8. GEOSPHERE MODELLING

8.1. Aim
This section considers geosphere modelling. In particular, it:
- provides a definition of the geosphere and considers its importance, and associated key issues, in safety assessments (Section 8.2);
- identifies the key flow and transport mechanisms that are typically identified when developing a conceptual model of the geosphere (Section 8.3);
- considers their representation in mathematical models (Section 8.4);
- identifies some example computer codes that are used for implementing the mathematical models (Section 8.5); and
- discusses typical data requirements for model formulation and implementation (Section 8.6).

8.2. Introduction

8.2.1. Definition
The geosphere consists of the rock and unconsolidated material that lies between the near-field and the biosphere. It can consist of both the unsaturated or vadose zone (which is above the groundwater table) and the saturated zone (which is below the groundwater table).

8.2.2. Importance and Key Issues
One of the radionuclide release pathways that is most commonly evaluated in safety assessments is the liquid release pathway. In the case of this release pathway, radionuclides are released from the near-field due to leaching by infiltrating water and then they migrate through the geosphere into the biosphere (see for example Figure 8.1). If the disposal facility is located in the saturated zone, a radionuclide plume will develop, with its longitudinal axis along the direction of flow with some lateral and vertical spread. If the disposal facility is in the unsaturated zone, the plume will spread vertically down from the facility to the watertable; some lateral dispersion will occur. Although the release of radionuclides via the leaching pathway can be limited by good engineering of the disposal facility, consistent with the multi-barrier concept, it is advantageous to limit radionuclide releases further. The geosphere can fulfil this role through acting as a natural barrier to prevent or inhibit the movement of radionuclides due to its physical, chemical or biological characteristics. It is this preventative/inhibiting role that needs to be evaluated as part of the safety assessment. Indeed, the IAEA safety requirements for near surface disposal of radioactive waste [IAEA, 1999] notes that “the waste disposal system shall provide for the isolation of waste and limitation of releases of radionuclides….., with account taken of the …..natural barriers associated with the site”.

In addition, depending on the depth of the disposal facility, the geosphere can also impact upon other radionuclide release pathways such as the gas, human intrusion, and natural disruptive events pathways. However, for the purpose of this section, the primary focus is on liquid release pathway since this is the pathway that is affected most by the geosphere and its characteristics and processes. This is especially the case for facilities that are located within a few metres of the ground surface since the gas, human intrusion, and natural disruptive events pathways essentially bypass the geosphere and result in the release of radionuclides directly from the near-field into the biosphere.
Anderson and Woessner [1992] identify a number of steps that can be applied to conceptual and mathematical modelling flow and transport in the geosphere (Figure 8.2), especially for the development groundwater flow models. Many of the steps are also applicable to the modelling of the near-field and biosphere. The level of detail at which the approach, described below and shown in Figure 8.2, is applied should be consistent with the assessment context and level of resources available.
Figure 8.2: Suggested Steps in Geosphere Flow and Transport Modelling [Anderson and Woessner, 1992]

- Definition of the purpose of the model. Information from the assessment context and scenario generation steps of the assessment approach can be used to define the purpose of the model.

- Development of the conceptual model using available site information concerning the geology, hydrogeology and geochemistry of the site, and the associated key processes that affect the geosphere. This information is used to conceptualise the movement of groundwater through the geosphere and to define the boundaries of conceptual model. At this stage, 3 dimensional visualisation software tools such as EarthVision [Dynamic Graphics, 2001] can be used to help develop and interpret the conceptual model and provide boundary conditions for the flow and transport models (see for example Figure 8.3).
Selection of governing equations (i.e. the fundamental equations upon which the model is based) and computer codes including the code verification by comparing the numerical solutions with one or more analytical solutions or with other numerical solutions.

Model design (e.g. grid generation required for numerical solution techniques, time step selection, boundary and initial conditions, and preliminary selection of input data).

Calibration and sensitivity analysis. The purpose of calibration is to establish that the model can reproduce any field-measured heads and flows (and contaminant concentrations if there are any data available, for example from tracer experiments). Calibration is accomplished by finding a set of parameters and boundary conditions that produce simulated heads and water fluxes (and concentrations), matching field data within a pre-established range of error (inverse problem). Most model calibrations are performed using steady-state data sets, but secondary transient calibrations can be performed using transient data sets. There are two methods of model calibration: manual trial-and-error adjustment; and automated parameter estimation. A sensitivity analysis can be performed in order to establish the effects of uncertainties on the calibrated model. Usually one parameter is changed at a time and the model response is examined. Calibration can only be undertaken for the time period for which data have been recorded.

Validation to establish greater confidence in the model by using the set of calibrated parameter values to reproduce the field data (see for example Figure 8.4). A model is considered validated when sufficient testing has been performed to ensure an acceptable level of predictive accuracy over the range of conditions over which the model may be applied. Validation is only possible over the short term for which data are available. As noted in Section 6.5, the validation of models for the long term evolution of a specific site is not possible over the long timescales of relevance to safety assessments.
- Estimation of quantities (heads, groundwater velocities, flows, concentrations) that are expected to change in the future including sensitivity analysis which quantifies the effect of uncertainty in input parameter values on the estimation (see for example Figure 8.5).

- Presentation of modelling design and results.

Figure 8.4: Observed versus Modelled Groundwater Heads (m) in the Lower Groundwater System at the Drigg Disposal Facility (negative values indicate the difference between observed and modelled heads) [BNFL, 2000]

Figure 8.5: Contaminant Pathline Analysis at the Hanford Site (heads in m) [Anderson and Woessner, 1992]
• A post-audit can be conducted several years after the initial modelling study once some new field data have been collected. If the model’s calculations are consistent with the new data, the model can be considered as validated for that particular site for the conditions that currently exist. Often the post-audit will lead to a new insight into system behaviour which may lead to changes in the conceptual model or in the input parameters and therefore the modelling process needs to be repeated.

8.3. Conceptual Models

Radionuclides released from the facility are transported in groundwater by advection, dispersion, and diffusion. If the disposal units are located below the water table, a radionuclide plume will develop, with its longitudinal axis along the direction of flow and a small lateral and vertical spread. If the disposal units are located above the water table, the conceptual model for groundwater should account for the fate and transport of radionuclides in the unsaturated zone. Downward advection usually is the primary mechanism for migration of radionuclides through the unsaturated zone to the water table. With its low moisture content, and low unsaturated hydraulic conductivity, unsaturated zone is usually acts as a natural barrier to migration of radionuclides to groundwater. On reaching the water table, radionuclides will be diluted due to mixing, and a plume will develop, predominantly in the lateral direction of the groundwater flow.

At sites with highly variable water table close to the bottom of the disposal units, the conceptual model may not account for transport through the unsaturated zone, leading to a conservative analysis. For long-term assessments, it is often sufficient to assume a steady-state flow field, with steady-state recharge. In the initial phase of an assessment, transport can be assumed to occur with a one-dimensional downward advection in the unsaturated zone,
and with one-dimensional advection and one or two-dimensional dispersion in the saturated zone.

The significance of transport through preferential pathways such as animal burrows, root channels, and fractures in the unsaturated zone, and of groundwater transport through fractures, and high-permeability lenses and channels can also be considered in developing the conceptual model. Conceptual model can also address the effects upon fate and transport of the radionuclides of matrix diffusion, colloidal transport, and various geochemical processes such as complexation if site characterisation indicates that these are processes of potential importance at the site.

When developing conceptual models of flow and contaminant transport in the geosphere, it is important to consider both internal processes (e.g. advection, dispersion, retardation - see below) within the geosphere, and external processes associated with the near-field and the biosphere. For example, near-field processes (see Section 7) can influence water flow and chemistry in the geosphere surrounding the disposal facility, whilst biosphere processes such as flooding, erosion, weathering, recharge, environmental change (including climate change) all can have an impact on the geosphere. In addition, the role of human activities such as abstraction of water and artificial recharge must not be ignored. Certainly decoupling the geosphere from other components of the disposal system should be undertaken with caution.

A range of processes occur in the geosphere that serve to transport contaminants to the biosphere through groundwater (Table 8.1). The key processes need to be considered when developing a conceptual model of radionuclide transport through the geosphere are considered below based on information provided in IAEA [2002a], Elert [1997], and standard groundwater text books such as Bear [1972], de Marsily [1986] and Freeze and Cherry [1979]. It should be remembered that the relative importance of these processes is site- and contaminant-specific.

Table 8.1: Example Fate and Transport Processes (after NRC [1990])

<table>
<thead>
<tr>
<th>Process</th>
<th>Definition</th>
<th>Impact on Transport</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mass Transport</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Advection</td>
<td>Movement of mass as a consequence of fluid flow.</td>
<td>Most Important way of transporting mass away from source</td>
</tr>
<tr>
<td>Diffusion</td>
<td>Mass spreading due to molecular diffusion in response to concentration gradients.</td>
<td>An attenuation mechanism of second order in most flows systems where advection and dispersion dominate.</td>
</tr>
<tr>
<td>Dispersion</td>
<td>Fluid mixing due to effects of unresolved heterogeneity in the permeability distribution.</td>
<td>An attenuation mechanism that reduces contaminant concentration in the plume. However, it spreads to a greater extent than predicted by advection alone.</td>
</tr>
<tr>
<td><strong>Physico-chemical processes</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Radioactive Decay</td>
<td>Irreversible decline in the activity of a radionuclide through a nuclear reaction.</td>
<td>An important mechanism for contaminant attenuation when the half-life for decay is comparable to or less than the residence time of the flow system. Also adds complexity in production of daughter products.</td>
</tr>
<tr>
<td>Sorption</td>
<td>Partitioning of a contaminant between the water and mineral or organic solids in the system.</td>
<td>An important mechanism that reduces the rate at which the contaminants are apparently moving. Makes it difficult to remove contamination at a site.</td>
</tr>
<tr>
<td>Dissolution/precipitation</td>
<td>The process of adding contaminants to, or removing them from, solution by reactions dissolving or creating various solids.</td>
<td>Contaminant precipitation is an important attenuation mechanism that can control the concentration of contaminant in solution. Solution concentration is mainly controlled either at the source or at a reaction front.</td>
</tr>
<tr>
<td>---------------------------</td>
<td>------------------------------------------------------------------------------------------------------------------</td>
<td>----------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Acid/base reactions</td>
<td>Reactions involving a transfer of protons (H⁺).</td>
<td>Mainly an indirect control on contaminant transport by controlling the pH of water.</td>
</tr>
<tr>
<td>Complexation</td>
<td>Combination of cations and anions to form a more complex ion.</td>
<td>An important mechanism resulting in increased solubility of metals in water, if adsorption is not enhanced. Major ion complexation will increase the quantity of a solid dissolved in solution.</td>
</tr>
<tr>
<td>Hydrolysis/substitution</td>
<td>Reaction of a halogenated organic compound with water or a component ion of water (hydrolysis) or with another anion (substitution).</td>
<td>Often hydrolysis/substitution reactions make an organic compound more susceptible to biodegradation and more soluble.</td>
</tr>
<tr>
<td>Redox reactions (biodegradation)</td>
<td>Reactions that involve a transfer of electrons and include elements with more than one oxidation state.</td>
<td>An extremely important family of reactions in retarding contaminant spread through the precipitation of metals.</td>
</tr>
<tr>
<td>Biologically mediated mass transfer</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Biological transformations</td>
<td>Reactions involving the degradation of organic compounds, whose rate is controlled by the abundance of the micro-organisms and redox conditions.</td>
<td>Important mechanism for contaminant reduction but can lead to undesirable daughter products.</td>
</tr>
</tbody>
</table>
8.3.1. Advection

Advection is the transport of dissolved contaminants by the bulk movement of flowing water. The magnitude of the flux is a function of the flow rate and the concentration of dissolved radionuclides in the water. In the context of safety assessments, movement of water is usually considered to be due only to hydraulic forces. Consequently, the hydraulic head gradient is usually the primary motive force for advectively driven contaminant transport. Although, when considering advective flow in the unsaturated zone, there is also a need to consider the moisture content of the unsaturated zone.

8.3.2. Dispersion

Dispersion is the term applied to the observed spreading of contaminants in an advective velocity field. It can arise from: radionuclides being transported by several paths with different transport times; and differences in flow velocities within a single transport path (see Figure 8.6). In geological media, dispersion due to the presence of multiple flow paths often dominates. Dispersion occurs in direction of flow (longitudinal dispersion) and perpendicular to flow direction (transverse dispersion).

Figure 8.6: The Contribution of Multiple Flow Paths and Velocity Distribution to Dispersion

Dispersion has several effects on radionuclide transport:
- a sharp pulse of radionuclide release will be spread out often causing a reduction in the peak concentration;
- a radionuclide may reach a discharge point much earlier than the mean travel time - this is of great importance for radionuclides that decay during their travel through the geosphere;
- the radionuclide may spread out over a larger area.
In the groundwater transport literature the term “dispersion” is considered to be the sum of two effects: mechanical dispersion (as described above); and molecular diffusion (see Section 8.3.3).

8.3.3. Diffusion
Diffusion is caused by random thermal movement of the molecules. This causes a transport of contaminants from areas with high concentration to areas with low concentration. The rate of transport depends on how large the difference in concentration is over a given distance (the concentration gradient) and the pore structure of the material. The influence of the pore structure is described by a material constant - the diffusivity. The difference in diffusion behaviour between various chemical compounds is usually relatively small. The most common representation for transport via diffusion is Fick's first law, which states that a diffusive flux for contaminant is linearly proportional to its concentration gradient.

Diffusion in natural barriers is of importance when the water flow rate is very small or non-existent. For example diffusion can contribute significantly to the transport through low permeability materials such as clays. Diffusion into parts of the geosphere with immobile water may also contribute significantly to the retardation of radionuclides. This is a very important retention mechanism in the case of radionuclide transport in fractured rock where the radionuclides can diffuse from the fracture into the rock matrix.

8.3.4. Sorption
Fixation of substances dissolved in water on solid surfaces, e.g. mineral surfaces, is usually called sorption. The effect is that the dissolved concentration is reduced. In most cases the fixated radionuclides can return to the solution when the concentration in the water phase is reduced. In such cases sorption is reversible.

Fixation may occur by three main processes.

- **Physical sorption** is usually rapid and reversible and occurs when solutes are attracted to solid surfaces by non-substance specific forces. Sorption of ions to charged mineral surfaces results in a non-specific bonding called electrostatic bonding. Since the mineral surfaces normally are negatively charges this process mostly affects cations. The cation exchange capacity (CEC) is a parameter often measured in soils.

- **Chemical sorption** is often slow and irreversible and a specific bonding takes place resembling an ordinary chemical bonding.

- **Precipitation** is actually not a sorption process, although it leads to the binding of radionuclides to the solid phase. The solubility of a radionuclide is greatly influenced by the chemical environment, e.g. pH, redox potential and the presence of other substances in the solution. In soils, precipitation usually takes place due to the influence of solid mineral surfaces. A variant of precipitation is co-precipitation, which means that one solute is precipitated with another with lower solubility and is incorporated in its precipitate. Co-precipitation can often occur with iron, aluminium and manganese hydroxides.

The effect of these processes, as well as ion exchange and isomorphic substitution, are usually lumped into a single linear sorption or distribution coefficient ($K_d$) for use in safety
assessments (see for example Figure 8.7). The reasons for this are that the computer codes for solving coupled geochemical effects with transport are relatively uncommon and intensive computationally, and existing geochemical databases and models are not sufficiently reliable to justify the additional modelling detail. Consequently the $K_{d}$ concept represents the most commonly used approach for modelling sorption in the framework of a safety assessment, although some assessments have used more detailed geochemical codes for assisting in the interpretation of geochemical processes (see for example BNFL [2000]).

**Figure 8.7: Evaluation of $K_{d}$ values for Cs in clay and sand environment from NEA OECD Sorption Database [Konopaskova et al, 1995]**

Figure 8.8 shows the relationship between concentration in solution and concentration in the solid phase varies under the influence of sorption and solubility limitations, respectively. When sorption processes dominate, the concentration in solution is proportional to the concentration in the solid phase. In the case of solubility limitations, the concentration in solution is not affected by the concentration in the solid phase.

**Figure 8.8: The Relationship between Concentration in Solution and in Solid Phase under the Influence of Sorption and Solubility Limitations**
8.3.5. Radioactive Decay

Radioactive decay is an important process for the reduction of radionuclide concentrations during the transport in the geosphere (assuming that there is no ingrowth of the radionuclide from a parent). Many radionuclides have half-lives much shorter than their transport time in groundwater and will thus decay before reaching the biosphere in significant concentrations. Other radionuclides have half-lives that are so long that the decay during the transport through the geosphere to the biosphere is negligible.

Radionuclides that are part of a decay chain need specific consideration for a number of reasons. First, the decay products may be radioactive isotopes of elements with different physical and chemical characteristics, e.g. different sorption capabilities (for example that the decay of Th to its progeny is often important as the decay products tend to be more soluble and mobile than the parent) and so could have different transport characteristics. Second, for certain decay chains, there can be a long-time period required for a parent and its daughter to reach secular equilibrium and so both might need to be explicitly considered. Third, whilst short-lived daughters might not need to be explicitly considered for groundwater transport calculations per se, they might significantly contribute to the radiological impact of groundwater releases (for example Pb-210) and so need to be accounted for in the estimated flux of radionuclides from the geosphere to the biosphere.

8.3.6. Colloidal Transport

As stated in Section 7, colloids are suspended particles with diameters less than ten microns. They can be composed of clay minerals, organic matter, or biological matter. They can form through precipitation of metal oxides or hydroxides, e.g. when a reducing leach water is mixed with a more oxidising groundwater. The stability of colloidal matter is dependent on pH and ionic strength so that high pH and high cation concentrations tend to destabilise colloids.

Since colloids usually have a large specific surface, radionuclides have a large affinity to them. Some radionuclides may also form colloids by themselves. Colloids have different transport properties than aqueous solution species and can serve as an important mechanism for increasing the mobility of radionuclides (by reducing the effect of certain sorption processes) or decreasing the mobility of radionuclides (due to the filtration of the colloids). Thus the transport of radionuclides by colloids may be an important pathway, especially for radionuclides that otherwise are immobile as solutes [Gardiner et al, 2001].

8.4. Mathematical Models

8.4.1. Mathematical Models of Flow

Before models of radionuclide transport in the geosphere can be generated, it is necessary to develop geosphere flow models. There is an immense literature on groundwater flow and hydrogeology. However a common fault is that site investigation programmes treat the hydrogeology in extreme detail, with large effort invested in flow predictions; whereas the subsequent transport and dispersion problems for radionuclides are considered by the
adoption of a few simplistic assumptions. There is a need to change this emphasis in order to focus the flow modelling towards the needs of the transport and dispersion calculations. It is necessary to ensure that the flow modelling is fit for purpose (i.e. input into transport calculations rather than water resource calculations) and that the hydrogeology of aquitards as well as aquifers is considered.

8.4.1.1. Unsaturated Flow

Unsaturated flow can be represented mathematically by Richards’ equation:

$$\nabla \cdot \left[ K_u(\theta) \nabla h \right] - \frac{\partial K_u}{\partial z} - \frac{\partial \theta}{\partial t} = 0$$

where
- $\theta$ is the moisture content [-]
- $h$ is the hydraulic head [m]
- $z$ is the depth [m]
- $t$ is the time [s]
- $K_u$ is the unsaturated hydraulic conductivity [m s$^{-1}$]

Alternatively a more simplistic representation of flow in the unsaturated zone can be adopted by assuming that the flow rate is equal to the net water infiltration rate (see for example IAEA [2002b]).

When modelling flow in the unsaturated zone using Richards’ equation, it is necessary to recognise the dependence of unsaturated hydraulic conductivity on moisture content and suction pressure (negative pressure head) in pores. The unsaturated hydraulic conductivity increases with increasing moisture content. There is a need to specify the functional relationship between unsaturated hydraulic conductivity and moisture content ($K_u$ vs $\theta$ curves) or hydraulic conductivity and suction pressure ($K_u$ vs $\psi$ curves). There are empirical relationships available to describe these curves but it is necessary to understand their range of applicability, and if possible calculations based on the empirical relations should be compared with actual data for a number of points in the field. In addition information is required on the variation of suction pressure with moisture content ($\psi$ vs $\theta$ curves). The characteristics curves describing the relationship between the suction pressure and moisture content may be expressed by the equation developed by van Genuchten [1980]:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + (\alpha |\psi|)^\beta \right]^{m}}$$

where
- $\theta$ is the moisture content [-]
- $\theta_r$ is the residual moisture content [-]
- $\theta_s$ is the moisture content in saturated conditions [-]
- $\psi$ is the suction pressure [m]
- $\alpha$ (m$^{-1}$), $\beta$, and $m = 1-1/\beta$ are empirical parameters.
The unsaturated hydraulic conductivity, $K_u$ [m y$^{-1}$], calculated by the van Genuchten relationship is expressed as a function of the saturated hydraulic conductivity, $K_s$ [m y$^{-1}$], and the effective saturation, $S_e$ [-]:

$$K_u = K_s S_e^{0.5} \left[ 1 - \left( 1 - \frac{S_e^{1/m}}{S_m} \right)^m \right]^2$$

where $S_e = (\theta - \theta_r) \left( \theta_s - \theta_r \right)$

Curves representing unsaturated hydraulic conductivity against moisture content for each medium can be obtained with these expressions.

8.4.1.2. Saturated Flow

It can be helpful to distinguish between flow in fractured and porous media (see for example Figure 8.6 and 8.9).

In fractured media (such as granite), flow is considered to be confined to well defined fractures or fracture zones. The intervening blocks often considered to be impermeable or contain only static water in pore spaces. The cross fracture average flow rate is calculated using:

$$\bar{u} = -\frac{h^2}{3\mu} \nabla p$$

where $\bar{u}$ is the cross fracture average velocity [m s$^{-1}$]

$h$ is the fracture width [m]

$\mu$ is the coefficient of dynamic viscosity [kg m$^{-1}$ s$^{-1}$]

$p$ is the pressure [kg m$^{-1}$ s$^{-2}$]

In porous media (such as unconsolidated gravel), different rock geometries and flow fields exist on microscopic scales but the existence of a representative elementary volume (REV) over which such microscopic variations can be averaged is assumed. The average real velocity (or pore water velocity) is calculated using:

$$v = \frac{v_d}{\theta_e}$$

where $v$ is the pore water velocity [m s$^{-1}$]

$\theta_e$ is the effective porosity (the fraction of rock volume available to the flowing water) [-] and,

$$v_d = -K \frac{\partial H}{\partial x}$$

where $v_d$ is the specific discharge (Darcy velocity) [m s$^{-1}$]

$K$ is the hydraulic conductivity [m s$^{-1}$]
\[ \frac{\partial H}{\partial x} \] is the head gradient [-]

It is also possible to consider some geological media to be dual porosity media (such as chalk), that exhibit both fracture flow and porous flow properties (see Figure 8.9).

When deciding upon the flow model to be used, it is important to consider the spatial scales over which the model is to be applied. If the fracture flow equation is used for a distribution of fractures (per unit volume), then an equivalent porosity and permeability can be calculated and the porous flow equation used. However, it should be noted that the porous flow equation is essentially empirical and its averaging of flow path geometry should be validated for particular media and scale under consideration.
Figure 8.9: Dual Porosity Medium with Fracture and Porous Flow [Savage, 1995]

8.4.2. Mathematical Models of Transport

The advection-dispersion equation for transport through unsaturated and saturated media (in two dimensions) with retardation and decay (but excluding colloid transport) is:

$$\frac{D_x}{\theta_e} \frac{\partial^2 C}{\partial x^2} + \frac{D_y}{\theta_e} \frac{\partial^2 C}{\partial y^2} - \frac{v_d}{\theta_e} \frac{\partial C}{\partial x} = R \frac{\partial C}{\partial t} + R \lambda C$$

where:
- $x$ is the groundwater flow axis
- $y$ is the transverse axis
- $C$ is the concentration of contaminant in the groundwater [kg m$^{-3}$]
- $D_x$ and $D_y$ are the dispersion tensors in the geosphere [m$^2$ y$^{-1}$]
- $\theta_e$ is the effective porosity or in the case of unsaturated flow the water filled porosity [-]
- $v_d$ is Darcy's velocity [m y$^{-1}$]
- $R$ is the retardation factor in the geosphere [-]
- $\lambda$ is the radioactive decay constant [y$^{-1}$]

$D_x$ and $D_y$ (the dispersion tensors in the geosphere) are defined as:

$$D_x = \theta D_e + \alpha_x |v_d| \approx \alpha_x |v_d|$$
$$D_y = \theta D_e + \alpha_y |v_d| \approx \alpha_y |v_d|$$

where:
- $\theta$ is the total porosity of the geosphere [-]
- $D_e$ is the molecular diffusion coefficient in pore water [m$^2$ y$^{-1}$]
\( \alpha_L \) and \( \alpha_T \) are the longitudinal and transversal dispersivities (respectively) in the geosphere [m]

R (the retardation factor in the geosphere) is calculate using:

\[
R = 1 + \frac{\rho_b K_d}{\theta}
\]

where:
- \( \rho_b \) is the dry bulk density of the geosphere [kg m\(^{-3}\)]
- \( K_d \) is the distribution coefficient in the geosphere [m\(^3\) kg\(^{-1}\)]
- \( \theta \) is the total porosity of the geosphere [-]

8.5. Computer Codes

Geosphere codes can be categorised using different criteria, for example:

- the basic simulation method (analytical or numerical, finite differences or finite elements);
- the zone of applicability (unsaturated zone, saturated zone or both);
- the treatment of flow and transport (just flow, just transport, both flow and transport);
- the number of solved phases (multi-phase, single-phase);
- the modelling approach used to represent flow and radionuclide transport (continuum, fracture, network, or compartment.

The latter approach is used below.

- **Continuum model** (e.g. VS2DT [Healy, 1990], FEMWASTE [Yeh, 1987]) – assumes porous media flow in 2 or 3 dimensions. Such models can be resource intensive in terms of data and computing and are generally too complex to be used directly in assessment calculations. However, they can be used to support the more simplified models that are used for assessments calculations.

- **Fracture model** (e.g. NAPSAC [Herbert et al, 1991], FracMan (www.fracman.golder.com)) – assumes fracture flow. Again data requirements might limit the applicability of such codes.

- **Network model** (e.g. NEFTRAN II [Olague et al, 1991], MONDRIAN [BNFL, 2000]) – can be used to represent either porous or fracture flow. This type of model is flexible and allows the direct representation of important flow paths through the geosphere in 1, 2 or 3 dimensions. It tends to be sufficiently simple to be used in assessment calculations, or to investigate ‘what if’ questions. However, there are a number of disadvantages: transverse flows and transport not directly represented; a network model may need to be ‘calibrated’ against a more complex model (e.g. a continuum model); the success of the model depends on the user making appropriate choices for network geometry; and the network geometry may need to be changed when boundary conditions change.
• **Compartment model** (e.g. AMBER [Enviros QuantiSci and Quintessa [2002], ModelMaker [FamilyGenetix, 2000]) – can be used to represent either porous or fracture flow. In addition to many of the advantages of the network approach, the compartment approach can be used to represent the near-field and biosphere. Thus it is possible to use one modelling approach to represent the entire disposal system thereby overcoming model interface problems. However, it needs to be ‘calibrated’ against a more complex model (e.g. a continuum model) and its successful application depends on the user making appropriate choices for network geometry.

Tables 8.2 and 8.3 list a range of codes for unsaturated zone flow and transport and saturated zone flow and transport, respectively, based on information in IAEA [2002a]. It should not be seen as an exhaustive list of codes that are available.

In addition to these general flow and transport codes, there are more detailed geochemical codes such as PHREEQC [Parkhurst, 1995]. PHREEQC performs a wide variety of aqueous geochemical calculations and has been derived from the code PHREEQE [Parkhurst et al, 1980]. Both these codes have been developed by the United States Geological Survey. PHREEQC is based on an ion-association aqueous model and has capabilities for:

- speciation and saturation-index calculations;
- reaction-path and advective transport calculations involving specified irreversible reactions, mixing of solutions, mineral and gas equilibria, surface complexation reactions and ion-exchange reactions; and
- inverse modelling, which finds sets of mineral and gas mole transfers that account for composition differences between waters, within specified compositional uncertainties.

### 8.6. Data

The broad range of data required to allow the modelling of the geosphere is described in Section 4.4 and summarised in Table 8.4. The specific parameters for which data need to be obtained will depend upon the precise models that are used but typically include:

- radionuclide half-life;
- water flow rates unsaturated and saturated zones;
- hydraulic gradients;
- hydraulic conductivities;
- effective and total porosities;
- radionuclide distribution coefficients;
- dispersion and diffusion coefficients.

IAEA [2002a] provides example compilations of such data. Further example data are provided in IAEA [2002c].

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1 Definitions for all terms appearing in italics are given in the glossary to these notes. Only terms that have not been used in previous sections are italicised in this section.
Table 8.2: Some Unsaturated Zone Flow and Transport Codes (based on information in IAEA [2002a])

<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>DR</td>
<td>The DRAF model had been developed as a mathematical tool for the safety assessment of near surface radioactive waste disposal facilities. The model solves the three dimension advection-dispersion equation with soil-solute interaction and radioactive decay by the finite differences method. The model has two versions, one for the saturated zone, another for the unsaturated zone.</td>
<td>Rives [1998]</td>
</tr>
<tr>
<td>HELP</td>
<td>HELP is a quasi two-dimensional hydrologic model of water movement across, into, through, and out of near surface disposal facilities. The model accepts climatologic, soil, and design data and utilises a solution technique that accounts for the effects of surface storage, runoff, infiltration, percolation, evapotranspiration, soil moisture storage, and lateral drainage. Disposal facilities systems, including various combinations of vegetation, cover soils, waste cells, and synthetic membrane covers and liners, may be modelled.</td>
<td>Schroeder et al [1988]</td>
</tr>
<tr>
<td>HY DRUS</td>
<td>One-dimensional, finite element model for flow and solute transport in the unsaturated zone.</td>
<td>Simunek et al [1996]</td>
</tr>
<tr>
<td>PT C</td>
<td>(Princeton Transport Code) A three-dimensional model for simulation of uncoupled transient flow and solute transport in confined or unconfined porous media. The model solves the advective-dispersive transport equation for reactive and non-reactive solutes using a hybrid finite element Galerkin technique coupled with a finite difference scheme.</td>
<td>Bentley and Kieper [1993]</td>
</tr>
<tr>
<td>UNSAT-H</td>
<td>UNSAT-H was developed to simulate the water dynamics of arid sites used or proposed for near surface waste disposal. UNSAT-H simulates one-dimensional water and heat flow in heterogeneous, unsaturated soils and sediments. Water vapour transport, evapotranspiration, and surface energy balance are also simulated. The Crank-Nicholson numerical scheme is used to solve Richards' Equation on a finite difference grid.</td>
<td>Fayer and Jones [1990]</td>
</tr>
<tr>
<td>VS 2DT</td>
<td>A finite-difference computer program for the simulation of water and solute movement in variably saturated porous media. The program solves the flow equation by combining the law of conservation of fluid mass with a nonlinear form of Darcy’s equation, and the advection-dispersion equation. The model can analyze problems in one and two dimensions with planar or cylindrical geometries. Solute transport options include first-order decay, adsorption, and ion exchange. Developed by the USGS.</td>
<td>Healy [1990]</td>
</tr>
<tr>
<td>Code</td>
<td>Description</td>
<td>Reference</td>
</tr>
<tr>
<td>--------</td>
<td>-----------------------------------------------------------------------------</td>
<td>----------------------------------</td>
</tr>
<tr>
<td>FEMWA</td>
<td>Two-dimensional finite element model for simulating steady state or transient flow in heterogeneous, saturated or unsaturated porous media, using triangular and/or quadrilateral elements.</td>
<td>Yeh and Ward [1980]</td>
</tr>
<tr>
<td>TER</td>
<td>Two-dimensional finite element model for transient solute transport simulation in saturated, or unsaturated porous media. Compatible with FEMWATER.</td>
<td>Yeh [1987]</td>
</tr>
<tr>
<td>FEMWA</td>
<td>Two-dimensional finite element model for transient solute transport simulation in saturated, or unsaturated porous media. Compatible with FEMWATER.</td>
<td>Yeh [1987]</td>
</tr>
<tr>
<td>X</td>
<td>Simple, semi-analytical computer code which calculates groundwater concentrations at selected receptor points. Employs the Green's function solution to the advection dispersion equation for an instantaneous release from an area source in a homogenous isotropic aquifer of infinite lateral extent and finite thickness. The groundwater flow is assumed to be constant and uniform across the porous medium. Also calculates groundwater fluxes and ingestion doses.</td>
<td>Codell et al [1982]</td>
</tr>
<tr>
<td>MIGRA</td>
<td>MIGRAD is designed to simulate the transport of radionuclides in unsaturated or saturated porous media. It solves the one-dimensional single contaminant transport equation with radioactive decay in one or two saturated porous media.</td>
<td>Pérez Guerrero and Ruperti [1998]</td>
</tr>
<tr>
<td>MOC</td>
<td>Two-dimensional, based on a hybrid finite difference and method of characteristics approach, for flow and solute transport in confined or water table aquifers. Developed by the USGS. Also available is the NRC version of MOC which accounts for adsorption and decay.</td>
<td>Harbaugh and McDonald [1996]</td>
</tr>
<tr>
<td>MODFL</td>
<td>Three-dimensional, finite difference model for time-dependent, or steady-state flow in confined and unconfined aquifers, capable of simulating the effects of wells, drains, rivers, recharge and leakage.</td>
<td>Harbaugh and McDonald [1996]</td>
</tr>
<tr>
<td>PORFLO</td>
<td>PORFLO is a deterministic, two-dimensional finite differences code applicable to an equivalent porous continuum. It is capable of simulating the coupled processes of saturated groundwater flow, contaminant transport, and heat transfer. The conceptual modelling approach used in PORFLO allows a 2-D heterogeneous system to be defined in either the horizontal or vertical plane. 3-D systems with axial symmetry (i.e., a cylinder) can also be modelled with PORFLO.</td>
<td>Kline et al [1983]</td>
</tr>
<tr>
<td>SUTRA</td>
<td>SUTRA simulates fluid movement and the transport of either energy or dissolved substances in a subsurface environment. It is a two-dimensional finite element code that simulates unsaturated or saturated flow in porous media and pollutant transport under either steady-state or transient conditions. The code can simulate transitions from unsaturated to saturated flow in heterogeneous and anisotropic media.</td>
<td>Voss [1984]</td>
</tr>
<tr>
<td>TOUGH</td>
<td>Three-dimensional model for simulating the flow of water, vapour, air and heat in porous and fractured media. Several code enhancements for considering e.g. radionuclide transport including diffusion, adsorption, hydrodynamic dispersion and radioactive decay, or solubility effects, are available</td>
<td>Pruess [1991]</td>
</tr>
<tr>
<td>VAM2D</td>
<td>Developed to simulate two-dimensional flow and transport in fully or variably saturated porous media.</td>
<td>Huyakorn et al [1989]</td>
</tr>
</tbody>
</table>
### Table 8.4: Example Data Required for Groundwater Conceptual Model Development
(after IAEA [2002a])

<table>
<thead>
<tr>
<th>Type</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geology</td>
<td>Lithology, Stratigraphy, Structure, Fracture density and aperture width in both unsaturated and saturated zones</td>
</tr>
<tr>
<td>Hydrogeology</td>
<td>Groundwater system boundaries, Aquifers, and confining units, Recharge and discharge zones, Hydraulic characteristics of the unsaturated zone: soil moisture, pressure, porosity, bulk density, saturated hydraulic conductivity, Hydraulic characteristics of the saturated zone: conductivity, porosity, Specific yield, and specific storage of aquifers, Potentiometric surfaces of aquifers: well water levels, Vertical gradients between aquifers</td>
</tr>
<tr>
<td>Geochemistry</td>
<td>Water chemistry of unsaturated and saturated zones, sorption, precipitation, complexation, redox</td>
</tr>
<tr>
<td>Well</td>
<td>Size and Depth of screen, Pumping Rate</td>
</tr>
</tbody>
</table>

### 8.7. Summary

The geosphere can act as a natural barrier to prevent or inhibit the movement of radionuclides due to its physical, chemical or biological characteristics. It is this preventative/inhibiting role that needs to be evaluated as part of the safety assessment especially when assessing the impact of the liquid release pathway. When modelling the geosphere, it is important to consider both internal processes within the geosphere, and external processes associated with the near-field and the biosphere. Potentially significant internal processes affecting the transport of radionuclides are advection, dispersion, diffusion, sorption and decay.

Before models of geosphere transport can be generated, it is necessary to develop geosphere flow models. It is necessary to ensure that the flow modelling is fit for purpose (i.e. input into transport calculations rather than water resource calculations) and appropriate to data availability (e.g. little point in using a detailed flow model if there are few data to support its use). Porous, fracture or dual porosity flow models can be developed depending upon the nature of the flow in the system to be modelled.

### 8.8. References


