The diffusion equation describes not only solute transport but also the flow of water, via Darcy's law. Of particular interest is transport in fractured rock where most of the flow is through the fractures while most of the storage is in the rock pores: a 'double-porosity' system. Hydrogeology remains a field that welcomes those who bring techniques from other areas of science to address problems as varied as water supply, radioactive waste disposal and geothermal energy.

Keywords: Diffusion, hydrogeology, groundwater, transport, subsurface, rocks.

1. Introduction

People with backgrounds in many different disciplines would refer to themselves as a hydrogeologist. For example there are those working in organizations such as the World Bank that deal primarily with socio-economic issues of water supply; then there are those who are concerned with physics relating to the safe disposal or radioactive waste. Many other people who contribute to hydrogeology consider themselves as working in different disciplines, e.g. soil physics. What all of these people have in common is that they are concerned about fluid, normally water, flow below the ground surface and transport within that fluid.

Here are some other activities, beyond water resources, where you would find hydrogeologists taking a major role if not the lead: geothermal energy exploration, remediation of contaminated land, ecological protection, landfill design, mine drainage, dewatering of construction sites, dam design, carbon dioxide sequestration, and radioactive waste disposal.

Hydrogeology is primarily an applied science aimed at aiding decision making and those decisions are almost invariably underpinned by modelling. Indeed almost any form of training in hydrogeology will involve an introduction to modelling and every year there are international conferences on that topic; sometimes those meetings even focus on the use of a particular model or a particular technique, such as the finite-element method.

Most of the models used by hydrogeologists deal with the flow of water and many also include a transport process: most commonly the transport of a dissolved substance but also heat and particle transport.

The aims of this paper are: to explain the occurrence of diffusion processes in hydrogeology; to outline some of the techniques that we use, both experimentally and in modelling; and to show that interesting challenges remain. Hydrogeology has always borrowed methods from other disciplines and the hope is that this paper will help continue that process. It is also possible that some of our approaches that I describe could be adapted for use in other fields.

A very readable introduction to hydrogeology was provided by Price [1].

2. The occurrence of the diffusion process in the subsurface

Water, solute and heat transport are all of importance in the subsurface, often these are coupled but we will consider them separately here. The flow of water is often the dominant transport process and, since it is least obvious why the flow of water should be regarded as a ‘diffusive’ process, it will be dealt with at some length.

2.1 Water flow

Water occurs in and flows through the voids in the subsurface which can vary greatly in their geometry and size. Whenever this flow occurs energy is lost due to viscous forces, hence water must flow from places where it has higher energy to places where it has lower energy. This problem was considered most eloquently by Hubbert [2] who showed that the energy per unit mass of a fluid can be written in the form:

$$H = \frac{v^2}{2} + gh + \frac{p}{\rho} \tag{1}$$

We often refer to H as the Hubbert potential but also as the total head as, relative to an appropriate datum, it is represented by the level that water will rise in a well. The above expression will be familiar to most readers as the quantity that remains constant along a flow path in the Bernoulli equation, which we recall applies to non-viscous flow.

We conclude that water will flow in the direction of decreasing total head, i.e. in the direction of the vector $-\nabla H$. However, this was known empirically long before considerations of the physics: most notably, 150 years ago, Darcy [3] showed that flow rate is proportional to head difference in a set of rather elegant experiments. Nowadays we would write the volumetric flow rate, volume of fluid per unit time per unit area, $\mathbf{q}$, as:

$$\mathbf{q} = -\mathbf{K}\nabla H \tag{2}$$

where tensor $\mathbf{K}$ is known as the hydraulic conductivity. In acknowledgment of Darcy’s work, often regarded as the first scientific contribution to hydrogeology, we both refer to this equation as Darcy’s Law and the quantity $\mathbf{q}$ as the Darcy velocity. Darcy’s equation is clearly equivalent to Fick’s first law; now we will see how groundwater flow gives rise to an equation equivalent to Fick’s second law.

Water and rock are compressible; they are not very compressible – for water $(\Delta V/V)/\Delta P \approx 5\times10^{-10}$ Pa^{-1} – but there is a lot of water below the ground surface. Most rocks of practical interest for water supply have porosities between 10% and 40%, so a small change in pressure can be associated with a significant exchange of water.

If we push a volume ΔV of water into unit volume of the subsurface then, assuming elastic behavior, this would be accompanied by a pressure change and hence a small change in head ΔH. If we assume elastic behavior we expect $\Delta V = \left(-\nabla.\mathbf{q}\right)\Delta t \propto \Delta H$. In fact we characterize the combination of the elasticity of the water and rock into a single parameter called the specific storage, S_s, and write $S_s \partial H / \partial t = \nabla.\mathbf{q}$. Combining this with Darcy's law given above we have an equation for transient groundwater flow

$$S_s \frac{\partial H}{\partial t} = \nabla.(\mathbf{K}\nabla H) \qquad (3)$$

which we recognize as equivalent to Fick's second law of diffusion. As the reader may have guessed, we could derive this same equation from the Navier-Stokes Equations. That approach would also result in a more general form where the fluid density and pressure are both scalar fields; that is the form normally employed in numerical models.

2.2 Solute transport

Let's move on now to consider solute transport in the subsurface. It needs little introduction and will come as no surprise that solute transport can often be described by an advection-dispersion equation:

$$n\frac{\partial c}{\partial t} + \mathbf{q}.\nabla c = n\nabla.(\mathbf{D}\nabla c) \qquad (4)$$

where c is concentration (mass/volume), n is the porosity, $\mathbf{q}$ is the Darcy velocity and $\mathbf{D}$ is a tensor with elements called the coefficients of hydrodynamic dispersion. For 1-D transport we would often write the longitudinal coefficient as

$$D_L = D_d + \alpha_L |v| \qquad (5)$$

where D_d is the molecular diffusion coefficient, v_L is the velocity and α_L is called the (longitudinal) dispersivity. The form of Eq. (5) has been confirmed in many laboratory experiments giving data such as that shown in Fig. 1.

2.3 Heat transport

Heat transport in the subsurface is analogous to solute transport and, as expected, this gives rise to transport equations such as:

$$\frac{\partial T}{\partial t} + \mathbf{q}.\nabla T = \kappa \nabla^2 T \qquad (6)$$

where T is the temperature and κ is the thermal diffusivity. The coupling between density, temperature and pressure is so strong that we rarely solve this equation in isolation and numerical models normally have to be used. An exception is for 'low enthalpy' geothermal systems.

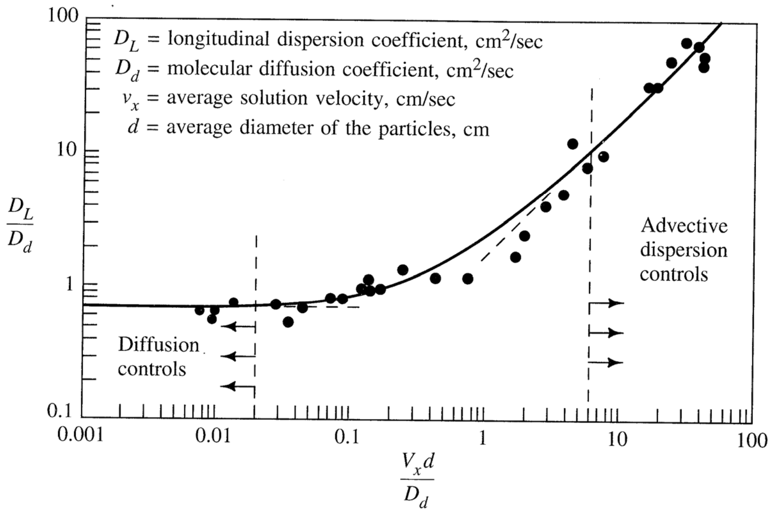

Fig. 1. The increase of longitudinal dispersion with velocity showing that the dispersion coefficient tends to the molecular diffusion coefficient for small velocity and becomes proportional to velocity at high velocities. (From [4].)

3. Why is hydrogeology difficult?

It would be quite reasonably to look at the equations above and think that hydrogeology must be really quite simple. The equations are normally linear and are very common, so numerous analytical solutions are available and numerical models that are capable of solving these equations abound. What makes the life of the hydrogeologist difficult is that:-

a) the subsurface is extremely heterogeneous;

b) the boundaries of our systems are uncertain;

c) the stresses on these systems are highly variable and uncertain (e.g. rainfall, pollution incidents); and, perhaps most importantly,

d) it is very difficult to access the subsurface to make observations either of the fabric of the rock or of the transport processes.

Heterogeneity in the subsurface is often a reflection of geological changes and stresses. Many rocks are fractured and flow through fractures often totally dominates over from the surrounding porous rock. For example, the intact rock, between the fractures, shown in Fig. 2 probably has a hydraulic conductivity of about 10^{-7} m/s. Suppose we had a kilometer thickness of such intact rock, then a single horizontal fracture with an aperture of just one millimeter would carry as much water as the intact rock for the same head gradient!

With regard to storage, however, the situation is reversed: typically the fractures will only contribute a few percent to the porosity. We refer to such systems, where fractures dominate flow while the rock ‘matrix’ pores dominate storage, as a ‘double-porosity’ system. The term ‘dual-porosity’ is also used. When considering water flow this is taken to occur in both the fractures and rock matrix, with a flow interchange between the two. Normally when considering solute or heat transport, the matrix pore water is approximated as being static and then we often refer to ‘mobile’ (fracture) water and ‘immobile’ (pore) water.

Fig. 2. Typical fractured rock (limestone). We would normally model this as a ‘double-porosity’ system. Note that it is difficult to determine the scale from such pictures.

In applied geology we take a very broad view of what can be regarded as ‘rock’. For example, I am currently involved in a large project on flow and transport in landfills: we regard this waste material as part of the fabric of the earth’s surface but with a few unusual heterogeneous features (e.g. plastic bags).

4. The hydrogeologist in the field

Imagine a hydrogeologist arriving on a Caribbean island with the remit to assess the water resources of the island. He will identify any wells and try to make sure these are properly surveyed so their relative elevations are known. Then he will find the depth to water in the wells and thus determine the relative heads. A contour plot of those heads gives the flow directions, in the same way that any topographical map indicates the slope of the land. In principle, the curvature of that surface should give an indication of the rainfall input, however, I have never seen data good enough to make that calculation.

But this only tells the hydrogeologist the direction of groundwater flow and the gradient of head. What he really wants is the hydraulic conductivity to put into Darcy's law to estimate flow rates.

4.1 The pumping test

The hydrogeologist would try to arrange for water to be pumped from some of the wells and for observations to be made of the response of the water levels in the same wells or (preferably) neighboring wells. Such a procedure is called a 'pumping test' and is normally carried out over a period of several days. If he can carry out such an experiment, he will start the analysis by plotting the data in various forms. He will hope and very often observe that the data will conform to the solution of the diffusion equation given by Theis [5], one of the most useful results in hydrogeology. This 'Theis solution' gives the change in head at radius r at time t in terms of the pumping rate, Q, and aquifer properties K and S_s:

$$\Delta H = \frac{Q}{4\pi bK} E_1(u) \quad \text{where} \quad u = \frac{S_s r^2}{4bKt} \tag{7}$$

where E_1 is an exponential integral and b is the thickness of saturated rock.

Indeed, it appears that the transient flow equation, Eq. (3) was first written, in relation to this problem of (cylindrical radial) flow to a well, by Theis [5]. And, since the solution is of such practical importance, Theis is rarely recognized for having been one of the first to identify the significance of elasticity, in the way that Fourier has been recognized for the equivalent result in heat transfer. Also it is a pity in that it is clear that the mathematical solution was obtained not by Theis himself but by a more mathematically skilled colleague.

At large times (small u) the E_1 function in Eq. (7) tends to a logarithm, so a plot of head change, ΔH, against $\ln(t)$ should tend to a straight line with slope $Q/4\pi bK$. So our hydrogeologist will commonly aim to construct this graph and estimate the hydraulic conductivity, K, as the long-time slope multiplied $4\pi b/ Q$. (Asymptotic analysis is very important for data analysis in hydrogeology.) In practice, that straight line will appear but often, especially for long pumping tests, with then increase in slope by a factor of two or decrease to zero. These features indicate the influence of a linear barrier (e.g. a fault) or a source of water (e.g. a lake), respectively, and can both often be analyzed by the method of images.

A remarkable finding is that this head versus log(time) slope analysis always appears to gives the arithmetic average permeability, K, of the subsurface, no matter how heterogeneous, but I am not aware of a general proof. One finding for which there is a general mathematical proof [6,7] is that if you pump at one point and observe the head changes at another, then if you reverse the points the same response will be obtained, no matter what the heterogeneity provided the flow remains diffusive, i.e. conforms to Eq. (3).

So, a good way to think of this pumping test is that it is a test that by its very nature overcomes the complexities (heterogeneities) of the subsurface. The same is true of the other field technique I want to mention, tracer tests.

4.2 The tracer test

There are written accounts of the use of tracers in relation to natural water flow going back at least to Roman times. For example, Roman historian Josephus reports, in his "Wars of the Jews", a test being carried out using chaff. The tracers commonly in use today are:-

- Particles: e.g. Lycopodium spores, Microspheres
- Microbiological: e.g. Bacteriophage
- Inorganic salts: e.g. Cl, Li
- Fluorescent dyes: e.g. Rhodamine WT, Fluorescein
- Fluorocarbons: e.g. SF6, Freon (including CFCs)
- Isotopes: e.g. Br-82, Cl-36, I, Tritiated water, Deuterated water

The list is restricted by a number of factors, particularly detectability and the avoidance of risk to health.

We can in this way establish connections from one place to another. Typically we put the tracer into a well and observe at another well. Often we never see our tracer again but if we are lucky we obtain concentration versus time data that we can analyze for transport parameters such as travel time and dispersivity.

Fig. 3 shows a collection of values of dispersivity, α_L, in Eq. (5) and this is seen to be dependent on the scale. Such scale dependence (sometimes referred to as 'anomalous dispersion') has been the subject of a great deal of speculation and innovation [8] but remains a problem. At the practical level of modelling, what most hydrogeologists are forced to do is to run their models with a variety of dispersivity values which is obviously inconsistent. At a theoretical level this has led to considerations such as transport on fractals and use of the continuous-time random walk theory [9].

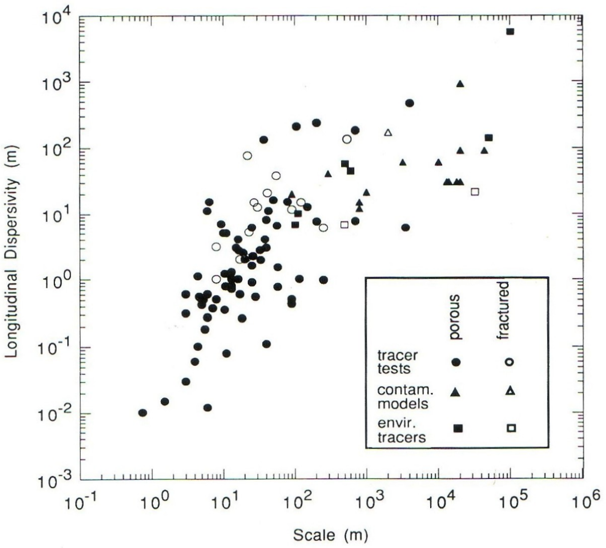

Fig. 3 Scale-dependence of dispersivity, α. (From [10].)

5. The hydrogeologist in the laboratory

The hydraulic conductivity of a rock is obviously amenable to measurement by passing water through a sample and measuring the head difference for a given flow rate. Often, however, we use gas instead of water to make such tests faster, and correct for the viscosity. Other corrections are sometimes applied due to ‘gas slippage’.

Hydrogeologists need molecular diffusion coefficients for their models. Much work has been done, in particular, to determine coefficients for the diffusion of radionuclides in various rocks, in relation to the subsurface storage of radioactive waste. Mostly the experiments are of the standard design with two cells separated by a thin sheet of rock. However, an experiment carried out by some of my colleagues in the British Geological Survey [11] used a rather unusual arrangement (Fig. 4). Essentially this is a reaction vessel with the blades of the stirrer replaced by a standard (‘one-inch’) rock core

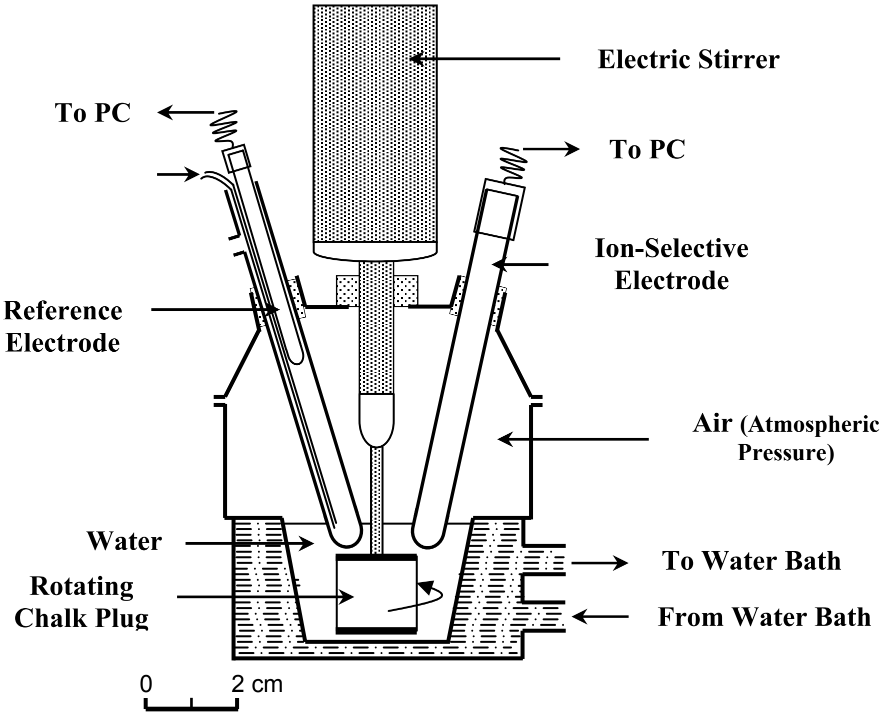

Fig. 4. Schematic representation of analytical equipment used to determine diffusion of chloride (or bromide) from consolidated porous plugs. (From [11].)

A very common type of experiment carried out in our laboratories is to pack a column with material and pass water and chemicals through, under a vertical head gradient. Normally we analyze what comes out of the bottom or top, a ‘breakthrough curve’, of such a column but sometimes the column is taken apart, sometimes after freezing, to obtain a spatial distribution.

6. Some modelling approaches

6.1. *Numerical modelling*

Given the heterogeneity of the subsurface and the complex boundaries involved, it is not surprising that modelling methods such as the finite element method have attracted much attention in hydrogeology. The method allows us to vary boundaries and regions of variable properties greatly as well as refine the mesh around points of specific interest. When the heterogeneity is not too great, the boundary integral equation method (equivalently, the boundary element method) becomes a particularly useful tool. However, finite difference models are also widely used and the most commonly used code, Modflow, is of this type.

Particular challenges to flow modelling are thrown up by the nonlinear behavior of the water table and seepage faces. Similarly, nonlinear sorption can cause difficulties for transport modelling.

6.2. Laplace-transform analytical solutions in hydrogeology

Consider advective transport through a channel containing blocks of rubble, Fig. 5.

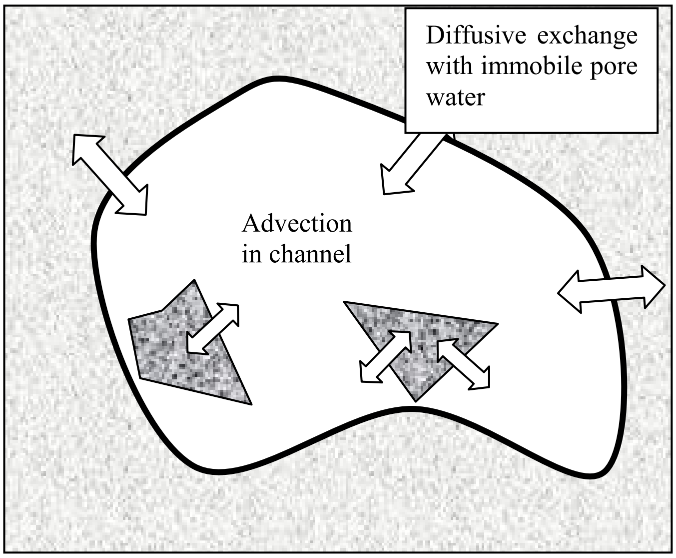

Fig. 5. An example of a 'double-porosity' system. Advective transport through a channel (into the page) with diffusive exchange (arrows) from mobile water into a relatively immobile pore water within internal 'blocks' and external to the channel.

Let's ignore dispersion and assume good mixing at any distance along the channel, so we have a single 'mobile' water concentration, $c(x,t)$, at any distance x along the channel. A Laplace transform solution can be written:

$$\bar{c}(x,p) = \int_0^\infty e^{-pt} c(x,t)dt \\ = \bar{c}(0,p)\exp\left\{-pt_a\left[1+\sigma \mathrm{B}\left(\sqrt{pt_{cb}}\right)+\rho \mathrm{C}\left(\sqrt{pt_{cc}}\right)\right]\right\} \tag{8}$$

Here p is the transform variable, $c(0,t)$ is the input concentration (assumed known), t_a is the travel time to point x, σ is the ratio of block porosity to channel porosity, ρ is the ratio of porosities outside and inside the channel. I refer to the two functions B and C as the 'Block Geometry Function' (BGF) [12,13] and 'Channel Geometry Function' (CGF), respectively. Chemical engineers will recognize B as being equivalent to their 'effectiveness factors' [14]. Simple examples are $\mathrm{B}(x) = \tanh(x)/x$ for slab-shaped blocks and $\mathrm{C}(x) = \mathrm{K}_1(2x)/[x.\mathrm{K}_0(2x)]$ for a circular channel. These functions depend *only* on the geometry of the blocks and the channel, respectively, and contain *all* of the relevant information: sizes are contained in the parameters t_{cb} and t_{cc}.

In the time domain, we can write a partial-integro-differential equation where the BGF appears, in inverse form, as the kernel of the integral: see [13]. Such equations are a natural basis for numerical modelling.

The characteristic time for diffusion across a block, t_{cb}, is equal to the square of the volume-to-area ratio divided by the diffusion coefficient within a block, as in Fick's second law. Similarly, the characteristic time for diffusion out of the channel, t_{cc}, is equal to the square of the channel area-to-perimeter ratio divided by the diffusion coefficient outside the channel.

A practical elegance of this formulation is that the B and C functions are readily replaced to reflect different geometries without affecting any other part of the formulation. Also, for mixtures of blocks of different shapes and sizes, we can write an effective function:

$$\mathrm{B}_{effective} = \sum_{i=1}^{n}\int_0^\infty P_i(\beta)\,\mathrm{B}_i\left(\frac{x\beta}{b}\right)d\beta \tag{9}$$

where $P_i(\beta)$ is the proportion by volume of blocks of shape i in the size range β to β+dβ (β = volume/area for a block).

To avoid the impression that the above form of solution is restricted solute transport through voids filled with blocks, I give a further solution for flow to a well in a fractured rock formation: imagine a hole drilled into the rock shown in Fig. 2. The change of head in the well when pumped at volumetric rate Q has the general form:

$$\overline{H}_w(p) = \frac{Q/(2\pi Kb)}{p\left[pt_1 + \mathrm{C}\left(\sqrt{pt_2(1+\sigma \mathrm{B}(\sqrt{pt_{cb}}))}\right)\right]} \tag{10}$$

where K and b are the hydraulic conductivity and thickness of the rock formation C characterizes the shape of the well, normally a tube, and B characterized the shapes of the porous blocks. Note that the B function is contained within the argument of the C function. (The times, t_1 and t_2, characterize the well storage and well diameter, respectively. Incidentally, if we set $t_1=\sigma=0$, so there is no well storage or matrix storage, Eq. (10) gives the Laplace transform of the Theis solution given in Eq. (7).)

The two functions B and C not only arise in relation to Laplace transform solutions of transient problems but also in relation to periodic behavior (when the Laplace transform variable p would be replaced by iω) and steady-state solutions with 'production', e.g. rainfall for flow or radioactive decay producing daughter products such as radon (when p would be replaced by the decay constant).

6.3. First-order exchange

In most branches of hydrogeology and transport science more generally, a first-order exchange approximation is assumed. This is for example called a 'dead-end pore model' (especially by soil scientists), 'quasi-steady-state model' and 'pseudo steady-state model': I'm sure there are other names

Normally this enters our transport equations in the form:

$$\frac{\partial \phi}{\partial t} = \frac{\alpha}{t_{cb}}(\Phi - \phi) + \text{other terms} \tag{11}$$

where ϕ is a potential (e.g. concentration, head or temperature) of the mobile phase and Φ is the average potential of the immobile phase, and α $[T^{-1}]$ is the exchange coefficient.

Formulated as a BGF this gives:

$$\mathrm{B}(x, \alpha) = \frac{\alpha}{\alpha + x^2} \quad \text{or, for transient problems,} \quad \mathrm{B}\left(\sqrt{pt_{cb}}, \alpha\right) = \frac{\alpha / t_{cb}}{p + \alpha / t_{cb}} \tag{12}$$

If diffusion is the true underlying exchange mechanism, this can be regarded as an approximation and an important issue is how to select the parameter α appropriately. Two approaches are: (a) to expand Eq. (12) and the BGF of interest as a Maclaurin series, then matching to giving $\alpha = -2/\mathrm{B}''(0)$, or (b) to compare partial fraction (Mittag-Leffler) expansions. For a slab geometry, $\mathrm{B}(x) = \tanh(x)/x$, these two approaches give $\alpha = 3$ and $\alpha = \pi^2/4$, respectively. For long-time asymptotic behavior (where α/t_{cb} becomes the decay constant), since $L^{-1}\{1/(p+k)\} = e^{-kt}$, the latter result ($\alpha = \pi^2/4$) is the more relevant. However, there remains considerable disagreement in the hydrogeology literature over the appropriate choice of the parameter α, if chosen to approximate a given BGF for a given block shape. My own view [13] has always been that either or neither approach may be valid given that the BGF can appear in so many different ways, as a functional, in a solution (e.g. Eq. (10)).

These issues have been revisited recently by one of my students [15] who has shown, for example, that the Maclaurin-expansion comparison method is equivalent to temporal-moment matching. It would be of interest to hear how this issue has been dealt with in other fields.

In more general terms, if we expand any BGF, for a specific geometry or as in Eq. (8), in partial fractions we obtain a sum of terms, such as that on the right of Eq. (12), which represent a set of first-order exchange coefficients. The existence of such a set has been the starting point for modelling by some researchers [16] and is possibly more popular than the BGF approach, at least in the US.

6.4. Numerical inversion of Laplace transforms

We tend to favor Laplace transform solutions as analytical inversion is often difficult if not impossible, for their simplicity, as exemplified above, and for the ease of extracting asymptotic behavior and moments. But of course, in practice we normally need time-dependent solutions: since analytical inversion is normally difficult and sometimes impossible, we use numerical inversion of the Laplace transform.

Although this inversion is an ill-conditioned problem, many methods have been proposed. For the types of transport problems I have encountered in hydrogeology I prefer to formulate my codes to use both the Talbot method [18] and the deHoog [19] method: the former tends to be quicker and can be very accurate, the latter is more robust but can be significantly slower. However, given that both of those methods require the transform to be given as a function with a complex argument, I often initially use a scoping code (only eight lines long) based on the Stehfest [20] algorithm where the transform function has a real argument.

It is worth mentioning that some use is made in hydrogeology of hybrid methods where we take partial differential equations and remove the $\partial\phi/\partial t$ term of the diffusion equation by the Laplace transform, giving $p\bar{\phi}-\phi(0)$, and then solve the spatial part of the problem by the usual finite-difference or finite element approaches. This approach was to the best of my knowledge first published in the heat transport literature in the 1970s.

6.5. Parameterization

What the above solution brings out is that we can normally parameterize these transport systems in terms of a set of times and storage ratios. This is often a great help in understanding the behavior of a system. For example, the three characteristic times in Eq. (10) can be ordered in 3! ways, so there are possibly six characteristic forms of behavior. (Hydrogeologists will probably note, however, that t_2 is, in practice, always smaller than the other two so there are really just two forms of behavior.)

Moreover, consideration of those times often helps us make approximations and formulate numerical solutions.

Of course we often have advantages in writing our equations in terms of dimensionless quantities. However, it is worth noting that commonly encountered dimensionless groups can be re-written in terms of the ratio of two times, e.g.:

$$Pe=\frac{vL}{D}=\frac{v}{L}\frac{L^2}{D}=\frac{t_{\text{Diffusion}}}{t_{\text{Advection}}} \tag{13}$$

By dividing each of the set of characteristic times for a given problem by the time of prime interest, one that will never be zero, the most appropriate groups will tend to arise.

For double-porosity systems the function $\mathrm{B}(x)$ tends to unity as x tends to zero hence, from the properties of the Laplace transform, we see that at long times $1+\sigma\mathrm{B}$ tends to $1+\sigma$. What this represents is that at long times the effective storage is the total storage and the t_{cb} parameter becomes unimportant. Similarly, $\mathrm{B}(x)$ tends to $1/x$ as x tends to infinity and this indicates that at short times $\sigma\,\mathrm{B}\left(\sqrt{pt_{cb}}\right)$ can be approximated by $1\Big/\sqrt{pt_{cb}/\sigma^2}$. This makes sense physically in that this expression represents 1D diffusion into the near surface of the blocks: the time t_{cb}/σ^2 represents the characteristic time for the fracture water to equilibrate with an equal volume of matrix pore water.

The general point to draw from this is that for double-porosity systems the single parameter t_{cb} / σ^2 is controlling at short times, both σ and t_{cb} at intermediate times, and σ alone at long times. The recognition of such behaviour, the change of effective parameters over time, which must occur in many transport problems, is particularly important to experimental design and to data analysis.

7. Flow dimension: anomalous hydraulic diffusion

I would now like to consider one implication of heterogeneity for flow: one that I have found particularly interesting.

If we consider flow to a well in a fractured rock system (e.g. Fig. 2) then it is not unreasonable to question a natural assumption in the Theis solution, Eq. (7), that the flow pattern is two-dimensional 'cylindrical' flow to the well.

I first began work on this issue in the 1980s when I was analyzing hydraulic data from a mine as part of a radioactive waste disposal investigation. I came to the conclusion that it is best to regard the flow dimension as a parameter that must be determined empirically and which may not have an integer value [21]. Incidentally, the generalization of the Theis solution, Eq. (7), is obtained by replacing the exponential integral $\mathrm{E}_1(u) = \Gamma(0,u)$ by the incomplete gamma function $\Gamma(d_f/2-1,u)$ where d_f is the flow dimension.

This idea of flow dimension has been applied quite widely over the last twenty years and tends to reveal dimensions in the range 1.3 to 1.8. The reason I favor as an explanation is shown in Fig. 6. This is the result of a simulation to flow in a randomly fractured medium to a central point in the plane. Most of the flow is confined to just 10% of the fractures (right) and clearly the flow pattern is rather like the spokes on a wheel: one-dimensional.

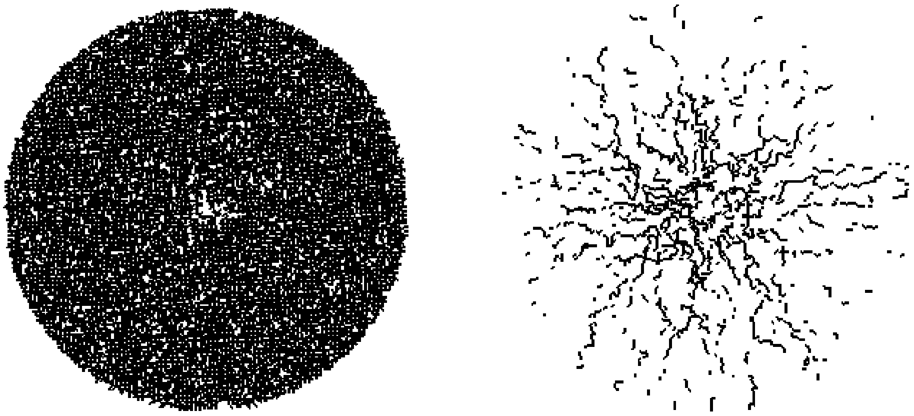

Fig. 6. Flow in a dense 2D random network (left) with variable conductivity gives rise to channeled flow (right) with dimension close to 1D.

However, a rather different approach has been taken in the petroleum literature [22]. The starting point of that approach is that rocks often look fractal (e.g. it is difficult to guess the scale for Fig. 2) and statistical analysis of fracture patterns in rock (e.g. box-counting) bear this out. This naturally leads to the idea that flow in fractured rock should be regarded as diffusion on fractals, and in [22] it is assumed that this should be described by a diffusion equation of the form:

$$\frac{\partial}{\partial t}H(r,t)=\frac{D_0}{r^{d_f-1}}\frac{\partial}{\partial r}\left(r^{d_f-d_w+1}\frac{\partial}{\partial r}H(r,t)\right) \tag{14}$$

This equation has the associated anomalous diffusion relation: $\langle r^2(t)\rangle \sim t^{2/d_w}$ in which $\langle r^2(t)\rangle$ is the mean squared distance covered in time t and d_w is the 'walk dimension'. This generalizes my approach where I had effectively assumed d_w=2. However, the above diffusion equation is just one of several that have been proposed [23].

Interest in this issue led us to simulate random walks on the Sierpinski gasket: we iterated the generators 9 times to obtain a 19,683×19,683 lattice. A typical result of that work is shown in Fig. 7.

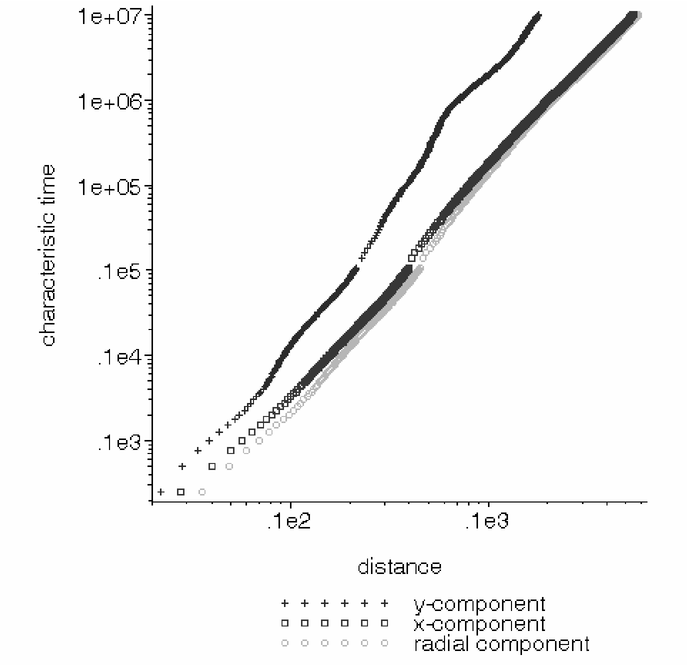

Fig. 7. Random walk simulation results for a Sierpinski carpet. Note the lack of consistency in dimension d_w both in direction and with time. (From [24].)

From Fig. 7 and numerous similar results it was concluded [24] that *none* of the proposed diffusion equations [23] properly represents diffusion on a fractal. One possible conclusion is that we should regard the proposed equations and their solutions as ‘hypotheses’ to be tested.

(This is obviously a topic that is being studied by many scientists with varying interests and it is therefore particularly difficult to keep up with the literature.)

8. The hydrogeology of radioactive waste disposal.

Having laid some of the foundations of the science of hydrogeology, we can deduce a few things about a particularly important problem that hydrogeologists work on: radioactive waste disposal.

Starting with the advection dispersion equation, we can see that it would be a good thing to minimize the flow rate so that the waste materials, especially the radionuclides, stay at or near the repository. From Darcy’s law, Eq. (2), we see that we therefore would like low permeability rock with low head gradients. Those are indeed amongst the main criterion used in site selection for repositories; other factors include the geological stability and the ability of the rock to sorb radionuclides. While we can seek sites with negligible flow rates we cannot stop other migration processes and in particular diffusion; i.e. we cannot reduce the hydrodynamic dispersivity below the molecular diffusion coefficient.

An obvious target material for disposal is clay with its very low permeability. Fig. 8 shows a profile of helium at a potential repository site, this has a shape that is consistent with a diffusive equilibrium which indicates negligible advection.

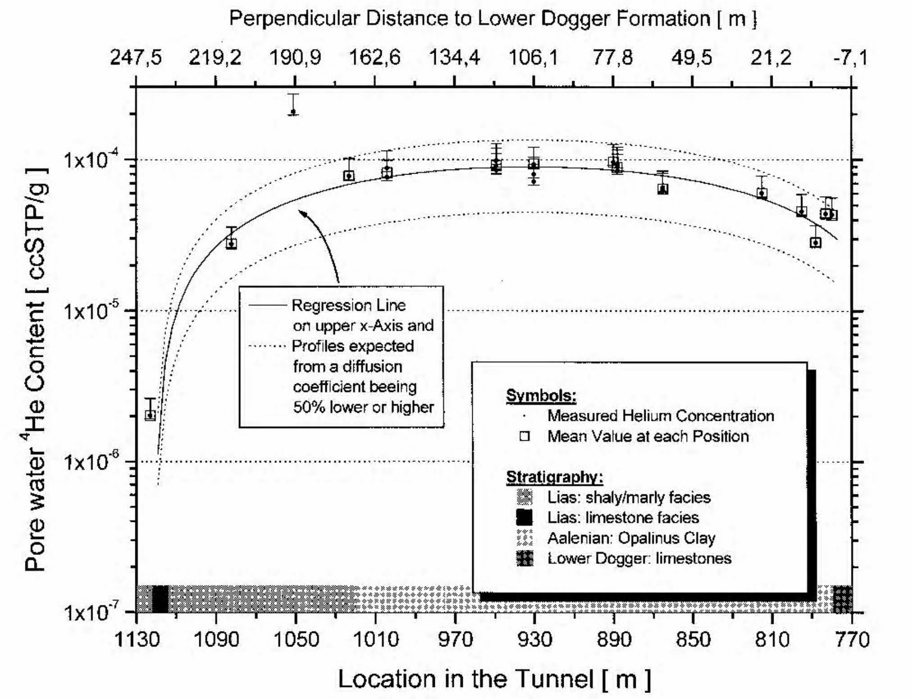

Fig. 8. Observed diffusion profile for helium in a clay formation with a fitted diffusion (with production) model. A *D* value of about 3×10^{-11} m^2/s over a distance of about 250 m gives a characteristic time of 10 to 50 millions of years. (From [25].)

Some countries, through the constraints of their geology, have to consider hard rocks (especially granite) for disposal of radioactive waste. While these materials are, like clay, of very low permeability they invariably contain cracks which are conduits for water flow. This was initially considered a significant problem until it was realized that diffusive exchange of solutes from flowing groundwater into the surrounding micro-fissures of the rock (i.e. the ‘double-porosity’ mechanism discussed earlier) would have a profound influence on the transport [26].

A good starting point for anyone new to radioactive-waste science and issues, is http://www.radwaste.org/.

9. Conclusions

Hydrogeologists spend a lot of their time investigating diffusive processes relating to water flow, the transport of solutes (normally contaminants) and, less commonly, heat. Although the relevant transport equations tend to be simple, the inaccessibility and heterogeneity of the subsurface cause significant difficulties. In the field we carry out experiments (pumping tests and tracer tests) which, at least partially, aim to cut across the complications caused by the heterogeneity.

This short paper cannot do justice to the very great efforts and wide-ranging literature relating to transport in the subsurface. The view presented is very much a personal one and another hydrogeologist would have given a different emphasis and different examples. In particular, the following topics deserved more attention:

- numerical modelling [27, 28],
- percolation theory [29, 30],
- the fractal nature of rocks [31],
- multiphase flow [32], and
- geostatistical methods [10, 33].

My main aim has been to show that the field of hydrogeology offers up a wide variety of challenges in relation to practical and theoretical aspects of transport theory. I sincerely hope that some of the younger readers will be encouraged to join in this effort. We all need water and we should apply our best science to the exploitation and preservation of this valuable resource.

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