Chapter 4

Probabilistic estimation of the radioactivity migration

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4.1 Introduction

This chapter deals with the probabilistic estimation of the radioactivity migration in a porous medium. In chapter 2, the deterministic parallel fracture model to estimate the migration of the radioactivity has been dealt with. There it is noted that a Laplace transform based analytical solution can be arrived at only when the source is assumed to be of constant strength. Moreover, this mode of solution has a major limitation with respect to the maximum distance of evaluation that turns out be about 200m in quadruple precision. To extend the solution beyond this limit, four different finite difference approximations have been tried and the results are reported in chapter 2. These schemes do not suffer from this distance limitation to a larger extent and they can also handle a non constant source. But the finite difference schemes have limitations with respect to greater accuracy and the memory utilization. This was the motivation to use the two variants of a pseudospectral method which could provide accurate results up to 300m. Although all these methods provide an estimation of the radioactivity migration, they still use a very simplified picture of a rock. The parallel fracture model is an idealization where the rock is thought to be a combination of an infinite array of identical parallel fractures separated by porous matrices of equal width.

In reality, a rock consists of porous blocks of uneven size in which several networks of randomly oriented and interconnected fractures are embedded. The schematic picture of a rock is given in fig. (1.1) of chapter 1. The pore water containing a radionuclide flows through these fractures. Due to the random network configuration, the effective path length traversed by the species from the source to an observation point located at the
The $z$ axis is higher than the linear distance between them. This will have an important bearing on the concentration. First, due to the increased path length, the concentration at a point of evaluation will be reduced. Secondly, with an increase in the path length, the retardation effects due to the porous matrix will also be enhanced. Hence due to these combined effects, the concentration will be significantly reduced and thus a realistic porous model will yield a less conservative estimate than the idealized parallel fracture model. *This is the motivation to address the present problem through a probabilistic route as the deterministic approach can not address this zigzag flow through a fracture network.*

An arbitrary single porous matrix with its embedded fracture network can be divided into several smaller blocks and the migration can be modeled by a random walk approach through this collection of smaller blocks. But as the number of porous matrices increases due to a larger domain as it happens in our case, the total number of smaller blocks increases enormously. Even though one can model the migration probabilistically in principle for this huge collection of blocks, in reality it becomes an impossible task. To circumvent this difficulty *we can assume that we can deal with a single porous matrix of an appropriate width* that reflects the averaging done over all the porous matrices of different shape, size and width that make up a real rock. We also calculate a quantity called the average migration length which is the average of several path lengths. With the average width and the average migration length, we can invoke the deterministic model to calculate required concentration profile as a function of time. Thus, we exploit the advantages of both the deterministic and the nondeterministic models.
4.2 A brief survey of literature

The probabilistic estimation of the migration of contaminant particles through a porous medium is a widely used technique. Using this approach, problems dealing with dispersion and diffusion have been handled since the middle of the last century \(^1\)\(^2\). For our porous flow problem, a number of realistic models have been proposed based on the probabilistic estimation. Williams \(^3\), \(^4\) reported a stochastic approach to address the migration of radioactive waste through a fracture-porous matrix system. This was based on an analogy with the neutron transport in a non multiplying medium. He considers the transport of radionuclides in pore water as a series of linear movements through the randomly oriented and interconnected fractures. The radionuclide flow can encounter a sudden change of direction at a node which is the intersection point of two or more fractures. These are treated as pseudo-scattering events. He introduced a scattering term to quantify the reaction rate (like a particle getting deposited on a solid surface which amounts to a removal). The direction of the motion at a node is indicated by an anisotropy related function. Though this approach gives an analytic estimation of the transport through a fracture network, it has a serious drawback. The diffusion of species into the porous blocks from the fracture is not taken into consideration. The numerical solution of this model was reported in a series of papers by Buckley et al. \(^5\), \(^6\), \(^7\).

The probabilistic model of Cvetkovic et al. \(^8\) considered the migration in both the fractures and the porous matrices. He implemented the deterministic single fracture model in a small domain and considered the flow velocity as a truly random parameter and thus he repeats the calculation to cover the total volume of rock. For simplicity, he
ignored the diffusion process within a fracture and assumed that the transport was a function of advection alone. The results provided an estimation of the escape probability of a radioactive species from a rock.

In the model of Giacobbo and Patelli \cite{9} the random walk of a particle in a phase space was governed by two quantities, a free flight kernel and a collision kernel characterizing a transition in the physical-chemical state of a particle (e.g. a particle encountering a node of fractures). They generated an effective path length between a source and an observation point using a random walk approach similar to that of Williams \cite{3}. This model too did not consider the matrix diffusion but assumed a constant adsorption and desorption rate to account for the retardation offered by the porous matrices.

4.3 A description of our present model

Throughout the chapter, meter is used as the unit of length. As mentioned earlier, the radionuclide is assumed to travel through a network of interconnected fractures. This random network of fractures is embedded in porous matrices of random shapes and sizes. This is a very complicated system and the exact modeling of the migration involving the network of fractures and porous matrices is difficult. As explained in the third paragraph of this chapter, we introduce the average porous matrix width and the average migration length and then invoke the deterministic model. We assume a uniform distribution of the fractures and the porous blocks throughout the medium. That is, the average densities of the fractures and the porous blocks are independent of the position.
The migration of a radioactive particle through this network is modeled in two stages. In the first stage, a randomly oriented path between the source and the observation point is generated. Following Williams [3], we assume that the flow through a network can be imagined as a series of straight line movements. The radionuclide can change its direction only at a node which is the intersection of two or more fractures. Thus there is no change of direction of movement between two consecutive nodes. In a practical situation, the shape, the width and the length of a fracture vary randomly. For simplicity, we assume that the first two quantities are identical for all the fractures whereas the length is assumed to follow a distribution. Buckley et al. [6] considered two models namely, the Picket Fence and the Fracture Angle models to sample the fracture length. By analogy with neutron transport, a term called the mean free path was introduced in these models. This is the average distance that a particle travels between two consecutive pseudo-scattering events. Cvetkovic et al. [8] assumed a uniform distribution of fracture length in the interval \([1, 10]\) and we follow the same distribution.

The next point to be considered is the orientation of a fracture at each node. The Fracture Angle model [6] assumes that at each node a fracture can have a orientation (with respect to the mean flow direction) that is uniformly distributed in the range \([-\phi_{max}, \phi_{max}]\). The same assumption was considered by Giacobbo and Patelli [9]. Now this angle that defines the new direction of flow at a node is called the branching angle. Using the above defined quantities, one can generate a migration length that a particle travels between the source and the observation point. By repeating this a number of times, we obtain an
average migration length. The steps involved in this statistical averaging are described below.

a. Sample a set of fracture lengths from a uniform distribution in the range \([1, 10]\).

b. Sample a set of branching angles from the range \([-\phi_{\text{max}}, \phi_{\text{max}}]\).

c. Select a fracture length and a corresponding branching angle from these two sets defined in the previous two steps.

d. The selected fracture is of length \(L_f\) and it is oriented at an angle \(\phi\) with respect to the mean flow direction. Then it has a projection of magnitude \(L_f \cos(\phi)\) in the mean flow direction. To cover a distance of length \(L_{SD}\) between the source and the observation point along the mean flow direction, one has to repeat steps (c) and (d) till the quantity \(\sum_{i} L_f^i \cos(\phi^i)\) equals \(L_{SD}\).

e. Steps from (a) till (d) will generate a value for the migration length. This is repeated a number of times to arrive at the average migration length between the source and the observation point.

The second stage of the modeling involves the migration of the radioactive species through the porous matrix by choosing an average width and then use it along with average migration length in the deterministic model. We choose this truly random quantity as follows. Let \(L_{f,\text{max}}\) denote the maximum length of a fracture and \(\phi_{\text{max}}\) denote the maximum branching angle for a rock sample. Then the maximum possible distance of separation of two consecutive fractures is \(\Delta = 2L_{f,\text{max}}\sin(\phi_{\text{max}})\) (fig. 4.1). On the other hand, the minimum distance of separation is zero (at a node). This implies that the average width of the porous matrix must fall in between 0 and \(\Delta\). We choose uniformly
distributed values from the interval \([0, \Delta]\) to represent the average width of the porous matrix.

![Diagram of fracture](image)

Fig. 4.1: Estimation of the maximum width of a porous matrix

With the average porous matrix width and the average migration length, we solve the coupled PDE's that were solved in second chapter using the same set of parameters that were used earlier [eq. (2.9) and eq. (2.19)].
4.4 Results and discussions

All the calculations reported in this chapter are performed in double precision for a period of 1000 yr. Three sets of values are chosen for $\varphi_{\text{max}}$, namely $30^\circ$, $60^\circ$ and $89^\circ$. For each of these values, we have followed the steps from (a) to (e) described in the previous section to arrive at an average migration length. The law of large numbers \[10\] states that the average of a set of independent and identically distributed random numbers tends to a mean value with an increase in the size of the sample space. In this present problem if the number of trials exceeds about $10^4$, we arrive at a mean value for the average migration length. Hence for all the values of $\varphi_{\text{max}}$, $10^5$ trials are performed to ensure a statistical convergence.

In the previous section, we have discussed in detail about the maximum and the minimum possible widths of the porous matrix for a rock sample. It was pointed out that the average width of a porous matrix is a function of $\varphi_{\text{max}}$ and $L_{f,\text{max}}$. In this present study, we are using three different values of $\varphi_{\text{max}}$ ($30^\circ$, $60^\circ$ and $89^\circ$) and $L_{f,\text{max}}$ is 10 in all the cases. So the maximum possible widths of the porous matrices are $10m$, $17.32m$ and $19.997m$ that correspond to $\varphi_{\text{max}} = 30^\circ$, $60^\circ$ and $89^\circ$, respectively. Following the parallel fracture model, we denote the separation distance between the mid points of two consecutive fractures by $2B$. We choose $2B$ values from the set \{1, 5, 10\} for all the values of $\varphi_{\text{max}}$. A radioactive element of very large half- life $T_{1/2} = 2.14E6$ is chosen so that the source strength can be considered as practically constant.
In figs.(4.2, 4.3) we plot the concentration as a function of the linear distance for all the values of $\varphi_{max}$. In these calculations, a fixed width of the porous matrix is considered. It is easy to note that there is a systematic decrease in the concentration value with the increase of $\varphi_{max}$. This can be understood very easily. A large $\varphi_{max}$ will result in a large migration length and this in turn causes the reduction in the concentration values. For comparison, we have plotted the results of parallel fracture model for the same value of $2B$. In the figs.(4.2, 4.3), these values are labeled as 'Parallel frac'. As expected, the values of the standard parallel fracture model form an upper bound.

Next we study the effect of the width of the porous matrix on the concentration values. The results are plotted in figs.(4.4-4.6). It is important to note that in all the plots, the concentration values decrease with the increasing width of the porous matrix. Moreover, it reaches a saturation when the width exceeds the value 5. We can easily explain these trends. A porous matrix of large volume can allow more diffusion and absorption. This in turn causes the decrease in the concentration at the observation point. On the other hand, the diffusion process is limited up to a distance of few diffusion lengths. So beyond a limit, the concentrations saturate and this explains the patterns observed in figs.(4.4- 4.6).

4.5 Conclusions

The structure of a rock has a complicated randomness and the modeling of the migration of a species through this medium demands a huge computational effort. We have tried to model realistically this complex mechanism subject to the limits of practical
computation. In this process, the ingredients from both the probabilistic and the deterministic approaches are used. We have used two randomly varying parameters, namely the fracture length and the branching angle and both of them are assumed to follow uniform distributions in their respective ranges. We attempt to mimic the migration of radioactivity within a rock by sampling over these two parameters. Subsequently, the calculations are performed within the framework of the deterministic parallel fracture model since this approach easily estimates the diffusion process through a porous block once the width of the porous matrix is known. Thus by blending the best of the deterministic and the probabilistic approaches, we try to improve the results of the simplified parallel fracture model.

From the results, it can be noted that the current approach gives a less conservative estimate when compared to its deterministic counterpart. This reduction of conservatism of concentration estimates is very desirable from both the radiological and environmental angles. The present model can be definitely improved if an analytical solution for a finite fracture embedded in a finite porous matrix is possible. As far we know, such solution is not available. This needs to be explored in future. If such a solution is made possible, then each segment of the zizzag path can be handled by this proposed new solution technique. This suggested approach will prove to be a much better probabilistic model of the porous medium than the present one that we have just indicated. Also, our present model has assumed a constant source. This is only to use the analytical results of the constant source parallel fracture model. Instead, if we resort to a finite difference solution for the parallel fracture model, then the requirement of a
constant source can be avoided. As a final remark, it must be mentioned that only experimental results can truly test the merits of all these models.

Fig. 4.2: Concentration vs. distance plot for $2B = 1$. 
Fig. 4.3: Concentration vs. distance plot for $2B = 5$.

Fig. 4.4: Concentration vs. distance plot for $\varphi_{\text{max}} = 30^\circ$
Fig. 4.5: Concentration vs. distance plot for $\varphi_{\text{max}} = 60^\circ$

Fig. 4.6: Concentration vs. distance plot for $\varphi_{\text{max}} = 89^\circ$
4.6 References


