

# Reliability Analysis of Contaminant Transport Models in Soils and Fractured Rocks

Geetha Manjari, K.<sup>1</sup> and Sivakumar Babu, G. L.<sup>2</sup>

<sup>1</sup>PhD student, Department of Civil Engineering, Indian Institute of Science, Bangalore 560012, India, Email: geetham@iisc.ac.in

<sup>2</sup>Professor, Department of Civil Engineering, Indian Institute of Science, Bangalore 560012, India

Abstract.Contaminant transport models play a fundamental role in understanding the potential impact of contaminant movement in the subsurface environment. The subsurface (i.e., geosphere) is mainly composed of soils and rocks, and these natural geological formations are highly heterogeneous and fractured. The presence of such complex medium influences the migration of contaminant reaching the biosphere which further affects the safety of the public health and environment. So, in this paper, various models are developed to predict the contaminant migration process in soil and rock media. However, the contaminant fate in subsurface is significantly influenced by uncertainties in natural geological media, and thus may affect model predictions. The effect of uncertainties in the geological and transport properties of the medium on the concentration patterns evolving in time and space are propagated and quantified by implementing efficient probabilistic techniques. The contaminant transport models thus developed are integrated into the probabilistic framework for assessing the performance of radioactive waste disposal systems. These models illustrated the effect of type of geological medium and different forms of uncertainties in the medium on the contaminant transport process and further, on the risk and reliability of the disposal systems.

**Keywords:** soil, rock, fracture patterns, contaminant transport models, numerical model, reliability analysis, near surface disposal facility, radioactive waste disposal facilities, performance assessment models

# 1 Introduction

Contaminant transport modelling in subsurface is the primary tool in understanding the physical, chemical and biological behaviour of contaminants with the surrounding geological medium. These models evaluate the extent of contaminant migration over spatial and temporal scales due to a possible source of subsurface pollution or, a contaminant spill. So, they are of utmost importance in handling geo-environmental problems like conducting risk assessments, remediating complex contaminated sites,

designing and monitoring barrier/disposal systems for contaminants (hazardous/nonhazardous) [1, 63, 64]. The subsurface contamination caused due to release of radionuclides from the radioactive waste disposal systems is raising environmental concerns globally from the past three decades. It is important that disposal sites be designed to prevent the possible contamination of the groundwater system in both short and long term [12, 42, 61]. Although they are designed to contain the waste from the surrounding environment, it is conceivable that significant pollution might occur in the long term. To estimate the risk and radiological impact caused by the migration of radionuclides to the biosphere, performance assessment models are developed. These models take into account the nature of the facility, radioactive inventory, geo-hydrological and geochemical behaviour of the site, release and transport of radioactivity to the biosphere.

Contaminant transport in the geosphere is central in assessing the overall performance of the disposal systems and one of the key factors that influences the contaminant transport process is the geological environment through which the contaminant migrates [11, 40]. So, modelling the transport of contaminant (i.e., radionuclides) in different geological media (ie., soils and rocks) is critical in monitoring the post-closure safety of disposal facilities for radioactive wastes [28, 70]. Several studies were carried out to model the migration of radionuclides in soils and rocks with an aim to understand their transport behaviour and the mechanisms that affect their movement. Analytical models were developed to predict the distribution and transport of radionuclides in porous media [33, 38, 70]. However, it becomes challenging to achieve a close form solution for problems with geometrical complexities, time varying boundary conditions and large-scale field studies. To overcome this issue, numerical models were developed that considered heterogeneity in the medium [43, 46], retention capacity of soils [Pique et al 2013], the influence of vadose/unsaturated zone [36, 60] and, decay chain with ingrowth of progenies [19, 22] to simulate the radionuclide transport process and estimate its concentration reaching the environment. Unlike soils, modelling the behaviour of contaminant in rocky medium is more complicated. It involves modelling two interacting subsystems namely fractures and the intact rock matrix [49]. Bear et al discussed various approaches to model flow and transport in fractured rock and also addressed the influence of various factors like fractures geometry, fracture aperture distribution, orientation distribution of fractures, diffusion in intact rock matrix on these models [9]. A number of analytical [30, 39, 62, 71] and numerical models [15, 40, 41, 52] were developed to predict the contaminant transport in fractured rocks. These models are deterministic and provide conceptual understanding and insight into the effects of different factors involved in a process, but lack in describing the transport of solutes through soils under the influence of uncertainty.

The theoretical model and field studies have recognized that the contaminant fate in subsurface is significantly affected by different forms of uncertainties in the geological media and thus may affect model predictions [25, 31, 56]. Failure to acknowledge and represent uncertainty can result in serious criticism of performance assessment [32]. The increasing awareness for these uncertainties led to an improved understanding of contaminant transport behaviour in subsurface. Uncertainty generally emerge in the form of inherent variability in the medium (soil properties/heterogeneity), measurement errors and modelling errors [7, 20]. The influence of spatial variability and design parameter uncertainties in geological and transport properties on contaminant transport process were studied [18, 27, 45, 50, 66]. Uncertainty analyses of environmental models needs to be performed to achieve a level of confidence in model results. The uncertainties in these models are quantified by carrying out reliability analysis where, the probability of radiation dose exceeding permissible limit is computed. Various probabilistic techniques like Monte Carlo simulation [42, 53], First Order Reliability Method (FORM)/ Second Order Reliability Method (SORM) [17], importance sampling methods [14] and subset simulation method [6, 48, 53] were adopted by researchers to quantify the uncertainties in geological systems. The choice of method of uncertainty analysis depends on the computational time for carrying out each simulation in the model. However, these studies did not explore the effect of various uncertainties in the geological medium under the framework of performance assessment modelling for radioactive waste disposal systems. Also, reliability and risk assessment of these systems needs to be studied by modelling radionuclide transport process in different geological media. So, as an integral part of performance assessment, uncertainty analysis is carried out to estimate the performance of the disposal systems. Overall, a probabilistic performance assessment modelling framework is developed by integrating efficient geosphere transport models. The objectives of the present study are:

- 1. To develop efficient geosphere transport models that can solve the radionuclide migration process in different geological media i.e., soils and fractured rocks.
- 2. Estimate the radiological impact caused due to radionuclide migration in the biosphere.
- 3. Characterize different forms of uncertainties in the geological properties of the medium and the transport properties of the contaminant.
- 4. Quantify the effect of these uncertainties on the radionuclide concentration, radiation dose by carrying out reliability analysis.

A broad outline of the general framework developed in the present study is represented in Fig. 1. A system/ analysis model is formulated with geosphere transport as one of its model components to estimate the performance of radioactive waste disposal systems. Geosphere transport is modelled numerically to predict the radionuclide transport in geological media. To carryout probabilistic analysis, the uncertain inputs (i.e., random variables/random process) are characterized and propagated through the analysis model

(via. geosphere transport model). Further, these uncertainties are quantified by carrying out reliability analysis where, the probability of failure of these systems due to radionuclide release is estimated. The steps followed in uncertainty analysis is automated by coding python programs.



Fig. 1. Sequence of steps followed in the present study

#### 1.1. Outline of the paper

The paper is organized into five sections. In Section 2, the details of the numerical model and the governing equation used to describe the radionuclide transport in soils and rocks are presented. In Section 3, different forms of uncertainties considered in the paper and the methods of uncertainty quantification are presented. Using the framework presented in the study (as shown in Fig 1.), three performance assessment models are developed, and they illustrate the influence of geological media and the uncertainties on the radionuclide transport process, on the performance of radioactive waste disposal systems. In Section 5, the major conclusions from the analysis are presented.

### 2 Contaminant Transport Models in Soils and Fractured Rocks

Numerical modeling has been extensively used in the study of groundwater contaminant transport in the past three decades and remains as a very effective way in dealing with these problems. They account for the geometrical complexities of the domain (heterogeneity, fracture network), seasonal variations in the properties of the geosphere and temperature fluctuations. So, in the present study the radionuclide transport is modelled numerically based on finite element method using FEFLOW 6.2, a numerical modelling software developed by Diersch [21]. This software handles complex boundary conditions, coupled groundwater flow, transport of solutes, and geochemical reactions between solid and aqueous phases. The governing equations for fluid flow and contaminant transport in soils and fractured rocks are presented below.

#### 2.1 Soils

In any geological medium, the main transport mechanisms that describe the movement of contaminant are advection, hydrodynamic dispersion (i.e., combination of molecular diffusion and mechanical dispersion), adsorption and radioactive decay. There can be an influence of other chemical and biological reactions barring from the previous transport mechanisms, depending on the reactive nature of contaminant. By conceptualizing the contribution from these factors into mathematical equations, models were developed by the researchers to describe the flow and mass transport of the contaminants. So, the geosphere transport (i.e., coupled flow and transport process) is represented by the governing equations for fluid flow (in a fully saturated medium) and contaminant transport which are given by

#### Fluid flow

$$S_0 \frac{\partial h}{\partial t} + \nabla . \left[ -K f_\mu (\nabla h + \chi e) \right] = Q \tag{1}$$

Mass transport

$$\varepsilon R_f \frac{\partial C}{\partial t} + q. \nabla C + \nabla . j + \varepsilon R_f v C = S$$
<sup>(2)</sup>

where  $S_{0}$ - specific storage coefficient,  $\partial \partial t^{h}$  – rate of change of hydraulic head, K – hydraulic conductivity,  $f_{\mu}$  – viscosity function,  $\nabla h$  – change in hydraulic head,  $\chi$  – buoyancy coefficient, e – gravitational unit vector, Q – specific mass supply;  $\varepsilon$  - porosity,  $R_{f}$  - retardation factor, j – diffusive flux, C - concentration,  $\nabla C$  – change in concentration,  $\frac{\partial C}{\partial t}$  - rate of change in concentration, v – radioactive decay, q - Darcy velocity, S –

Key Note Lecture 9

source/sink term.

#### 2.2 Fractured rocks

Discrete fracture network (DFN) modelling approach is implemented to model contaminant transport in fractured rocks. The model is developed numerically, where, the porous media and the set of fractures are represented as two distinct interacting subsystems coupled through interfaces [21]. Usually, the spatial dimension of fractures is lower than the domain (i.e., for a two-dimensional domain, the fractures are modelled as one-dimensional elements). The governing equations for fluid flow and contaminant transport are considered separately in porous medium (given eq 1 and eq 2) and the same equations are lowered by spatial dimension in the case of fractures. To solve for concentration of contaminant, the discrete features (fractures) and the porous medium are treated as a unitary feature, where all components are integrated into the solution domain consisting of the joint porous-medium domain  $O_p$  and a number of non-overlapping discrete feature domains  $O_f$ .

$$0 = O_p \cup \sum_F O_f$$
(3)

The contributions from porous medium and the corresponding fractures are assembled and, the overall concentration from both the systems are estimated. The above equations are used to build new radionuclide transport models and the details of these models are discussed elaborately in section 4.

#### **3** Uncertainty Analysis

Uncertainty analysis has the important goal of extending understanding and quantifying the effect of variabilities in the parameters and, achieve a reasonable assurance associated with the safety of the system. Generally, these uncertainties occur in the form of heterogeneity in hydrogeological properties of the medium and, the physical, chemical and biological properties of the contaminants being released and transported. In the present study, the uncertainties addressed are:

- 1. Uncertainty due to heterogeneity in the medium
- 2. Uncertainty in the design parameters of the model

#### 3.1. Random field modelling

The inherent randomness in the properties of natural materials extending over space is modelled based on random field theory [72]. Let  $\Omega$  be a set  $\mathbb{R}^n$  describing the system geometry such that  $x \in \Omega$ , then,  $H(x, \theta)$  is defined as random field, which is a collection of random variables indexed by the parameter x. The statistical descriptors of a random field

are (i) mean (ii) standard deviation and (iii) auto correlation function. Further, the random field is discretised to replace a continuous random process by a finite set of random variables. In this study, the random field is discretized using Karhunen-Loeve (K-L) series expansion. This method is based on the concept of spectral decomposition of its autocovariance function  $C(x, x') = \sigma(x)\sigma(x')\rho(x, x')$ , which is bounded, symmetric, and positive definite.

$$\int_{\Lambda} C(x, x')\phi_i(x')d\Lambda_{x'} = \lambda_i\phi_i(x)$$
(4)

 $\lambda_i$  and  $\phi_i$  are the eigen values and eigen vectors of the autocovariance function respectively which are computed analytically.

#### 3.2 Uncertainty in design parameters

The uncertainty in physical parameters in subsurface contaminant transport models are manifested in the form of physical, chemical and biological properties of the contaminant and the surrounding medium. So, in the present study, the geohydrological and transport properties of the medium and, the contaminant are treated as random variables and their coefficient of variation are chosen from the literature. The statistical properties of these variables are presented in section 4.

#### 3.3 Reliability analysis

Reliability is defined as the probabilistic measure of the assurance achieved on the performance of a system over time under specified conditions and it is expressed as reliability index ( $\beta$ ) and the probabilistic measure of its complementary event is called the probability of failure denoted by  $P_f$ . In the present study, reliability analysis is employed to quantify the uncertainties mentioned above. So, the geohydrological and transport properties of the medium and the contaminant are treated as a vector of random variables denoted by X, [ $X = X_1, X_2 \dots X_n$ ], where 'n' denotes the number of random variables. The performance function is defined as

 $g(X) = D_{max} - D(X)$  (5) where  $D_{max}$  - permissible radiation dose or concentration of the contaminant recommended for design, D(X) - the radiation dose or concentration of contaminant estimated from the model (function of random variables).

Subset simulation. Estimating the probability of failure of a rare event is challenging as they have very small failure probabilities. An efficient technique called subset simulation is developed to estimate the  $P_f$  for such rare events [5, 13]. The underlying idea in subset simulation is to break down a rare event into a sequence of frequently occurring events. The failure event is nothing but the intersection of all the intermediate events

 $F_m = \bigcap_{i=1}^m F_i$ . By sequentially conditioning on the event  $F_i$ , the failure probability  $P_f$  can be written as

$$P_f = P(F_1) \prod_{j=1}^{r-1} P(F_{j+1}|F_j)$$
(6)

 $P(F_1)$ , the first failure event is determined by DMC. Further, the conditional samples are generated by means of a Markov chain designed so that the limiting stationary distribution is the target conditional distribution of some adaptively chosen intermediate event. This gradually populates the successive intermediate regions up to the target failure region. This is carried out by following Modified Metropolis Hastings algorithm.

#### 3.4. Python programming interface

The computational efficiency of the model is improved by coding python programs where the probabilistic analysis to generate random realizations of geological and radionuclide transport parameters and, estimate the probability of failure using subset simulation are automated.

# 4 Reliability Analysis of Radionuclide Transport Models for Radioactive Waste Disposal Facilities in Soils and Fractured Rock

Radioactive waste disposal is a global challenge which is gaining increased attention due to thealarming effects caused by its exposure to human health and the environment. To provide long-term isolation and containment of the radioactive waste, disposal systems are designed which depend on the type of waste (nonhazardous/hazardous), its physical state (solid/liquid/gaseous) and the concentration of radioactivity (low level (LLW) / intermediate level (ILW) / high level waste (HLW)). The disposal systems are constructed a few meters to a few thousands of meters from the surface based on concentration of activity (i.e., radioactivity) in the waste. The wastes are conditioned, immobilized and then placed in the disposal systems. According to the present practices in India for the storage and disposal of various categories of solid waste, the LLWs and ILWs are placed in the Earth/Stone Lined trenches, RCC trenches and Tile holes (which are also known as near surface disposal facilities (NSDF)); and HLWs are disposed into deep geological repositories [57]. The post-closure safety of the disposal systems are assessed by developing performance assessment models that predict the extent of safety achieved due to isolation of these wastes and estimate the amount of risk caused by the failure of these systems by taking into account various scenarios of release and pathways of intrusion. The

significance of radionuclide transport models in estimating the performance of radioactive waste disposal systems are illustrated in the following three models.

#### 4.1 Numerical model to describe the flow and transport of radionuclide in soil

A numerical model is developed to simulate three-dimensional radionuclide transport process in soil and this model is integrated into performance assessment modelling framework for near surface disposal facility (NSDF). The national (Atomic Energy Regulatory Board (AERB)) and international (International Atomic Energy Agency (IAEA)) regulatory bodies have developed safety guides to assess the performance of NSDFs and these guidelines are followed in the present study to develop performance assessment models [2, 34]. In any performance assessment model, initially, the pathway leading to the failure of the radioactive waste disposal system should be identified [69, 73]. Here, it is assumed that the disposal facility failed due to infiltration of water into the system that resulted in radionuclide release in groundwater and transport in geosphere. Once the failure scenario is recognised, the source term and geosphere transport modelling are carried out. Typically, the critical processes involved in performance assessment are judged based on sensitivity of the process. The focus of this study is mainly on discerning the behaviour of radionuclides in the geosphere and its impact on the radiation dose values of radionuclide at the endpoint. So, a simple source term model is considered followed by, three-dimensional geosphere transport model.

**Source term model**. The source term denotes the inventory of radioactivity (i.e., waste dumped) within the facility at any given time. The concentration of the radionuclide at the source area is computed using the following equations [46].

~~~

$$C(t) = \frac{C(t)}{\theta V R_f} exp[-(\lambda_p + K_l)t]$$

$$K_l = \frac{vS_r}{\varepsilon V R_f(8)}$$

$$\frac{dc}{dt} = -(\lambda_p + K_l)C_{(9)}$$
(7)

with the initial condition  $C(t = 0) = C_0$  where *C* is the inventory of the nuclide (atoms) at time *t*; *K* is the leach rate or fractional release rate of the nuclide; *t* is the time (T); *L* is the length, *B* is the width and *H* is the height (m) of the disposal facility; *v* is the infiltration rate of water from the disposal facility (m/s); *S*, *V* are the surface area and the volume of the disposal facility respectively;  $\theta$  is the porosity of soil;  $C_0(t)$  is the concentration of the nuclide at the source area (atoms L<sup>3</sup> or mol); *C*(*t*) is the activity of the radionuclide at time

t (atoms); and  $C_0$  is the initial concentration of radionuclide. Using the above equations, the source term is assigned as decaying mass boundary condition in the numerical model.

**Geosphere transport model**. The radionuclides released in the groundwater migrate towards the biosphere and this process is modelled using FEFLOW 6.2. The transport mechanisms of radionuclide transport are formulated into basic governing equation as shown in eq (1). The plan, sectional view and the point of location of the source of the domain are shown in Fig. 4(a). A triangular finite element mesh is generated with 55,496 nodes and the three-dimensional view of 1000m x 1000m x 6m domain is presented in Fig. 4(b). The groundwater velocity considered in the model is 0.1 m/day. The initial and boundary conditions for flow and radionuclide transport are presented in Table 1 and eq (5).



(b) **Fig. 4.** Domain considered for the study (a) plan and sectional of the domain (b) three-dimensional view of finite element mesh

Fluid flow

| Section | Туре      | Value  |                             |
|---------|-----------|--------|-----------------------------|
| A-E-H-D | -         | -      | -                           |
| A-B-C-D | Dirichlet | H=150m | Pervious boundary (Inflow)  |
| E-F-G-H | Dirichlet | H=130m | Pervious boundary (Outflow) |
| B-F-G-C | -         | -      | -                           |

Table 1. Boundary conditions for fluid flow

Mass transport

$$\mathcal{C}(x, y, z, 0) = 0 - \infty < x < \infty; -\infty < y < \infty; 0 < z < d - \infty < x < \infty; -\infty < y < \infty;$$

0 < z < d

$$\mathcal{C}(\pm\infty, y, z, t) = 0 - \infty < y < \infty, 0 < z < d, t > 0$$

$$(10)$$

$$\frac{\partial}{\partial z}C(x, y, 0, t) = \frac{\partial}{\partial z}C(x, y, d, t) = 0 - \infty < x < \infty - \infty < y < \infty, \quad t > 0$$

C(u + u - t) = 0 is cut is 0 < t < t < 0

The model is run by assigning the above initial and boundary conditions and the concentration of the radionuclides at different distances are obtained.

*Validation with an analytical model*. To check the efficiency of the numerical model and the extent of convergence achieved from the FE mesh refinement, the results from numerical model are compared with an analytical solution developed by Park and Zhan [51]. They developed a closed form solution for contaminant transport from a point, line and an area sources in a finite aquifer system. The results of non-reactive contaminant movement over time at 10 m from the source is computed from the analytical model and the numerical model, and, presented in Fig 5. From the figure it can be observed that, the results from the numerical model match well with the analytical solution. So, the numerical model could efficiently solve the contaminant migration process in a three-dimensional medium. Now, the numerical model is used predict the transport behavior of radionuclide Iodine (<sup>129</sup>I) released from NSDF. The reason for choosing this radionuclide for the analysis is because the previous studies reported that among different LILW (low and intermediate level waste) in NSDF, radionuclide <sup>129</sup>I delivered the highest

concentration in groundwater leading to high risk to human health and environment [24, 44, 66].



Fig. 5. Concentration versus time at 10 m from the source

The inventory and geo-chemical properties of <sup>129</sup>I and, the geo-hydrological properties of the medium are presented in Table 2 and Table 3 respectively. This data of radioactive waste originating from PHWR (Pressurised Heavy-Water Reactor) nuclear reactor operation and fuel reprocessing near Trombay Site, India is considered for the study [44, 58]. To reduce computational time of the model, the inventory values are reduced to around 100 times the actual inventory value and the evolution of source over time is estimated from eqs (7-9) and its trend is plotted in Fig. 6.

Table 2. Decaying source concentration and other properties of the four radionuclides

| Radionuclide | Inventory* | Half<br>life | Distribution | Ingestion dose |
|--------------|------------|--------------|--------------|----------------|
|              | (Dq)       | (y)          | (ml/g)       | (Sv/Bq)        |
| Iodine       | 1.1E6      | 1.7E7        | 1            | 1.1E-7         |

| S. No | Property                              | Value          |
|-------|---------------------------------------|----------------|
| 1.    | Infiltration velocity (m/sec)         | 1E-08          |
| 2.    | Volume (L*B*H) of the barrier $(m^3)$ | 15 x 2.5 x 4.8 |
| 3.    | Porosity                              | 0.3            |
| 4.    | Hydraulic conductivity (m/day)        | 5              |

Table 3. Input parameters to estimate the decaying source concentration



Fig. 6. Decaying source concentration evolving in time

**Radiological model.** The consequence of radionuclide migration to human habitat is estimated by radiation dose. The radiological model evaluates radiation dose to a member of the critical group due to consumption of ground water for drinking. It is mathematically expressed as

$$rd = C \times w_{in} \times d_{in} \tag{11}$$

Key Note Lecture 9

226

where rd- is the radiation dose (mSv/y); *C* - concentration of radionuclide in ground water (Bq/m<sup>3</sup>); *w*<sub>in</sub>- drinking water intake (l/day); *d*<sub>in</sub> - ingestion dose coefficient (Sv/Bq). Further, the risk to a member of the critical group due to the waste disposal practice is also estimated. The drinking water intake is assumed to be 2.2l/day [44]. For the analysis, the risk to a member of the critical group from the disposal practice is evaluated by considering the effect of risk factor and ingestion dose coefficient. The total risk factor to the public as recommended by International Commission of Radiological Protection (ICRP) [35] is  $7.3 \times 10^{-5}$  mSv<sup>-1</sup>. The product of the risk factor and the dose received gives the risk to the individual. These values are estimated and compared with the threshold dose and risk values used as design criteria. Thus, the results from radiological model quantifies the performance of radioactive waste disposal facility.

**Deterministic analysis**. The concentration and radiation dose of the radionuclides are measured upto 200m from the source as the values become negligible beyond these points. The model is run for 2000000 days and the concentration versus time trends evolving in time at critical distances of 50, 100, 150 and 200m are estimated. The trends are plotted for time periods before the arrival of maximum concentration (i.e., pre-peak) and presented in Fig. 7. It can be observed that the concentration values are decreasing with an increase in the distance from the source. In the process of contaminant transport, the radionuclides get sorbed to the neighbouring porous media and thus the concentration reduces with the distance. The concentration of radionuclides is highly dependent on the inventory value, distribution coefficient and its half-life. Iodine delivers the high concentration and radiation dose because of its low distribution coefficient, high inventory value and ingestion dose coefficient. Since the source concentration decays after few years, the concentration at any point reaches a maximum value and then reduces to zero. When the distribution coefficient value is low, there is no redardation which inhibits the mobility of the contaminant. The radiation dose through drinking water pathway is calculated and the results are compared with the dose limit  $(1 \text{ mSv.y}^{-1})$  to a member of the public) recommended by ICRP and shown in Fig. 8. From Fig. 8, it can be noticed that the radiation dose values did not exceed the dose limit for the given hydro-geological conditions of the domain. Further, the peak value of risk to a member of critical group due to iodine is estimated as 6.5 x 10<sup>-5</sup> y<sup>-1</sup> which is lower the risk due to background radiation and the risk from accidents and catastrophes  $(1 \times 10^{-3} - 1 \times 10^{-4} \text{ y}^{-1})$  and natural background radiation  $(1.8 \times 10^{-4} \text{ y}^{-1})$ .



**Proceedings of Indian Geotechnical Conference 2020** December 17-19, 2020, Andhra University, Visakhapatnam

Fig. 7. Concentration versus distance for iodine before the arrival of maximum concentration (Pre-peak)



Fig. 8. Radiation dose versus time for iodine

**Probabilistic analysis .** A deterministic model used for risk assessment ignores the uncertainties in the subsurface might cause severe consequences such as damage to human health and environment. So, various techniques need to be employed to address the effects of these uncertainties. In this example, the uncertainty in the geological and transport properties i.e., groundwater and soil medium, are considered as random variables. The statistical properties of the parameters considered for the analysis are mentioned in the Table 4. The coefficient of variation (COV) and probability distribution reported in literature have been considered for the study [17, 24, 45].

**Table 4.** Statistical properties of the input parameters

| S. No. | Property                                        | Iodine  |      | Distribution |
|--------|-------------------------------------------------|---------|------|--------------|
|        |                                                 | Mean    | COV  | -            |
| 1.     | Longitudinal dispersivity - $\alpha_L(m)$       | 3       | 0.09 | lognormal    |
| 2.     | Transverse dispersivity- $\alpha_T$ (m)         | 0.3     | 0.09 | lognormal    |
| 3.     | Porosity - θ                                    | 0.3     | 0.09 | lognormal    |
| 4.     | Distribution coefficient- k <sub>d</sub> (ml/g) | 1       | 0.1  | lognormal    |
| 5.     | Diffusion coefficient- D (m <sup>2</sup> /s)    | 5.9E-08 | 0.08 | lognormal    |

These uncertainties are propagated through the model as shown in Fig. 1. and quantified by carrying out reliability analysis to estimate probability of failure  $(P_f)$ . The probability of failure is defined as the probability of radiation dose exceeding the permissible value  $(D_{max} = 0.77 \text{ mSv/y})$ . To run the model in a computationally efficient way, a code is developed using the built-in python interface in FEFLOW 6.2 that integrates the deterministic and probabilistic part of the analysis. Using eq (6), the simulations are carried out and  $P_f$  value is estimated using subset simulation. The  $P_f$  value obtained from the analysis is  $3.5 \times 10^{-9}$  which is very low, and this value indicates that the disposal system is safe. To check the variability of estimates, the sample COV of failure probability over 25 independent subset simulation runs. A comparison is made between the coefficient of variation and number of samples per subset and; the effect of number of samples per subset and probability of failure. From the results it was observed 20,000 samples per subset was ideal to obtain a convergent solution. Thus, the example presented a performance assessment model where, the complexity involved in a migration process of radionuclide in three-dimensional medium has been addressed by developing a numerical model. Further, the influence of variability in the input properties of geological medium that describe the migration process has also been quantified.

# 4.2 Numerical model to describe the flow and transport of radionuclide in spatially varying soils

In the previous model, the uncertainty in the design parameters and their effect on the radionuclide transport process have been handled effectively. However, the heterogeneity in the geological medium and the effect of modelling spatial variability in the properties of the medium due to heterogeneity were not considered. Since the importance of reckoning with this form of uncertainty is discussed in the previous section, it is imperative to model spatial variability in the medium. This model presents the effect of spatial variability in the medium on the performance assessment of radioactive waste disposal system. The features, events and processes (FEP) leading to the failure of disposal system and the source term model remains the same as mentioned in previous model. The next component i.e., the geosphere transport is modelled for a spatially variable medium, where, the heterogeneity in the soil properties is described by using random field theory which is presented in section (2.1). The random field is approximated by KL expansion and given by

$$H(x,\theta) = \left[\mu + \sum_{i=1}^{M} \sqrt{\lambda_i} \phi_i(x) \xi_i(\theta)\right]_{(12)}$$

For the present study, the parameter (hydraulic conductivity) is modelled as a log-normal random field. So, the expansion becomes [16]

$$H(x,\theta) \approx exp\left[\mu_{ln} + \sum_{i=1}^{m} \sqrt{\lambda_i} \phi_i(x) \xi_i(\theta)\right]$$
(13)

where  $\mu_{ln}$  - the mean of underlying normal field.

The statistical parameters of log-normal random field are given as

$$\sigma_{ln} = \sqrt{\ln(1 + (\sigma/\mu)^2)} \tag{14}$$

$$\mu_{ln} = \ln \mu - 0.5\sigma^2 \tag{15}$$

The random field presented in the above equation is discretized analytically using the method given by Ghanem and Spanos [26]. These equations are coded in python program and, the stochastic analysis to generate the random field are automated. The hydraulic conductivity of soil was described as two-dimensional isotropic log-normal random field. The statistical parameters of the random field are  $\mu = 0.05$  m/day, COV = 10%, and auto-

correlation length of 2m. Using the python program, the values of a random field (for a given realization) at different points of the soil mass are computed. Typical realization of random field in the numerical model is presented in Fig. 9. The random field values are assigned to different elements of a deterministic mesh which is indicated by the colour bands throughout domain in Fig. 9. However, the hydraulic conductivity is same at any given point in both x and y directions confirming the isotropic nature of the medium.



Fig. 9. Spatially varying hydraulic conductivity along the domain

**Deterministic analysis.** The deterministic analysis is performed by generating a domain and assigning mean value of hydraulic conductivity. The timeframe considered for the analysis is 200000 days (i.e., around 550 years) and beyond this time period the concentration values reached insignificant levels. Fig. 10 presents the concentration trends evolving in time at different distances from the source. The results show decrease in peak concentration value with the increase in distance from the source.

# 

Proceedings of Indian Geotechnical Conference 2020 December 17-19, 2020, Andhra University, Visakhapatnam

Fig. 10. Concentration versus time at observation points located 80 m and 100 m from the source

As mentioned in the previous example, the reduction in concentration value with distance is due to the influence of decaying source concentration and, the distribution coefficient which retards the mobility of the contaminant. The endpoints of assessment, maximum radiation dose and corresponding risk values of <sup>129</sup>I reaching the human habitat through drinking water pathway are computed by using the radiological model given in section 4.1.3 as 0.66 mSv/y and  $4.95 \times 10^{-5}$  y<sup>-1</sup> respectively. These values are within the regulatory limits and, the risk due to LILW radioactive waste disposal has an almost negligible radiological impact from the disposal facility on the human health and environment.

**Probabilistic analysis:** Integrating the K-L expansion and subset simulation. To estimate the failure probability, subset simulation algorithm and K-L expansion are linked. This methodology is presented by Ahmed and Soubra [3]. The general algorithm of subset simulation remains the same as mentioned in section 4.1. Two steps are introduced to the algorithm in order to integrate both the methods. They are

- 1. The vector  $\xi_i$ ,  $\{i = 1 \dots M\}$  generated in the first step of subset simulation is substituted in the K-L expansion. Then, these values are assigned at the centres of the different elements of the deterministic finite element mesh to simulate the random field.
- 2. By assigning these values to the mesh a new deterministic model (i.e., realization) is created each time. Using this model, the corresponding system

response is computed. This process is repeated till the random field belonging to the last failure region is estimated.

The above methodology is coded in python to automate the simulations. The stochastic responses (i.e., concentration trends evolving in time) for spatially variable soil medium ( $l_{lnx} = 5$  m, COV = 50%) is illustrated by running a set of Monte Carlo simulations. These responses were compared with the result for deterministic case and presented in Fig. 11.



Fig.11. Concentration versus time for various cases



Fig. 12. Probability of failure versus correlation length for different cases

In the deterministic case, same hydraulic conductivity is assigned all over the domain indicating that themedium is homogeneous and, this result is represented by thesolid line. In the spatially variable case (i.e., heterogeneous medium), the concentration trend at mean is represented by dash dot line. The spectrum of concentration trends (blue lines) occur due to the randomness in the system, which is ignored in the deterministic case. So, Fig. 11. highlights the need to account for spatial variability and quantify its uncertainty by adopting probabilistic techniques. The probability of radiation dose exceeding its permissible value i.e., probability of failure  $(P_f)$  is determined using subset simulation method and the results are presented in Fig. 12. In the figure, it can be observed that, the  $P_f$  values lie in the range of  $10^{-9}$ - $10^{-1}$ . The  $P_f$  value is highest for homogeneous soil (black lines in Fig. 11) due to faster rate of radionuclide movement through the medium. In spatially variable case, the probability of failure increased with the increase in autocorrelation distance. In Fig. 12. it can be observed that, an increase in autocorrelation length  $(l_{inx})$  from 2 m to 5 m, showed reduction in failure probability by a factor of 10<sup>3</sup>. Further an increment of  $l_{inx}$  from 5 m to 10 m and more, the reduction in  $P_f$  is 10 times which is not very significant. So, there is a notable influence of auto-correlation distance between 2 m - 5 m which suggests that in this range the parameter is sensitive to radionuclide transport. For small correlation length, the scale of transition in the conductivity values become more often along the length and cause the radionuclide to travel slower. For very high auto-correlation length, radionuclide concentration becomes independent of variance and tries to attain a value close to the homogeneous case. Thus, the results from this study shows that the extent of heterogeneity influences the safety of the system, and it is important to consider spatially variability in the medium to understand the behaviour of radionuclide transport and assess the radiological impact from the disposal system.

# 4.3 Numerical model to describe the flow and transport of radionuclide in fractured rock

The presence of a complex geological environment near the disposal facility affects the geosphere transport component and this effectively contributes to the overall performance assessment of radioactive waste disposal systems. The influence of this factor with soil as the geological medium of transport is discussed in the previous two models. In this example, probabilistic performance assessment framework for an NSDF is developed, where, the radionuclide transport in modelled in fractured rocks. Thus, the radiological impact caused by radionuclide release from an NSDF into the groundwater, which further lead to its migration through fractured rock mass is assessed. As mentioned in the previous examples, the failure of disposal facility is caused due to the infiltration of water leading to an eventual release of radionuclides into geosphere. Further, the radionuclides get transported in groundwater to the near-field geosphere which is a fractured rock medium. So, the radiological impact caused due to the radionuclide transport through

rocks to the nearby environment is assessed from the model. Typically rocks possess properties like low-permeability, low groundwater velocity and, molecular diffusion is the primary solute migration process. However, fractures, the natural discontinuities within the rock can form pathways for the migration of radioactive waste released to the subsurface environment. A simple source-term model as given in section 4.1.1 is used to estimate the inventory value of radionuclide evolving in time. Once the radionuclide is released into the geosphere, the transport process in described by geosphere transport model which is presented below.

**Geosphere transport model.** The contaminant transport through fractured rock mass is described by generating fractures and developing a model that predicts the contaminant transport through the fractured medium. A statistical rule-based algorithm developed by Riley [59] is employed to generate fractures observed in layered sedimentary rocks. Using this algorithm, the fracture trace length distributions and fracture spacing distributions are derived for a given fracture density and orientation distribution of layered rocks. The parameters of the fracture generation model are fracture density  $\rho_k$ ; orientation distribution,  $\theta_k$ ; speed of fracture propagation  $u_k$  and; the fixed probability that fracture terminates  $p_k$ , given a fracture set k. The first two parameters  $(\rho_k, \theta_k)$  are determined from field data. The other parameters  $(u_k, p_k)$  are used to match the statistical distributions of fracture trace lengths estimated from the method with those determined from field observations. Let us consider two fracture sets, set1 and set 2.  $u_1$  is given by the speed of crack propagation from set 1 and  $\theta_{12}$  represents the angle between fracture sets 1 and 2. The fracture from set 2 intersects with an already existing fracture from set 1. By incorporating the concepts of probability theory, the fracture trace length distribution for two fracture sets (set 1 and set 2) is given by the equation

$$P_{12}(x) = 1 - exp \left[ -2(1 - p_1)\rho_2 \sin(\theta_{12}) \int_{0}^{x} \int_{0}^{\frac{u_2}{u_1}\xi} exp \right]$$

$$\left( -2(1 - p_1)\rho_2 \sin(\theta_{12}) \int_{0}^{r} \int_{0}^{\frac{u_2}{u_1}\zeta} 1 - P_{12} \, dx \, d\zeta \right) dr \, d\xi$$
(16)

where *x*, *r* are displacements of fracture 1 and fracture 2 from the seed points and  $\xi$ ,  $\zeta$  are growing tip of fractures 1 and 2 respectively. The above equation can be implemented as an iterative scheme for simultaneously calculating  $P_k(x)$  and the fractures generated from these realizations become the conductive elements in a fracture network. In this study a two-dimensional finite element model is developed with a fractured network generated

based on discrete fracture network concept. Based on the formulation developed for fractures and porous matrix in FEFLOW 6.2 (discussed in section), an integrated fractured rock network is generated.

**Validation with analytical model**. The efficiency of numerical model is tested by comparing the numerical model results with an analytical solution. The analytical solution developed by Tang et al [67] is used to predict the contaminant migration through a horizontal fracture. A two-dimensional finite element mesh is generated with 3288 nodes. The fracture is modelled as 1D discrete finite elements sharing the edges of rock matrix and they are assumed to follow Hagen-Poiseuille law of flow motion. A typical non-reactive contaminant is considered for the analysis and the concentration of contaminant varying over time is estimated at 0.76 m from the source point and the results are presented in Fig. 13.



Fig. 13. Comparison of relative concentration versus time for analytical and numerical models with different molecular diffusion values

From the figure it can be observed that, the concentration trends from numerical and analytical solutions match well. It is evident that the movement of contaminant through fracture can be simulated efficiently using the numerical model.

Modelling the aperture variations along the fracture. One of the popular concepts of describing the local aperture variations is by adopting local parallel plate concept. In this study, the local aperture variations along the fracture are simulated by approximating each fracture as a series of 456  $'N_p'$  discrete segments with different aperture sizes. Each segment within the fracture is modelled as a parallel plate. The number of segments in each fracture is a function of the length of each element in finite element mesh, the length of fracture and also the extent of variations observed from in-situ investigations. By integrating the effect of all these factors, maximum number of segments in a fracture is given by

$$N_p = \frac{l_f}{l_e(18)}$$

Where  $N_p$ ,  $l_f$  and  $l_e$  are the maximum number segments in each fracture, length of fracture and the length of element in the finite element (FE) mesh respectively. In the present study, each fracture is segmented into five parts and the range of aperture values considered are  $1 \times 10^{-5}$  m to  $5 \times 10^{-5}$  m [29, 74]. A random combination of aperture sizes are considered for the analysis as shown in Fig. 14. To examine various factors involved in contaminant transport modelling through fractured rock mass, a geosphere transport model has been developed that includes generating fractures, generating a finite element mesh that can model fluid flow and contaminant transport process in fractures and intact rock matrix and, generating aperture variation along the fracture. These three components are integrated by coding in python programming interface. The computational efficiency of the model increased by automating these components.



Fig. 14. Schematic of aperture variation along the fracture

Input parameters considered in the model. The input properties of radionuclide to solve the source term which include the inventory and geo-chemical properties of Iodine and the geo-hydrological properties of the medium are taken from the literature and presented in the previous models (Table 2 an Table 3). From the previous studies, it could be noted that the general range of fracture orientations observed from the field and modelling investigations was  $0^{\circ} - 130^{\circ}$  [8, 47, 75]. In the present study, fracture orientations ( $\theta_k$ ) considered are 45°- 90°. The input parameters considered for fracture generation are presented in Table 5. The geological and transport properties of fractured rock mass are taken from the literature and presented in Table 6. The distribution coefficient in the intact rock matrix is calculated using empirical equation given 480 by Krishnamoorthy et. al., [38].

$$K_r = \frac{K_f \rho_s r}{3} (19)$$

Where  $K_f$  - distribution coefficient in fracture (m1/g);  $\rho_s$  - specific density (g/cm<sup>3</sup>); r - particle radius (cm). A rock mass of size 20 m × 20 m with fracture network of dimension 10 m × 10 m is modelled within the domain and it is shown in Fig. 15.



Fig. 15. Finite element mesh generated for the problem

This domain is discretized into a two-dimensional quadrilateral mesh with 40401 nodes and the fractures are modelled as one-dimensional discrete elements. To model the inclined fractures in FE mesh, each quadrilateral element is divided further into four small triangular elements leading to 80401 nodes in the mesh, are shown in Fig. 15. The flow motion along the fracture is assumed to follow Hagen-Poiseuille law. The contaminant

flow is considered both along x-direction and y-direction to examine the influence of heterogeneity in fractures. The fluid flow and mass boundary conditions (bc) for flow along x-direction are presented in Table 7. The same bc conditions are applied in y-direction for the cases when the contaminant flow is along y-direction.

| Sr. | Property                                                    | Value       |
|-----|-------------------------------------------------------------|-------------|
| No  |                                                             |             |
| 1   | Length of domain in x-direction (m)                         | 10          |
| 2   | Length of domain in y-direction (m)                         | 10          |
| 3   | Number of fracture sets                                     | 1, 2, 3     |
| 4   | Density of fractures (m <sup>-1</sup> )                     | 1,2         |
| 5   | Probability of continuation after fracture intersection (m) | 0, 0.1, 0.2 |
| 6   | Velocity of propagation                                     | 2,1         |
| 7   | Inhibition distance for initial point simulation (m)        | 0.1         |

Table 5. Input data considered for fracture generation

Table 6. Geological properties of rock and transport properties of the contaminant

| Quantity                               | Value                |  |  |  |  |
|----------------------------------------|----------------------|--|--|--|--|
| Intact rock matrix                     |                      |  |  |  |  |
| Isotropic hydraulic conductivity (m/s) | 10-9                 |  |  |  |  |
| Porosity                               | 0.13                 |  |  |  |  |
| Molecular diffusion $(m^2/s)$          | 5×10-10              |  |  |  |  |
| Longitudinal dispersivity (m)          | 1                    |  |  |  |  |
| Transverse dispersivity (m)            | 0.05                 |  |  |  |  |
| Fracture                               |                      |  |  |  |  |
| Fracture area (m <sup>2</sup> )        | 6×10 <sup>-5</sup>   |  |  |  |  |
| Hydraulic aperture (m)                 | $1.2 \times 10^{-4}$ |  |  |  |  |
| Hydraulic radius (m <sup>2</sup> )     | 6×10 <sup>-5</sup>   |  |  |  |  |
| Longitudinal dispersivity (m)          | 0.1                  |  |  |  |  |
| Molecular diffusion $(m^2/s)$          | 5×10 <sup>-9</sup>   |  |  |  |  |
| Distribution coefficient (ml/g)        | 2.6                  |  |  |  |  |

Section Value Quantity Fluid Flow AB Dirichlet type bc at LHS  $(-5 \le y \le 15; x = -5)(m)$ 10 DC Dirichlet type bc at LHS  $(-5 \le y \le 15; x = 15)(m)$ 0 Mass Transport Initial condition of contaminant concentration  $(Bq/m^3)$ 1 EF Decaying mass bc at LHS  $(0 \le y \le 10; x = -0 m)$ 0.05  $(Bq/m^3)$ 

Table 7. Fluid flow and mass transport boundary conditions

**Deterministic analysis.** The movement of radionuclide in the fractured medium is nonintuitive due to the presence of an interconnected system of randomly oriented fractures. Some critical observation points are considered for the analysis and shown in Fig. 16. The evolution of contaminant concentrations over time are evaluated at these points. From Fig. 16 (a) and 16 (b), it can be noted that observation points are ordered along x-direction and y-direction. The results of contaminant concentrations are evaluated at different observation points spread along and across the network. To investigate the radionuclide migration through a fractured rock mass and demonstrate the efficiency of the radionuclide transport model, the simulations are presented for  $45^{\circ}$ -  $90^{\circ}$  fracture network. The fracture network generated from the algorithm is shown in Fig. 17.



Fig. 16. Observation points when the contaminant flow is (a) along x-direction (b) along y-direction



Fig. 17. 45°- 90° Fracture pattern generated from fracture generation algorithm

When two fracture sets are considered a total of 200 fractures are generated and the results of concentration trends for flow along x and y directions are presented in Fig. 18. These results give an idea of the concentration profiles for the  $45^{\circ}$ - 90° fracture set. Fig. 18 (i) and Fig. 18 (ii) present the concentration trends evolving in time when the contaminant flow is along x-direction and y-direction respectively. Due to the reactive nature of the contaminant, there is a postpeak decay in the concentration trends. Through visual inspection, it can be observed that the concentration trends in Fig. 18 (i) and Fig. 18 (ii) are not similar. So, the pathway of radionuclide movement is different (i.e., preferential movement) when the is flow along x and y direction indicating the effect of heterogeneity in the fracture network. The time of arrival of maximum concentration (around 150 years) is same in both the cases, however, the peak concentration is around 8000 Bq/m<sup>3</sup> in the Fig. 18 (i)), whereas, it increased to around 12000 Bq/m<sup>3</sup> in Fig. 18 (ii). The influence of local aperture variation on the radionuclide transport process is tested by running simulations for scenarios with and without considering the variations.



**Proceedings of Indian Geotechnical Conference 2020** December 17-19, 2020, Andhra University, Visakhapatnam

(ii) Along y direction

Fig. 18. Concentration versus time for 45°- 90° fracture set

It is interesting to note that, the peak concentration value remained almost same in both the cases, however, the time of arrival of maximum concentration increased by twofold (i.e., increased from 149 years to 354 years). These results suggest that the time taken to reach the endpoint of interest changes drastically when the local aperture variations along the fractures are taken into account in the model. The same observation is made both for flow along x-direction and y-direction. Further, the radiation dose and risk to a member of the critical group through consumption of ground water for drinking are calculated from

the radiological model. The risk estimated falls in the range of  $10^{-4}$  to  $10^{-5}$  y<sup>-1</sup>. These values are low in comparison to the risk due to natural catastrophes and natural background radiation. Similar observations were made for risk values calculated in the case of contaminant flow along y-direction. Hence, the risk values evaluated for deterministic analysis fall within the safe limits indicating safe disposal of radioactive waste.

**Probabilistic analysis.** An integrated safety assessment model considers the effect of uncertainties. So, probability that the quantities (i.e., radiation dose or risk) exceed the design threshold is estimated by carrying out reliability analysis. This value provides a prior indication of radionuclide contamination in the environment due to any release of radionuclide from disposal facility. The mean values (underlying normal distribution) of the input parameters (in Table 4), the probabilistic distribution and coefficient of variation (COV) [4, 10, 55,59 65] have been assumed from literature and presented in Table 8. The  $P_f$  values are estimated as 6.7 ×10<sup>-6</sup> for 15% COV and for 30% COV from subset simulation. These values indicate that, with the increase in the COV, the  $P_f$  increases by a factor of 10<sup>4</sup>. So, higher is the radiological impact and risk to the near-field biosphere in the second case and the disposal system needs immediate attention to stop intrusion of radiation further to the environment.

| S.No | Property                                  | Iodine |          | Distribution |  |
|------|-------------------------------------------|--------|----------|--------------|--|
|      |                                           | Mean   | COV      |              |  |
|      | Intact Rock matrix                        |        |          |              |  |
| 1    | Distribution coefficient (ml/g)           | 2.6    | 0.15,0.3 | Lognormal    |  |
| 2    | Porosity                                  | 0.13   | 0.15,0.3 | Lognormal    |  |
|      | Fracture                                  |        |          |              |  |
| 3    | Fracture aperture (part 1) (µm)           | 50     | 0.15,0.3 | Lognormal    |  |
| 4    | Fracture aperture (part 2) (µm)           | 10     | 0.15,0.3 | Lognormal    |  |
| 5    | Fracture aperture (part 3) (µm)           | 20     | 0.15,0.3 | Lognormal    |  |
| 6    | Fracture aperture (part 4) (µm)           | 40     | 0.15,0.3 | Lognormal    |  |
| 7    | Fracture aperture (part 5) (µm)           | 30     | 0.15,0.3 | Lognormal    |  |
| 8    | Diffusion coefficient (m <sup>2</sup> /s) | 5×10-9 | 0.15,0.3 | Lognormal    |  |
| 9    | Longitudinal dispersivity (m)             | 10     | 0.15,0.3 | Lognormal    |  |

Table 8. Input data considered for fracture generation

The results from this model reiterates the need to account for the contributions from fractures, local aperture variations in fractures, geological and radionuclide transport properties in the fractured rock media to estimate the performance of the radioactive waste disposal facility.

### 5 Conclusions

Various contaminant (i.e., radionuclide) transport models are developed to predict the subsurface contamination caused by the migration of contaminants in the geosphere. These models are integrated to the probabilistic performance assessment modelling framework to quantitatively estimate the radiological impact and risk caused due to the release of radionuclides from radioactive waste disposal systems to the biosphere. The influence of the geological media (ie., soil, rocks) and the different forms of uncertainties (ie., spatial variability, parameter uncertainties) on the performance of radioactive waste disposal systems (ie., NSDFs) are encapsulated in these models. The main conclusions from each model are:

(a) Numerical model to describe the flow and transport of radionuclide in soil

- 1. A three-dimensional radionuclide transport model with a decaying source concentration is modelled 564 numerically and the concentration, radiation dose of radionuclide Iodine (<sup>129</sup>I) is computed.
- 2. The deterministic analysis results showed that potential risk due to <sup>129</sup>I to the nearby human habitat through drinking water pathway calculated from the model is and it is observed to be lower than the risk observed from industrial accidents and natural catastrophes  $(1 \times 10^{-3} 1 \times 10^{-4} y^{-1})$ .
- 3. The uncertainties in the input parameters porosity, hydraulic conductivity, groundwater velocity, diffusion coefficient and distribution coefficient are propagated through the model and quantified. The probability of failure (i.e., radiation dose exceeding permissible value) is 10<sup>-9</sup>. The low value of probability of failure show that the system is safe from the risk due to radiation through the drinking water pathway.

(b) Numerical model to describe the flow and transport of radionuclide in spatially varying soil0

- 1. The transport of radionuclide in geosphere is modelled numerically to understand the influence of spatial 574 variability in soil on radionuclide transport process.
- 2. From the deterministic analysis, the risk values of <sup>129</sup>I reaching the endpoint through drinking water pathway 576 is calculated as  $4.95 \times 10^{-5}$  y<sup>-1</sup> which is lower than the risk observed from industrial accidents and natural catastrophes.
- 3. The radionuclide migration process in a homogeneous medium (traditional case) and spatially varying medium are compared and, the results showed that the rate of movement of radionuclide was faster in a homogeneous medium than the latter case. In the spatially varying case, the frequent fluctuations in conductivity led to a slower rate of flow leading to lower concentration at the endpoint.

- 4. The  $P_f$  values increased monotonically with an increase in the spatial correlation length and its value is maximum for homogeneous case. The range of autocorrelation length that has significant effect on  $P_f$  is identified from the probabilistic analysis indicating its sensitivity on the radionuclide transport process. From the design point of view, by modelling the medium to be homogeneous the possibility of failure in the system is overestimated which is uneconomical.
- (c) Numerical model to describe the flow and transport of radionuclide in fractured rock:
  - 1. A numerical model that describes the flow and transport behaviour of a contaminant in fractured rock mass is developed. It simulates the fracture patterns from a stochastic algorithm, models the flow and transport of contaminant (through fractures and rock) and, quantifies the contaminant migration through the system.
  - 2. The risk estimated from the model for  $45^{\circ}$   $90^{\circ}$  fracture set is  $10^{-5}$  y<sup>-1</sup> and this value is low in comparison to the risk due to natural catastrophes and natural background radiation.
  - 3. The influence of local aperture variations along the fracture is also investigated. The results showed that by incorporating the local aperture variations, the time of arrival of maximum concentration increased by twofold. Since the temporal aspect of contaminant plume movement is also critical in the safety assessment, it becomes critical to account for this factor in the geosphere transport modelling in fractured rocks.
  - The uncertainties in the geological properties of fractures and intact rock matrix, 4. transport properties of radionuclide iodine are propagated through the model and the effect of these uncertainties are quantified using subset simulation. The probability of failure values are estimated as  $6.7 \times 10^{-6}$  for 15%COV and  $6 \times 10^{2}$ for 30% COV. With the increase in the COV of random variables, the  $P_f$  value increased. The  $P_f$  value for 30% COV is very high indicating a higher probability of risk and radiological impact on biosphere. The results from each model demonstrates their computational efficiency, highlights the influence of the groundwater contaminant transport process in analyzing the safety of the disposal systems and the need to account for various uncertainties in the geosphere (which include the geohydrological properties of the medium and the contaminant transport properties) to estimate the risk and radiation caused by the radionuclides on the environment and public health. The probabilistic performance assessment modelling framework presented in this paper helps in improving the quality of risk and radiological impact assessment for the practitioners.

#### Acknowledgements

The work presented in this paper is part of research work carried out in the project "Development of probabilistic design and analysis procedures in radioactive waste disposal in NSDF and design of NSDF closure" sponsored by Board of Research in Nuclear Science (BRNS). The discussion with scientists of Bhabha Atomic Research Center (BARC) and their financial assistance is gratefully acknowledged.

#### References

- 1. Abriola, L. M. (1987). Modeling contaminant transport in the subsurface: An interdisciplinary challenge. *Reviews of Geophysics*, 25(2), 125-134.
- 2. AERB (Atomic Energy Regulatory Board). 2006. *Near surface disposal of radioactive waste (Tech. Rep.)*. Guide No: AERB/NRF/SG/RW-4, Mumbai, India: AERB.
- 3. Ahmed, A., &Soubra, A. H. (2018). Application of the subset simulation approach to spatially varying soils. In *Risk and Reliability in Geotechnical Engineering* (pp. 591-625). CRC Press.
- Aladejare, A. E., & Wang, Y. (2017). Evaluation of rock property variability. *Georisk:* Assessment and Management of Risk for Engineered Systems and Geohazards, 11(1), 22– 41.
- 5. Au, S. K., & Beck, J. L. (2001). Estimation of small failure probabilities in high dimensions by subset simulation. *Probabilistic engineering mechanics*, *16*(4), 263-277.
- Au, S. K., & Beck, J. L. (2003). Subset simulation and its application to seismic risk based on dynamic analysis. *Journal of Engineering Mechanics*, 129(8), 901-917.
- 7. Baecher, G. B., & Christian, J. T. (2005). *Reliability and statistics in geotechnical engineering*. John Wiley & Sons.
- Bai, T., & Pollard, D. D. (2000). Fracture spacing in layered rocks: A new explanation based on the stress transition. *Journal of Structural Geology*, 22(1), 43–57. doi: 10.1016/S0191-8141(99)00137-6
- 9. Bear, J., Tsang, C.-F., & De Marsily, G. (1993). Flow and contaminant transport in fractured rock. Academic Press.
- Benaafi, M., Hariri, M., Bertotti, G., Al-Shaibani, A., Abdullatif, O., &Makkawi, M. (2019). Natural fracture system of the cambro-permianwajid group, wadi al-dawasir, swsaudiarabia. *Journal of Petroleum Science and Engineering*, 175, 140–158.
- 11. Berkowitz, B. (2002). Characterizing flow and transport in fractured geological media: A review. *Advances in water resources*, 25(8-12), 861-884.
- Boguslavsky, A. E., Gaskova, O. L., Naymushina, O. S., Popova, N. M., & Safonov, A. V. (2020). Environmental monitoring of low-level radioactive waste disposal in electrochemical plant facilities in Zelenogorsk, Russia. *Applied Geochemistry*, 104598.
- Cadini, F., D. Avram, N. Pedroni, and E. Zio. (2012). "Subset Simulation of a Reliability Model for Radioactive Waste Repository Performance Assessment." *Reliability Engineering* and System Safety 100. Elsevier: 75–83. doi:10.1016/j.ress.2011.12.012.

- Cadini, F., Gioletta, A., & Zio, E. (2015). Estimation of passive systems functional failure probabilities by the modified meta-IS algorithm. *Progress in Nuclear Energy*, 81, 134-140.
- Cao, X., Zheng, L., Hou, D., O'Connor, D., Hu, L., & Wu, J. (2020). Modeling the risk of U (VI) migration through an engineered barrier system at a proposed Chinese high-level radioactive waste repository. *Science of The Total Environment*, 707, 135472.
- Cho, S. E., & Park, H. C. (2010). Effect of spatial variability of cross\_correlated soil properties on bearing capacity of strip footing. *International Journal for Numerical and Analytical Methods in Geomechanics*, 34(1), 1-26.
- Chopra, M., Rastogi, R., Kumar, A. V., Sunny, F., & Nair, R. N. (2013). Response surface method coupled with first-order reliability method based methodology for groundwater flow and contaminant transport model for the uranium tailings pond site. *Environmental Modeling & Assessment*, 18(4), 439-450.
- Ciriello, V., Di Federico, V., Riva, M., Cadini, F., De Sanctis, J., Zio, E., & Guadagnini, A. (2013). Polynomial chaos expansion for global sensitivity analysis applied to a model of radionuclide migration in a randomly heterogeneous aquifer. *Stochastic Environmental Research and Risk Assessment*, 27(4), 945-954.
- Cotta, R. M., Naveira-Cotta, C. P., Genuchten, M. T., Su, J., & Quaresma, J. N. (2020). Integral transform analysis of radionuclide transport in variably saturated media using a physical non-equilibrium model: application to solid waste leaching at a uranium mining installation. *Anais da Academia Brasileira de Ciências*, 92(1).
- Der Kiureghian, A., &Ditlevsen, O. (2009). Aleatory or epistemic? Does it matter?. Structural safety, 31(2), 105-112.
- 21. Diersch, H. J. G. (2013). FEFLOW: finite element modeling of flow, mass and heat transport in porous and fractured media. Springer Science & Business Media.
- Elango, L., Brindha, K., Kalpana, L., Sunny, F., Nair, R. N., &Murugan, R. (2012). Groundwater flow and radionuclide decay-chain transport modelling around a proposed uranium tailings pond in India. Hydrogeology Journal, 20(4), 797-812.
- Elango, L., Thirumurugan, M., Sunny, F., & Chopra, M. (2016). Modeling of Radionuclide Transport in Groundwater. In *Groundwater Assessment, Modeling, and Management* (pp. 283-297). CRC Press.
- Geetha Manjari, K., & Sivakumar Babu, G. L. (2018). Probabilistic analysis of groundwater and radionuclide transport model from near surface disposal facilities. *Georisk: Assessment* and Management of Risk for Engineered Systems and Geohazards, 12(1), 60-73.
- 25. Gelhar, L. W. (1993). *Stochastic subsurface hydrology* (Vol. 390). Englewood Cliffs, NJ: Prentice-Hall.
- Ghanem, R. G., & Spanos, P. D. (2003). Stochastic finite elements: a spectral approach. Courier Corporation.
- Ghanem, R., & Dham, S. (1998). Stochastic finite element analysis for multiphase flow in heterogeneous porous media. *Transport in porous media*, 32(3), 239-262.
- Glinskii, M. L., Glagolev, A. V., Speshilov, S. L., Grachev, V. A., Plyamina, O. V., &Evseenkova, T. A. (2020). Development of Environmental Monitoring in the Vicinity of Nuclear Energy Facilities. *Atomic Energy*, 127(3), 166-173.
- 29. Graf, T., & Therrien, R. (2005). Variable-density groundwater flow and solute transport in porous media containing nonuniform discrete fractures. *Advances in water resources*, 28(12), 1351–1367.

- Grisak, G. E., & Pickens, J. F. (1980). Solute transport through fractured media: 1. The effect of matrix diffusion. *Water resources research*, 16(4), 719-730.
- 31. Hassan, A. E., Pohll, G., Pohlmann, K. F., & Chapman, J. B. (2020, August). Incorporating subsurface heterogeneity and uncertainty in groundwater flow and transport modeling: Three approaches for three different environments. In *Hydrology and Water Resources: Volume 5-Additional Volume International Conference on Water Resources Management in Arid Regions*, 23-27 March 2002, Kuwait (p. 223). CRC Press.
- Helton, J. C. (1993). Uncertainty and sensitivity analysis techniques for use in performance assessment for radioactive waste disposal. *Reliability Engineering & System Safety*, 42(2-3), 327-367.
- Higashi, K., & Pigford, T. H. (1980). Analytical models for migration of radionuclides in geologic sorbing media. *Journal of Nuclear Science and Technology*, 17(9), 700-709.
- IAEA (International Atomic Energy Agency). 2014. Near surface disposal facilities for radioactive waste. IAEA SAFETY STANDARDS SERIES (No. GS-R-3). Vienna, Austria: IAEA.
- 35. ICRP (International Commission on Radiological Protection). 1990. *Recommendations of the international commission on radiological protection*. ICRP Publication 60. Annals of the ICRP 1 (3). Oxford: Pergamon Press.
- Jakimavičiūtė-Maselienė, V., Mažeika, J., &Motiejūnas, S. (2016). Application of vadose zone approach for prediction of radionuclide transfer from near-surface disposal facility. *Progress in Nuclear Energy*, 88, 53-57.
- Krishnamoorthy, T. M., Nair, R. N., &Nambi, K. S. V. (1997). Evaluation of disposal limits for shallow land burial facilities: Application to the back end of nuclear fuel cycle. *Applied radiation and isotopes*, 48(9), 12031209.
- Krishnamoorthy, T. M., Nair, R. N., &Sarma, T. P. (1992). Migration of radionuclides from a granite repository. *Water Resources Research*, 28(7), 1927-1934.
- Kumar, G. S., & Sekhar, M. (2005). Spatial moment analysis for transport of nonreactive solutes in fracturematrix system. *Journal of Hydrologic Engineering*, 10(3), 192-199.
- Lei, Q., Latham, J.-P., & Tsang, C.-F. (2017). The use of discrete fracture networks for modelling coupled geomechanical and hydrological behaviour of fractured rocks. *Computers and Geotechnics*, 85, 151–176.
- Long, J. C. S., Hestir, K., Karasaki, K., Davey, A., Peterson, J., Kemeny, J., &Landsfeld, M. (1991). *Fluid flow in fractured rock: Theory and application*. In Transport Processes in Porous Media (pp. 203-241). Springer, Dordrecht.
- 42. Marseguerra, M., & Zio, E. (2001). Looking at Monte Carlo simulation for describing nonlinear sorption in groundwater contaminant transport. *Mathematics and computers in simulation*, 55(1-3), 167-176.
- Miller, A. W., Rodriguez, D. R., &Honeyman, B. D. (2010). Upscaling sorption/desorption processes in reactive transport models to describe metal/radionuclide transport: A critical review. *Environmental science & technology*, 44(21), 7996-8007.
- Nair, R. N., & Krishnamoorthy, T. M. (1999). Probabilistic safety assessment model for near surface radioactive waste disposal facilities. *Environmental Modelling & Software*, 14(5), 447-460.

- Nair, R. N., Mayya, Y. S., &Puranik, V. D. (2006). A generic method to evaluate the reasonable upper-bound dose from near-surface radioactive waste disposal facilities through drinking water pathway. *Nuclear technology*, 153(1), 53-69.
- Nair, R. N., Sunny, F., & Manikandan, S. T. (2010). Modelling of decay chain transport in groundwater from uranium tailings ponds. *Applied mathematical modelling*, 34(9), 2300-2311.
- 47. Narr, W., &Suppe, J. (1991). Joint spacing in sedimentary rocks. *Journal of Structural Geology*, *11*(9), 1037–1048. doi: 10.1016/0191-8141(91)90055-N
- Nazeeh, K. M., & Sivakumar Babu, G. L. (2018). Reliability analysis of near-surface disposal facility using subset simulation. *Environmental Geotechnics*, 6(4), 242-249.
- Neuman, S. P. (2005). Trends, prospects and challenges in quantifying flow and transport through fractured rocks. *Hydrogeology Journal*, 13(1), 124-147.
- Pannecoucke, L., Le Coz, M., Houzé, C., Saintenoy, A., Cazala, C., & de Fouquet, C. (2019). Impact of spatial variability in hydraulic parameters on plume migration within unsaturated surficial formations. *Journal of hydrology*, 574, 160-168.
- Park, E., & Zhan, H. (2001). Analytical solutions of contaminant transport from finite one-, two-, and threedimensional sources in a finite-thickness aquifer. *Journal of Contaminant Hydrology*, 53(1-2), 41-61.
- 52. Parker, B. L., Cherry, J. A., & Chapman, S. W. (2012). Discrete fracture network approach for studying contamination in fractured rock. *AQUA mundi*, *3*(2), 101-116.
- Patelli, E. (2012). An upscaling approach for uncertainty quantification of stochastic contaminant transport through fractured media. *In International Conference on Scalable Uncertainty Management* (pp. 261-272). Springer, Berlin, Heidelberg.
- Piqué, À., Arcos, D., Grandia, F., Molinero, J., Duro, L., & Berglund, S. (2013). Conceptual and numerical modeling of radionuclide transport and retention in near-surface systems. *Ambio*, 42(4), 476-487.
- Piscopo, V., Baiocchi, A., Lotti, F., Ayan, E. A., Biler, A. R., Ceyhan, A. H., ... Ta,skin,M. (2017). Estimation of rock mass permeability using variation in hydraulic conductivity with depth: experiences in hard rocks of western Turkey. *Bulletin of Engineering Geology and the Environment*, 1–9. doi: 10.1007/s10064-017-1058-8
- Qin, X. S., Huang, G. H., & Chakma, A. (2008). Modeling Groundwater Contamination under Uncertainty: A Factorial-Design-Based Stochastic Approach. *Journal of Environmental Informatics*, 11(1).
- Raj, K., Prasad, K. K., & Bansal, N. K. (2006). Radioactive waste management practices in India. *Nuclear Engineering and Design*, 236(7-8), 914-930.
- 58. Rakesh, R., Yadav, D., Narayan, P., & Nair, R. (2005). Post closure safety assessment of radioactive waste storage and management site, trombay (Tech. Rep.). Bhabha Atomic Research Centre, India.
- 59. Riley, M. S. (2004). An algorithm for generating rock fracture patterns: mathematical analysis. *Mathematical geology*, *36*(6), 683-702.
- 60. Robinson, B. A., Houseworth, J. E., & Chu, S. (2012). Radionuclide transport in the unsaturated zone at Yucca Mountain, Nevada. *Vadose Zone Journal*, *11*(4).
- 61. Rowe, R. K., & Booker, J. R. (1985). 1-D pollutant migration in soils of finite depth. *Journal of Geotechnical Engineering*, 111(4), 479-499.

- 62. Sarkar, S., Toksoz, M. N., & Burns, D. R. (2004). *Fluid flow modeling in fractures (Tech. Rep.).* Massachusetts Institute of Technology. Earth Resources Laboratory.
- 63. Shackelford, C. D., & Rowe, R. K. (1998). Contaminant transport modeling. In *Environmental Geotechnics* (pp. 939-956).
- 64. Sharma, H. D., & Reddy, K. R. (2004). *Geoenvironmental engineering: site remediation,* waste containment, and emerging waste management technologies. John Wiley & Sons.
- Sharma, P. K., Joshi, N., & Ojha, C. (2013). Stochastic numerical method for analysis of solute transport in fractured porous media. *Journal of hydro-environment research*, 7(1), 61–71.
- 66. Sujitha, S., Manjari, K. G., Datta, S., & Babu, G. S. (2016). Risk and reliability analysis of multibarrier system for near-surface disposal facilities. *Journal of Hazardous, Toxic, and Radioactive Waste, 20*(2), 04015014.
- 67. Tang, D. H., Frind, E. O., &Sudicky, E. A. (1981). Contaminant transport in fractured porous media: Analytical solution for a single fracture. *Water resources research*, 17(3), 555-564.
- Tang, D. H., Frind, E. O., &Sudicky, E. A. (1981). Contaminant transport in fractured porous media: Analytical solution for a single fracture. *Water resources research*, 17(3), 555-564.
- 69. Thangarajan, M., & Singh, V. P. (Eds.). (2016). Groundwater Assessment, Modeling, and Management. CRC Press.
- Thiessen, K. M., Thorne, M. C., Maul, P. R., Pröhl, G., &Wheater, H. S. (1999). Modelling radionuclide distribution and transport in the environment. *Environmental Pollution*, 100(1-3), 151-177.
- Trinchero, P., Cvetkovic, V., Selroos, J. O., Bosbach, D., &Deissmann, G. (2020). Upscaling of radionuclide transport and retention in crystalline rocks exhibiting micro-scale heterogeneity of the rock matrix. *Advances in Water Resources*, 103644.
- 72. Vanmarcke, E. (2010). Random fields: analysis and synthesis. MIT press, Cambridge, Massachusetts, USA.
- 73. Wattal, P.K. (2013). "Indian programme on radioactive waste management." *Sadhana, Indian Acedamy of Sciences*, 38(5), 849-857.
- Wendland, E., &Himmelsbach, T. (2002). Transport simulation with stochastic aperture for a single fracture– comparison with a laboratory experiment. *Advances in water resources*, 25(1), 19–32.
- Yue, L., Sun, S., Liu, J., Wei, J., &Wu, J. (2017). Research on crack initiation mechanism and fracture criterion of rock-type materials under compression shear stress. *Advances in Mechanical Engineering*, 9(10), 1–13. doi: 782 10.1177/1687814017720087