Dissertation for the degree of Doctor of Philosophy

**Mass Transport Analysis**
**In The Near Field Of Geologic Repository**

Doo-Hyun Lim  
Department of Nuclear Engineering  
University of California, Berkeley

December 2002
This work was performed as part of the project supported by the Japan Nuclear Cycle Development Institute.

Comments and notification of any errors in this report would be appreciated.

Joonhong Ahn
Principal Investigator of the project
Department of Nuclear Engineering
University of California
Berkeley, CA 94720
USA

ahn@nuc.berkeley.edu
Table of Contents

1. INTRODUCTION AND SUMMARY ............................................................................................. 1
   1.1 INTRODUCTION ..................................................................................................................... 1
   1.2 STATE OF THE ART ................................................................................................................. 1
   1.3 OBJECTIVES ............................................................................................................................ 3
   1.4 SCOPE AND SUMMARY ......................................................................................................... 3
2. LITERATURE REVIEWS .................................................................................................................... 7
   2.1 LITERATURE REVIEW FOR MASS TRANSPORT IN FRACTURED ROCK ........................................ 7
       2.1.1 Water Flow Modeling in Fractured Rock ........................................................................... 7
       2.1.2 Solute Transport Modeling in a Fractured Rock ................................................................. 7
   2.2 LITERATURE REVIEW FOR FRACTURE GEOMETRY PARAMETERS ............................................. 9
       2.2.1 Fracture Size ....................................................................................................................... 10
       2.2.2 Aperture ............................................................................................................................. 12
       2.2.3 Orientation Angle ................................................................................................................. 14
       2.2.4 Location .............................................................................................................................. 14
       2.2.5 Linear Frequency, Spacing, and Number Density ................................................................. 15
   2.3 SUMMARY ................................................................................................................................. 17
3. WATER FLOW ANALYSIS IN THE NEAR FIELD OF GEOLOGIC REPOSITORY ................................. 18
   3.1 INTRODUCTION ....................................................................................................................... 18
   3.2 MODEL SPACE .......................................................................................................................... 18
   3.3 FRACTURE NETWORK GENERATION ...................................................................................... 18
       3.3.1 Generation of Fracture Segments ...................................................................................... 19
       3.3.2 Flow-Bearing Cluster (FBC) of Fractures ......................................................................... 22
       3.3.3 Identification of FBC ......................................................................................................... 22
   3.4 TRANSFORMATION OF FBC INTO EQUIVALENT CONTINUUM ............................................... 24
       3.4.1 Transformation of FBC into a Heterogeneous Continuum .................................................. 24
           3.4.1.1 Equivalent porosity ....................................................................................................... 24
           3.4.1.2 Equivalent hydraulic conductivity ............................................................................... 25
       3.4.2 Transformation of the FBC into a Homogeneous Continuum ............................................. 26
   3.5 GOVERNING EQUATION AND SIDE CONDITIONS .................................................................. 27
       3.5.1 Solution for Governing Equation by Finite Element Method .............................................. 28
       3.5.2 Example for Results of Water Flow Analysis .................................................................... 33
       3.5.3 Finite-Element Mesh Size ............................................................................................... 35
   3.6 NUMERICAL RESULTS ............................................................................................................. 36
       3.6.1 Fracture Network Generation and Occurrence of FBC ....................................................... 36
       3.6.2 Effects of Heterogeneity of NFR on Flow Rate .................................................................. 38
           3.6.2.1 Determination of the number of realizations .................................................................. 39
           3.6.2.2 Effect of Length distribution ....................................................................................... 39
           3.6.2.3 Effects of Aperture Correlation .................................................................................... 44
       3.6.3 Effect of Modeling Approach for NFR on Flow Rate ......................................................... 46
List of Figures

Figure 1.1  (a) Schematic view of the Swedish (KBS-3) repository design, showing the small hole in the canister and the location of the various escaper routes. Path $Q_1$, release directly to the flowing water in a fracture intersecting the deposition hole. Path $Q_2$, release to the disturbed zone around the tunnel. Path $Q_3$, release to the tunnel backfill and further to a fracture (zone) intersecting the tunnel. Path $Q_4$, release through the rock to a nearby fracture or fracture zone [Romero, et al., 1995 (a), (b); Gylling, 1997]. (b) The compartmentalization of the repository; each box (solid line) is a compartment, and dashed lines are finer subdivisions of the boxes. The arrows show the various pathways followed by the species from the canister to the flowing water. Drawing is not to scale. [Romero, et al., 1995 (b)]. .................................................................2

Figure 1.2  (a) Conceptual model of Japanese HLW repository. (b) Conceptual model for nuclide transport in the EBS of the repository. In (b), hypothetical, water-filled region is considered to separate the vitrified waste and the buffer [JNC, 2000 (Vol.1, p.V-16)]. .................................................................3

Figure 1.3  Schematic diagram of the transformation of the flow-bearing cluster (FBC) of fractures. Local homogenization and uniformization are defined in Chapter 3. Shaded region represents the flowing-bearing region. .................................................................4

Figure 2.1  Probability density functions of lognormal distributions for length of fracture segments for the crystalline rock at depth below than 150m based on literature review. Three different distributions, $(\alpha_l=1.0$, $\beta_l=1.0m)$, $(\alpha_l=0.1$, $\beta_l=1.0m)$, and $(\alpha_l=0.1$, $\beta_l=3.0m)$, are described by the thick lines, and will be used in this study. An area under each curve is unity. .......................11

Figure 2.2  Probability density functions for aperture based on literature review. Lognormal distribution is assumed. A distribution with $\alpha_a=0.833$ and $\beta_a=7.07\times10^3$ (i.e. mean and standard deviation of 100$\mu$m) is described by the thick line, and will be used in this study .................................13

Figure 2.3  Probability density function for orientation angle ..................................................................14

Figure 2.4  Probability density function for location of the primary fractures .....................................14

Figure 2.5  Probability density function for location of the secondary fractures .................................15

Figure 3.1  Model space .........................................................................................................................18

Figure 3.2  Determination of coordinates for one end of a fracture segment ........................................19

Figure 3.3  Determination of length ($l$) and aperture ($a$) .................................................................19

Figure 3.4  Determination of orientation ($\theta$) ....................................................................................19

Figure 3.5  Determination of the location ($r$, $\phi$), length ($l$), and aperture ($a$) of a second fracture segment .................................................................................................................20

Figure 3.6  Possible two cases for two fractures ..................................................................................20

Figure 3.7  Fracture network generation ...............................................................................................21

Figure 3.8  Three realizations of fracture network by the same statistics .............................................21

Figure 3.9  Fracture clusters. Thick lines represent the FBC of the DFN, whereas the thin lines represent the DEC in the DFN .................................................................22

Figure 3.10 Intersection between two fracture segments. In (a), intersection is counted once ...............22

Figure 3.11 An example for the identification of the FBC in a fracture network .....................................23

Figure 3.12 FBC for the fracture network in Figure 3.11 ........................................................................23

Figure 3.13 FBC for the fracture network in Figure 3.7 ........................................................................24

Figure 3.14 Calculation of an equivalent porosity for a triangular element ........................................25

Figure 3.15 Concepts of the specific surface area ................................................................................26

Figure 3.16 Water-flowing region (i.e. FBC and buffer) in the model ..................................................27

Figure 3.17 Triangular element in the domain ......................................................................................29

Figure 3.18 Coordinates of three nodes in a triangular element by global coordinate system $(x, y)$ .........................................................................................................................30

Figure 3.19 Triangular elements covering the FBC and buffer region ..................................................32

Figure 3.20 Triangular mesh generation on the FBC (Figure 3.13) and the buffer region .....................33
Figure 3.21  Darcy velocity for the FBC in Figure 3.13.................................................................34
Figure 3.22  Domain discretization by four different sizes of mesh..................................................35
Figure 3.23  The relationship between the connectivity and the number of fractures for three realizations (I, II, and III). Statistics for Case 2 in Table 3.3 is used.................................................................37
Figure 3.24  Frequency for the threshold connectivity for three cases in Table 3.3................................38
Figure 3.25  CDF for FBC occurrence. Labels 1, 2, and 3 indicate the cases shown in Table 3.3 ..........38
Figure 3.26  CDF of total discharge at the outer boundary for a model with a heterogeneous NFR by the local homogenization for 100 realizations for 9 cases in Table 3.4.........................................................39
Figure 3.27  Fracture networks, FBCs, and Finite element mesh, and Darcy velocity distribution for a selected realization for 9 cases..................................................................................43
Figure 3.28  Total discharges at the outer boundary by the local homogenization for 9 cases with 90% confidence intervals..................................................................................................................44
Figure 3.29  CDF of total discharge at the outer boundary for a model with a heterogeneous NFR for cases A and B (correlated and uncorrelated)..................................................................................44
Figure 3.30  Darcy velocity distributions in the model space both for correlated and uncorrelated cases.................................................................................................................................45
Figure 3.31  Comparison of the 90% confidence intervals of total discharges at the outer boundary between a model with a homogenized NFR by the uniformization (thick lines) and a model with a heterogeneous NFR by the local homogenization (thin lines) for 9 cases. .................................................................46
Figure 4.1  Model space for the mathematical model..........................................................................49
Figure 4.2  Potential and stream functions for 3 cases..........................................................................56
Figure 4.3  Domain discretization for numerical solution by FFDF.....................................................57
Figure 4.4  Analytical vs. numerical for (case1: \( K_1/K_2 = 1 \) and 144 points).....................................59
Figure 4.5  Analytical vs. numerical for (case 3: \( K_1/K_2 = 1 \) and 280 points).................................59
Figure 4.6  Analytical vs. numerical for (case 5: \( K_1/K_2 = 1 \) and 560 points).................................59
Figure 4.7  Analytical vs Numerical for (case 2: \( K_1/K_2 = 0.1 \) and 144 points)...............................60
Figure 4.8  Analytical vs Numerical for (case 4: \( K_1/K_2 = 0.1 \) and 280 points)...............................60
Figure 4.9  Analytical vs. numerical for (case 6: \( K_1/K_2 = 0.1 \) and 560 points)...............................60
Figure 4.10  Average difference and number of points.........................................................................61
Figure 5.1  Probability density function of \( x(t) \) for 3 cases..................................................................74
Figure 5.2  Particle transport for different time steps 0, 10\( \tau \), and 200\( \tau \) for water velocity in Figure 3.21.78
Figure 5.3  Tracks of all particles for water velocity in Figure 3.21....................................................78
Figure 5.4  Tracks of all particles for water velocity in Figure 3.21 for higher diffusion coefficients in the NFR (FBC and non-FBC) region than Figure 5.3.........................................................78
Figure 5.5  Cumulative distribution functions of the residence times of \( 10^4 \) particles........................80
Figure 5.6  Cumulative distribution functions of the residence times for correlated aperture for case A..82
Figure 5.7  Cumulative distribution functions of the residence times for correlated aperture for case B.................................................................83
Figure 5.8  Cumulative distribution functions of the residence times of \( 10^4 \) particles for the model with a heterogeneous NFR by the local homogenization (solid line) and for the model with a homogenized NFR by the uniformization (dashed line) for 9 cases...............................................85
Figure 5.9  Comparison of the 90% confidence intervals of residence times for the entire model space between a model with a homogenized NFR by the uniformization (thick lines) and a model with a heterogeneous NFR by the local homogenization (thin lines) for 9 cases..........................86
Figure 5.10  Fractional absorption rates at the outer boundary for \( 10^4 \) particles for cases A, B, and C with heterogeneous NFR ((a)–(c)) and homogenized NFR ((d)–(f))..................................................................................87
Figure 6.1  Model space for tortuosity estimation.................................................................................91
Figure 6.2  (a) Fracture network generation in unit square domain, (b) Interconnected fractures connecting the left and right boundaries, (c) Interconnected fractures with assigned labels at the intersections..................................................................................92
Figure 6.3  Fracture network with assigned the label at the intersections and boundary conditions for water flow. .................................................................93
Figure 6.4  Cumulative distribution functions (CDFs) of \( \tau_0, \tau_a \) and \( \tau_p \) for \( l=1.0 \) (a), and \( l=0.75 \) (b), and \( l=0.5 \) (c) for 100 realizations .................................................................95
Figure 6.5  Fracture network, interconnected fractures (thick lines) connecting the left and right boundaries, and interconnected fractures forming the actual flow paths for a selected realization for each case .................................................................96
Figure 7.1  Model space for flow rate calculation .................................................................................................................................98
Figure 7.2  A fracture network with \( N_f=7 \) for constant length \( (l=1.0) \), aperture \( (b=10^{-2} \) m), and uniform location and orientation ...........................................................................99
Figure 7.3  Distribution of hydraulic head at the intersections of fractures .........................................................................................100
Figure 7.4  CDFs of the flow rate by DFN (solid) and homogeneous continuum (dashed) approaches for 100 realizations for four cases in Table 7.3 .................................................................................................................................102
Figure A.1  Polar coordinates .........................................................................................................................................................111
Figure A.2  Lognormal distribution by Analytical solution using (2.1) and by numerical solution using equations (A.10, A.11) .................................................................................................................................112
Figure B.1  Fracture network generation ........................................................................................................................................113
Figure B.2  Fracture network generation with constant orientation ........................................................................................................113
Figure B.3  Fracture network with the constant length of 0.3m (short fractures) ................................................................................114
Figure B.4  Fracture network with the constant length of 3.0m (long fractures) ..................................................................................114
Figure B.5  Fracture network with constant length (3.0m) and orientation (0.25 \( \pi \)) .................................................................114
Figure B.6  Fracture network with the constant aperture .....................................................................................................................115
Figure C.1  Simple example for water flow analysis .......................................................................................................................116
Figure F.1  (a) Gap regions (shaded), and (b) the imaginary absorbing boundary ................................................................................121
Figure F.2  Calculation of the maximum thickness of the gap region \( h_{gap} \) ..........................................................................................................122
Figure G.1  Interconnected fracture network same as Figure 6.2 (c) ........................................................................................................123
Figure G.2  Identification of paths from the list in Table G.1 ...............................................................................................................124
Figure H.1  Simple example of fracture network ........................................................................................................................................125
Figure H.2  A fracture network with boundary conditions ................................................................................................................125
Figure I.1  A fracture network in Figure H.2 (b) .................................................................................................................................127
Figure I.2  A fracture network which has two inlets .........................................................................................................................128
Figure I.3  Equivalent array of resistors to the fracture network in Figure I.1 (a) and the fracture network in Figure I.2 (b). \( R_{ij} \) [ohm] denotes the resistance between points \( i \) and \( j \) in electrical circuit .................................................................................................................................129
Figure I.4  Simplified array of resistors from Figure I.3 (b) by Ohm’s law for resistors in parallel .......................................................129
List of Tables

Table 2.1 Combinations of Modeling Approaches for Water Flow and Solute Transport ............................................. 9
Table 2.2 Number of Fractures Calculated with Experimental Data for Frequency ................................................................. 16
Table 2.3 Statistics of Fracture Geometry Parameters ...................................................................................................... 17
Table 3.1 Statistics of Fracture Geometry Parameters Used to Generate Figure 3.7 ................................................................. 21
Table 3.2 Mesh Size Effect on Water Flow Calculation ...................................................................................................... 36
Table 3.3 Statistics of the Fracture Geometry Parameters for Three Curves in Figure 3.25 ................................................. 36
Table 3.4 Statistics of the Fracture Geometry Parameters for 9 cases ................................................................................ 38
Table 3.5 Statistical Results of Total Discharges at the Outer Boundary and at the Interface for a Model with a Heterogeneous NFR for Different Number of Realizations for Case E in Table 3.4. ................ 39
Table 3.6 Statistical Results of Total Discharges for 100 Realizations at the Outer Boundary and at the Interface for a Model with a Heterogeneous NFR by the Local Homogenization for 9 cases .......... 40
Table 3.7 Statistical Results of Total Discharges for 100 Realizations at the Outer Boundary and at the Interface for a Model with a Heterogeneous NFR by the Local Homogenization for Correlated Aperture Cases ........................................................................................................ 44
Table 3.8 Total Discharges of a Particular Realization for Cases A and B with the Correlated Aperture in Figure 3.30 (b) and (d) .................................................................................................................................. 45
Table 3.9 Total Discharges at the Outer Boundary for a Model with a Heterogeneous NFR and a Model with a Homogenized NFR for 100 Realizations for 9 cases ........................................................................ 46
Table 4.1 Input Parameters for Graphical Representation of Analytical Solution .................................................................. 55
Table 4.2 Numerical Values of Coefficients in Analytical Solution ....................................................................................... 56
Table 4.3 Input Parameters for Comparison .................................................................................................................... 56
Table 4.4 Difference for K1/K2=1 ........................................................................................................................................ 58
Table 4.5 Difference for K1/K2=0.1 ........................................................................................................................................ 58
Table 4.6 Comparison of Total Discharge at the Outer Boundary and at the Interface .................................................. 61
Table 5.1 Input data for numerical simulation for 3 cases ................................................................................................ 74
Table 5.2 Comparison of \( <x(t)> \) (Analytical and Numerical) ............................................................................................. 74
Table 5.3 Comparison of \( <x(t)\\^2> \) (Analytical and Numerical) ............................................................................................... 74
Table 5.4 Statistics of Residence Time for the Entire Model Space and the Buffer Region for 9 Cases ............................................... 79
Table 5.5 Statistics of Residence Time for the FBC and Non-FBC Regions for 9 Cases .............................................................. 79
Table 5.6 Number of Particles Which Has Zero Non-FBC Residence Times ........................................................................ 81
Table 5.7 Statistics of Residence Time for the Entire Model Space and the Buffer Region for Correlated Aperture for Cases A and B .................................................................................................................................... 83
Table 5.8 Statistics of Residence Time for the FBC and non-FBC Regions for Correlated Aperture for Cases A and B ....... 83
Table 5.9 Statistics of Residence Times for the Entire Model Space and the Buffer Region for 9 Cases by the Uniformization ........................................................................................................................................ 84
Table 5.10 Statistics of FBC Residence Times for 9 Cases by the Uniformization .................................................................................. 84
Table 5.11 Maximum Fractional Absorption Rate at the Outer Boundary ........................................................................... 87
Table 6.1 List of Connected Points for Figure 6.2 (c) ................................................................................................................. 92
Table 6.2 List of Connected Points based on Potential Distribution in Figure 6.3 ................................................................ 93
Table 6.3 Statistics of the Fracture Geometry Parameters for Tortuosity ................................................................................ 95
Table 6.4 Statistics of \( \tau_2, \tau_0 \) and \( \tau_{\phi} \) ................................................................................................................................. 95
Table 6.5 Median Values of \( \tau_2, \tau_0 \) and \( \tau_{\phi} \) .................................................................................................................. 95
Table 7.1 Uniformized Hydraulic Properties for the Fracture Network in Figure 7.2 ................................................................. 100
Table 7.2 Flow Rates through the Fracture Network in Figure 7.2 ..................................................................................... 101
Table 7.3  Parameters for Water Flow Rate ................................................................. 101
Table 7.4  Flow Rates by DFN ($Q_{DFN}$) and Homogeneous Continuum ($Q_{HOMO}$) Approaches for 100 Realizations for 4 Cases in Table 7.3. ....................................................................................... 101
Table G. 1  List of Connected Points for Figure G.1 ................................................................. 123
1. Introduction and Summary

1.1 Introduction

A geological repository is considered as the most favorable option for safe disposal of the High-Level radioactive Waste (HLW). The main roles of the repository are to isolate and confine the HLW and to mitigate the radiological effect to the human environment for a sufficiently long period of time. The safety of the repository can be evaluated, based on the amount of radionuclides released from the waste matrix to the human environment. Two regions of interest have been considered for the performance assessment of HLW repository, i.e., the near field and the far field. The point of interest of this dissertation is mass transport analysis in the near field for a water-saturated HLW repository.

The near field region is considered [Romero, et al., 1995 (a), (b); Gylling, 1997; JNC, 2000 (Vol.1, p.V-5)] to consist of the Engineered Barrier System (EBS) and part of the surrounding host rock, which is called the Near-Field Rock (NFR) in this dissertation. Better characterization of the groundwater flow and radionuclide transport especially in the near field is crucially important for improving the performance assessment of HLW repository [Ahn, et al., 1996; Ahn, et al., 1998]. Processes affecting the EBS performance are carried by groundwater through the NFR, such as bentonite swelling, waste-matrix dissolution, and canister corrosion. The short-lived radionuclides would decay within a short distance from the waste canister [Ahn, et al., 1996], whereas the concentrations of long-lived radionuclides can build up in the water stream containing multiple failed canisters in the repository [Ahn, et al., 1998]. Radionuclides released from the waste-matrix will be transported by groundwater through the NFR, and eventually to the human environment.

Previous near-field models [Romero, et al., 1995 (a), (b); Gylling, 1997; JNC, 2000] have not taken into account the heterogeneity of the NFR for the radionuclide transport analysis. Romero, et al. [1995 (a), (b)] and Gylling [1997] treated the NFR as a homogenized compartment represented by the averaged hydraulic and transport properties. JNC [2000 (Vol. 4, p.V-48)] called the near-field rock the Excavation Disturbed Zone (EDZ), which is modeled as a highly permeable continuum represented by averaged values of hydraulic properties.

The NFR generally has a low permeability except where it is fractured [National Research Council, 1996]. The fractures are major conduits for groundwater flow and radionuclide transport. The geometry of the fractures in the NFR can affect significantly the groundwater flow and the radionuclide transport through the rock [National Research Council, 1996; Lim, et al., 2001(a); Lim, et al., 2001(b); Lim, et al., 2002]. Therefore, the heterogeneity of the NFR should be taken into account in the simulations of groundwater flow and radionuclide transport in the near field of HLW repository.

1.2 State of the Art

Transport in a fractured rock is substantially different, depending on whether the pores and fractures in the rock are saturated with water or not. While the United States is considering a HLW repository above the water table in Yucca Mountain, many other countries, such as Canada, Finland, France, Japan, Sweden, and Switzerland, are considering constructions of HLW repositories in a crystalline rock below the water table. In this dissertation, the HLW repository below the water table in the water-saturated region is considered.

The performance assessments of Swedish and Japanese HLW repository concepts, which are typical for water-saturated HLW repository, are summarized in this section.

The performance of Swedish HLW repository concept was assessed by an integrated model, which consists of sub-models for transport in the near-field (NUCTRAN) and in the far-field (CHAN3D) [Gylling, 1997]. The near-field model calculates the release rate of the radionuclides from the canister [Romero, et al., 1995 (a), (b)]. The far-field model is based on the channel network (CN)” concept, and is used for an analysis of radionuclide transport to the human environment.

In the Swedish model, the near-field includes a waste canister, a bentonite-filled buffer, and a NFR (see Figure 1.1 (a)). The near-field is represented as a number of compartments [Romero, et al., 1995 (a), (b)] (see Figure 1.1 (b)). Averaged properties are defined for these compartments.

---

* NFR is considered to be fractured in this dissertation. It is assumed that water flows only through the fractures in the NFR, and the rock matrix is impermeable.

** Detail is given in Section 2.1
Radionuclides leaking out through the damaged hole of a canister diffuse into the bentonite-filled buffer and then migrate through various pathways into the flowing water in rock fractures. Figure 1.1 shows four possible pathways. Because the nuclide transport through one specific pathway is influenced by the release in the other paths, the release should be calculated simultaneously for all paths [Gylling, 1997].

Gylling [1997] takes the following three steps to simulate the groundwater flow and radionuclide transport from the waste canister to the human environment. First, the flow rate of groundwater is calculated by using the far-field model (CHAN3D) in the system including the near field. The calculated flow rate is used as input data for the near-field transport. Second, the radionuclide transport in the near field is simulated by the near-field model (NUCTRAN). The output of the transport analysis in the near field is used as input data for the far-field transport. Third, the radionuclide transport in the far field is simulated by CHAN3D.

In the Swedish performance assessment, heterogeneity of the near-field for radionuclide transport is represented by four major channels (or paths). However, effects of fracture network geometry in the NFR are not explicitly considered. Thus, the heterogeneity due to discrete fracture network has not been taken into account for radionuclide transport in the near field.

JNC [2000] performed the safety assessment for a conceptual HLW repository for Japanese geologic environment. Their concept is similar to Swedish concept [Romero, et al., 1995 (a), (b); Gylling, 1997]. The near field consists of the EBS and a limited volume of the surrounding host rock, which is called the EDZ (see Figure 1.2 (a)).

An integrated model is also developed for the radionuclide transport from the repository to the human environment. First, the groundwater flow rate in the near field is calculated by using the three-dimensional discrete fracture network (DFN) code (FracMan/Mafic). Then, the EDZ is treated as a homogeneous continuum, whose equivalent hydraulic property such as transmissivity is obtained from a discrete-fracture network model. Second, the flow rate obtained by 3D DFN model in the EDZ is used as input data for the nuclide migration analysis in the near field. The radionuclide transport in the EBS is simulated by MESHNOTE, which treats simplified one-dimensional geometry of a waste canister, and bentonite-filled buffer, and the homogenized EDZ (see Figure 1.2 (b)).

* Detail is given in Section 2.1
Radionuclides released from the buffer are assumed to be mixed instantly and completely with groundwater flowing through the EDZ. Total nuclide flux enters fractures intersecting the EDZ. Third, the radionuclide transport in the far field is simulated by one-dimensional multi-pathway model (MATRICS), which takes into account heterogeneity of the host rock by a one-dimensional planar-fracture model. A planar fracture in the model represents a major channel of radionuclide transport.

Figure 1.2  (a) Conceptual model of Japanese HLW repository. (b) Conceptual model for nuclide transport in the EBS of the repository. In (b), hypothetical, water-filled region is considered to separate the vitrified waste and the buffer [JNC, 2000 (Vol.1, p.V-16)].

As has been reviewed above, in Swedish and Japanese performance assessment studies, the NFR is treated as a homogeneous continuum for radionuclide transport analysis, while the heterogeneity of NFR was recognized for water flow analysis and implicitly incorporated into their near-field transport models. However, this simplification introduced in previous assessment studies has not yet been verified to be conservative or acceptable.

A near-field model incorporating the heterogeneity of the NFR not only for the groundwater flow analysis but also for the radionuclide transport analysis is needed to check the validity of the simplification applied in the previous studies for the performance assessment of HLW repository.

1.3 Objectives

The objectives of this dissertation are:

1. to develop a near-field model incorporating the heterogeneity of the NFR for the groundwater flow and particle transport analyses for a hypothetical water-saturated HLW repository in a two-dimensional space,

2. to investigate effects of the heterogeneity of the NFR on the groundwater flow rate and particle transport, and

3. to investigate effects of the modeling approach for the NFR on the groundwater flow rate and particle transport.

1.4 Scope and Summary

In this study, the near field consists of the waste canister, the bentonite-filled buffer, and the neighboring surrounding host rock. The waste canister would fail due to corrosion. The waste canister is assumed to confine radioactive materials for 1000 years after the emplacement in the repository. In the 1000 years after emplacement, the heat generation from the canister will rapidly decrease, and the temperature in the repository will settle down to the ambient temperature [Ahn, et al., 1995]. The time period after the temperature has settled down to the ambient is considered in this study.

Bentonite is considered as a basic material for the buffer in the water-saturated HLW repository. The buffer is considered to compensate the mechanical fluctuation around the EBS, to inhabit the water penetration into the waste canister, and to retard radionuclide transport. In this study, 100wt% bentonite is assumed as a buffer material [JNC, 2000 (Vol. 3, p.IV-68)].
A “one-waste canister” configuration (see Figure 3.1) in a two-dimensional model is considered for the groundwater flow and particle transport analyses in the near field in this study. The NFR region with the radius of 5m is considered [JNC, 2000 (Vol. 3, p.IV-134)].

Chapter 2 shows the literature reviews for the modeling of the water flow and solute transport in fractured rock. Statistical distributions of fracture geometry parameters are also summarized based on literature review.

Based on the literature survey for the fracture geometry parameters, lognormal distributions are assumed for the length and aperture of fractures. The uniform and exponential distributions are assumed for the spatial distributions of the primary and secondary fractures, respectively*. The uniform distribution is assumed for the orientation angle of fractures.

Chapter 3 is a key chapter in this dissertation. A two-dimensional near-field model is developed for the one-waste canister configuration to simulate the groundwater flow for a hypothetical water-saturated HLW repository.

![Diagram of transformation of flow-bearing cluster (FBC)](image)

**Figure 1.3** Schematic diagram of the transformation of the flow-bearing cluster (FBC) of fractures. Local homogenization and uniformization are defined in Chapter 3. Shaded region represents the flowing-bearing region.

A Discrete-Fracture Network (DFN) is generated in the NFR based on distribution functions of the fracture geometry parameters by random sampling (i.e. length, aperture, orientation, and location). The water-flowing fracture segments in the DFN in the NFR are determined by checking the interconnectivity of the fractures. The Flow-Bearing Cluster (FBC) of fractures is transformed into an equivalent continuum in two different ways** (see Figure 1.3). First, a transformation is applied to the FBC locally, resulting in a heterogeneous continuum. Thus, the NFR is divided into the flow-bearing region (i.e. heterogeneous continuum transformed from the FBC) and the water-stagnant region. Second, the FBC is uniformized over the entire NFR. The NFR is transformed into a

* Definitions of the primary and secondary fractures are given in Section 2.2.4

** The first and second approaches are called the local homogenization and the uniformization, respectively, in this dissertation. Details are given in Chapter 3.
homogeneous continuum. The entire NFR is the flow-bearing region. The second approach is similar to those used in the near-field models in the Japanese and Swedish HLW repository performance assessment studies as discussed in Section 1.2. The permeability for the transformed continuum is evaluated by the Kozeny-Carman equation. The flow rate of groundwater is calculated by solving a steady-state potential equation numerically by the finite element method.

Effects of the heterogeneity of the NFR and effects of the modeling approach for the NFR are investigated for different sets of statistics of fracture geometry parameters by comparing the groundwater flow rates between the model with a heterogeneous NFR by the local homogenization and the model with a homogenized NFR by the uniformization. The connectivity, defined as the ratio of the total number of intersections to the total number of fractures, is used as a measure that expresses the degree of heterogeneity of the NFR.

Numerical results for effects of the heterogeneity of the NFR (see Figure 3.28) show (1) that the network with a greater connectivity exhibits a greater water flow rate, and (2) that a low connectivity gives a greater uncertainty for water flow rate.

Numerical results for effects of the modeling approach of the NFR (see Figure 3.31) show (1) that the median values of the water flow rates obtained by the two approaches are close to each other, (2) that the flow rates obtained by the local homogenization gives a greater uncertainty, (3) that, at a large connectivity, two approaches give a similar result, and (4) that the homogenized NFR by uniformization does not necessarily overestimate the water flow rate, compared to the heterogeneous NFR by local homogenization. The last result implies that the homogenized NFR by uniformization may not be applied to the water flow analysis for a conservative performance assessment.

In Chapter 4, numerical results obtained by the model with a homogenized NFR, developed in Chapter 3, are bench-marked against an analytical solution. Analytical solutions for the steady-state potential distribution and stream functions are obtained for the model with a homogenized NFR. With the analytical solution, the water flow rate is evaluated. The numerical results obtained by the model, developed in Chapter 3, are compared with those obtained by analytical solutions.

The numerical results for the values of hydraulic potential differ from those by analytical solution by an average difference less than 1.17 x 10 \(^{-3}\) (see Table 4.5). The numerical results for the total discharges of water in the model space differ from those obtained by analytical solutions by a relative difference less than 0.55% (see Table 4.6).

In Chapter 5, the random walk tracking model is developed for particle transport in combination with the flow model, which is developed in Chapter 3. The RWTM is applied because of such advantages as (i) a simple algorithm, (ii) easy incorporation with the flow model, and (iii) no numerical dispersion.

Effects of the heterogeneity of the NFR and effects of the modeling approach for the NFR are investigated for different sets of statistics of fracture geometry parameters by comparing the particle residence times and the mass absorption rates at the outer boundary between the two approaches as shown in Figure 1.3 for transforming a FBC into a continuum.

Numerical results show (1) that the network with a greater connectivity exhibits a shorter residence time of particles (see Figure 5.9), (2) that the effect of the length and aperture correlation on the residence time of particles in the near-field is negligible (see Figure 5.6 (a) and Figure 5.7(a)), (3) that the residence time of particles for the homogenized NFR is mainly determined by the bentonite-filled buffer region (see Table 5.9 and Table 5.10), (4) that the homogenized NFR by uniformization gives the conservative results, i.e., underestimation of the residence time (see Figure 5.9) and overestimation of the mass absorption rate at the outer boundary (see Figure 5.10), compared to the heterogeneous NFR by local homogenization, and (5) that, by uniformizing the DFN over the entire NFR, the residence times in the entire model space and mass absorption rate at the outer boundary of the NFR are hardly affected by the connectivity of fractures (see Figure 5.9 and Figure 5.10 (d)–(f)). The last two results imply that the homogenized NFR by uniformization may be applied for a conservative performance assessment, but not for repository site selection or design, where differentiating one rock medium to another is of primary interest.

In Chapter 6, the coefficient C in Kozeny-Carman equation for permeability is discussed. The equation includes a coefficient, C, which can be determined by the tortuosity (τ) and the shape of cross-sectional area of the flow path normal to the flow (c₀). In Chapter 3, C is assumed to be one. In Chapter 6, a single value of the coefficient C for the entire FBC is evaluated based on the fracture network geometry. If flow through a parallel-plate channel is assumed, the value for c₀ is known to be 3 [Carman, 1956]. Tortuosity (τ) needs to be estimated by taking into account fracture-network geometry because the flow rate is estimated by the transformation of the FBC into a continuum in Chapter 3 and Chapter 5.

Two formulae for tortuosity are considered in the fracture network. In one formula, tortuosity is defined as \(τ_L = (L/c_0)^2\), where \(L\) is the average length of the paths through a fracture network, and \(L\) is the geometrical length of
the medium [Bear, 1972]. In the other formula, tortuosity is defined as \( \tau_0 = \langle \cos^2 \theta \rangle \) [Fowler, et al., 1940; Carman, 1956] or \( \tau_\theta^* = \langle \cos^2 \theta^* \rangle \), where \( \theta \) is the orientation angle of all fractures included in the FBC (see Figure 3.4), and \( \theta^* \) is the orientation angle of all fractures forming the actual flow paths in the FBC.

Numerical results show (1) that \( \tau_0 \) gives the smallest value among the three, whereas difference between \( \tau_0 \) and \( \tau_\theta^* \) is not significant (see Figure 6.4), and (2) that, by using \( \tau_0 \) instead of \( \tau_\theta \), conservative (over)estimate can be made for the water flow rate in the fractured rock.

In Chapter 7, the homogeneous continuum model, transformed by the second approach (or uniformization) with the coefficient \( C = \tau_0 / c_0 \) is compared with the conventional DFN model for the same fracture network.

Numerical results show that the homogeneous continuum model with tortuosity correction overestimates water flow rates, compared with those by the DFN model (see Figure 7.4).

In Chapter 8, the conclusions that have been derived from this study are summarized.
2. Literature Reviews

Literature reviews have been made in this chapter for (1) the mass transport modeling in fractured rock, and (2) the fracture geometry parameters.

2.1 Literature Review for Mass Transport in Fractured Rock

A stochastic approach has been employed to represent the heterogeneity of the fractured rock due to a discrete fracture network because the measurement and characterization of all fractures are totally impractical [Andersson, et al., 1987]. Three types of stochastic models have been used to simulate the water flow and solute transport in fractured rock [Geier, et al., 1992; (1) Discrete Fracture Network (DFN) model, (2) Stochastic Continuum (SC) model, and (3) Channel Network (CN) model.

2.1.1 Water Flow Modeling in Fractured Rock


Two-dimensional DFN models were developed and tested by various researchers, such as Long, et al. [1982; 1987], Schwartz, et al. [1983], and Andersson, et al. [1986]. Three-dimensional DFN models were also developed [Long, 1985; Elsworth, 1986; Anderson, et al., 1987; Dershowitz, et al., 1994].

The major advantage of DFN models is the explicit representation of the geometrical and physical properties of fractures for a fractured rock [Geier, et al., 1992; National Research Council, 1996]. A fracture network of various scales can be treated [Geier, et al., 1992]. The major disadvantages of DFN models are (1) statistical fracture geometric data especially at depth are difficult to obtain [National Research Council, 1996], (2) when sampling locations are not well distributed, extrapolation is required [Geier, et al., 1992], (3) the model can be complex and computationally intensive for realistic fracture density [National Research Council, 1996; Liu, et al., 2000], and (4) the model to relate information about fracture geometry to the hydraulics of fractured rock is in question [Neuman, 1988].

Neuman [1988] applied the Stochastic Continuum (SC) concept to a heterogeneous fractured rock. The SC model is based on the representation of hydraulic properties in terms of probability models that describe the medium as a random field. The SC models make it computationally feasible for large-scale flow modeling because they do not take into account the individual fracture geometry to represent the heterogeneity of the rock. In the SC model, however, due to the weak coupling between fracture geometry and the hydraulic properties, the transport properties, which are sensitive to the heterogeneity of the medium, may be different from the DFN model [Dverstorp, et al., 1992].

The Channel Network (CN) model has been developed to incorporate an uneven flow distribution in a fractured rock, and to reflect the stochastic appearance of natural properties [Gylling, 1997]. The basis of the CN model [Moreno, et al., 1993; Moreno, et al., 1997; Gylling, 1997] is that flow through a fracture network is confined to discrete effective one-dimensional pathways known as channels. In the CN model, a large number of channels are constructed in the 3D system to represent a fractured rock. Each channel has a hydraulic conductance taken stochastically from a distribution. The flow rate is calculated by solving the pressure distribution in the system with mass balance at each intersection point.

For the flow modeling in the NFR, the DFN approach might be appropriate because the fractures representing the heterogeneity of the NFR could control the groundwater flow in the NFR. Also, difficulties for DFN approach, such as limitation of the field data and large-scale modeling, would not be the case for the near-field region of the HLW repository because relatively large amount of field data will be available in the near-field, and because the near field region around a waste canister is not so large as the far field [JNC, 2000 (Vol. 1, p. V-5)].

2.1.2 Solute Transport Modeling in a Fractured Rock

The models for solute transport in a fractured rock are summarized based on literature survey for the cases where flow velocity profile in the rock is known and not affected by the solute transport.

In the discrete network models such as the DFN and CN models, solute transport through a network of fractures or pipes was modeled by representing the tracer as a finite number of particles, i.e., a particle-following
A particle-following method has been developed to simulate the mass transport through the discrete fracture network [Schwartz, et al., 1983; Robinson, 1984]. In this method, a large number of particles are added initially to a single fracture at the upstream boundary of the system [Schwartz, et al., 1983] or to the intersections along a side of the network [Robinson, 1984]. Particles move by advection through the fracture network based on water velocity for individual fracture segments. At an intersection, the direction of particles is determined from probabilities weighted according to the relative quantities of flow moving away from the intersection with assumption of perfect mixing. As a consequence of the perfect mixing at the intersections, mass disperses as it moves by advection through the network. Thus, large-scale dispersion is modeled in this way. However, the particle-following method by Schwartz, et al. [1983] and Robinson [1984] does not take into account the matrix diffusion, which is one of the most important mechanisms for retardation of the radionuclides [Neretnieks, 1980; Ahn, 1988].

Yamashita et al. [1990] introduced a particle-following method incorporating the matrix diffusion for a single fracture model with an infinite porous rock matrix. They described the effect of matrix diffusion in terms of the residence times of particles because of the fact that a particle may reside in the matrix for some time in addition to its residence time in the water in the fracture. The residence time of each particle is determined by a probability density function of the particle residence time, which is obtained by normalizing the mass flux. This method is adopted by Moreno et al. [1997] to simulate the solute transport in the CN model.

Dershowitz et al. [1995] described an implementation of a DFN model in which the matrix diffusion was modeled by a probabilistic particle-following technique. The solute concentration is obtained analytically from the one-dimensional diffusion equation with a constant effective diffusivity. Then, the fraction of the number of particles residing in the matrix is calculated by integrating the total mass transfer rate across the fracture-matrix boundary, and enables to evaluate the probability of finding a particle in the matrix and in the fracture. Similar to the model by Yamashita et al. [1990], the total residence time of a particle is calculated by summing the residence time in fractures and residence time in matrix.

For continuum based models such as the SC model, two basic approaches were used to simulate the solute transport: (1) the Finite Difference Method (FDM) or Finite Element Method (FEM), and (2) the Random Walk Tracking Method (RWTM).

The FDM or FEM is a numerical approach to solve a differential equation by expressing the differential equation as a set of linear equations by domain discretization. Although this method is well developed for solving the transport equation in a mathematical sense, there are disadvantages. First, computational work to solve the \( N_{eq} \) equations per time step is intensive. Also, the solution may include the parts of domain, which never traversed by solutes [Tompson, et al., 1987]. Second, the use of finite difference or finite element causes numerical errors due to the numerical dispersion and/or oscillation [Bear, 1987; Tompson, et al., 1987; Kinzelbach, 1988; Uffink, 1988].

The numerical dispersion is caused by the approximation of the first-order derivative, which involves error of the order of magnitude of the second-order derivative [Bear, et al., 1987]. The numerical dispersion is severe when the advection is dominant \((P_e > 2-10)\)** [Huyakorn, et al., 1983; Tompson, et al., 1987]. The numerical error caused by the numerical dispersion can be made small by decreasing the size of mesh [Bear, et al., 1987; Huyakorn, et al., 1983; Tompson, et al., 1987; Kinzelbach, 1988]. However, a fine mesh is not always possible [Huyakorn, et al., 1983], and sometimes the most impractical option [Tompson, et al., 1987]. Various finite difference methods to overcome the numerical dispersion have been summarized by Huyakorn, et al. [1979].

The RWTM is an analogue process that obeys the transient advective-dispersive transport equation. Advantages of this method are as follows. First, the algorithm is simple and can easily be applied in large, three-dimensional as well as unsaturated problem [Tompson, et al., 1987; Kinzelbach, 1988]. Also, this method can be easily combined with any flow model [Kinzelbach, 1988]. Second, there is no numerical dispersion since the random walk method is not a direct numerical solution of the differential equation [Tompson, et al., 1987; Kinzelbach, 1988; Uffink, 1988]. Third, the computational effort per time step is proportional not to the number of nodes but to the number of particles. Hence, the storage requirement will be dramatically reduced from any finite element or finite difference method [Tompson, et al., 1987].

---

* In some studies [Schwartz, et al., 1983; Yamashita et al., 1990; Dershowitz et al., 1995], it is called a particle-tracking method.

** Peclet number, \( P_e \), defines the ratio between the rate of transport by convection to the rate of transport by molecular diffusion [Bear, 1972].
There are disadvantages of RWTM. A solute mass is represented as a large collection of particles. In order to obtain consistent and reliable results, a large number of particles are required [Tompson, et al., 1987]. The statistical fluctuation of numerical results can be avoided by increasing the number of particles. However, increasing total number of particles does not show the same degree as an improvement of results because this fluctuation is proportional to the square root of the number of particles [Kinzelbach, 1988]. The application of source/sink conditions is complicated [Tompson, et al., 1987] and the prescribed total flux boundary condition is difficult to simulate in RWTM [Kinzelbach, 1988]. The RWTM, which is well developed in continuum such as porous medium, has a difficulty in applying to the fractured rock represented by dual continua [Liu, et al., 2000].

Table 2.1 shows the summary and combination of the applicable modeling approaches for the water flow and solute transport analyses based on the literature review.

In previous studies, if the network models (i.e., DFN and CN) are used for water flow, the particle-following method is usually used for the solute transport as summarized in Table 2.1. One of the major differences between the DFN and the CN is that the system by the DFN approach conducts water only if the system is percolated, whereas the system by the CN approach always conducts water. This is because the hydraulic conductance for the CN approach is determined stochastically not by the fracture geometries but by assigning for each channel from the distribution.

The SC approach for water flow is suitable for coupling with FEM/FDM or with RWTM for solute transport, but has a difficulty in incorporating matrix diffusion because fracture-geometry is not explicitly considered.

Table 2.1 Combinations of Modeling Approaches for Water Flow and Solute Transport

<table>
<thead>
<tr>
<th>Water flow</th>
<th>FEM / FDM: causes severe numerical dispersion if advection is dominant ($P_r &gt; 2-10$).</th>
<th>RWTM: 1) developed for continuum models. 2) simple algorithm, easy incorporation on flow models, and no numerical dispersion.</th>
<th>Particle-following: 1) developed for network models, 2) takes into account the large-scale dispersion due to the mixing at fracture intersections.</th>
</tr>
</thead>
<tbody>
<tr>
<td>DFN</td>
<td>Not discussed in this study</td>
<td>Difficult to combine RWTM with DFN with matrix diffusion</td>
<td>Applicable</td>
</tr>
<tr>
<td>SC</td>
<td>Applicable</td>
<td>Applicable</td>
<td>Not applicable</td>
</tr>
<tr>
<td>CN</td>
<td>Not discussed in this study</td>
<td>Difficult to combine RWTM with CN with matrix diffusion</td>
<td>Applicable</td>
</tr>
</tbody>
</table>

In this study, to take into account the heterogeneity of the NFR, a discrete fracture network is generated in the NFR. A flow-bearing fracture cluster is determined from the fracture network. Thus, the NFR is divided into the flow-bearing region and the stationary water region. To compare the modeling approaches, the flow-bearing cluster (FBC) of fractures is transformed into not only a heterogeneous continuum but also a homogeneous continuum. The hydraulic properties of the transformed continuum are determined by averaging fractures included in the flow-bearing region. In the stationary water region, matrix diffusion of the solute is considered to take place (see Chapter 5). Therefore, the water-flow model developed in this study is considered to apply a Stochastic Continuum (SC) approach, in a sense that hydraulic properties are determined by stochastically distributed fractures. But, the major difference between the previous SC approach and the present one is that the flow-bearing region is first determined by checking percolation of a fracture network and that the hydraulic properties are determined over that flow-bearing region. It should be noted that by constructing a continuum this way the heterogeneity resulting from fracture network is incorporated and utilized.

In following section, the fracture geometry parameters, which characterize the discrete fractures in fractured rock, are reviewed based on the literature survey.

2.2 Literature Review for Fracture Geometry Parameters

Fracture geometry parameters are the fracture size (or the length for a two-dimensional description), aperture, orientation, and location. The statistical distributions of the parameters are reviewed. Other parameters for a fracture network, such as frequency, spacing, and number density of fractures, are also reviewed.

2.2.1 Fracture Size

The size of a fracture can be characterized differently based on the shape of a fracture. For a two-dimensional line fracture, the size is represented by its length. For a three-dimensional disk-shaped fracture, its radius represents the size. The shape of a fracture may be approximated by polygonal, circular, elliptical, or irregular shape [Long, 1985; Geier, et al., 1992].

Baecher, et al. [1977] reviewed the literature on length distribution. The length was reported to vary lognormally or exponentially. Long [1985] mentioned that trace lengths are distributed either lognormally or exponentially. Long, et al. [1987] chose a lognormal distribution for the length of fractures for a granite rock at depth of 320m at Fanay-Augères in France. Mean (μ) and standard deviation (σ) of the fracture length range between 0.53m and 1.14m, and 0.5m and 1.33m, respectively (see Figure 2.1). Cacas, et al. [1990(a)] mentioned that the empirical trace length distribution could reasonably be approximated by a lognormal distribution for highly fractured granite 150m below ground at Fanay-Augères in France. Mean and standard deviation of the trace length vary from 0.74m to 1.16m, and from 2.03m to 2.72m, respectively (see Figure 2.1). Hestir, et al. [1990] considered the lognormal and exponential distributions for length of fractures to estimate permeability in the fracture network. Odling, et al. [1991] obtained experimentally that fracture lengths are distributed lognormally for 12m×14m area on the bedding surface of a sandstone bed of Devonian in Norway. Mean and standard deviation of lengths in a log scale are -0.821 and 0.981, respectively. Niemi, et al. [2000] studied the crystalline rock, which is the potential HLW repository site in eastern Finland, at depth of 200m up to 1000m. This site is considered as a representative of a low-conductivity fractured rock. The sizes of fracture are distributed lognormally with mean values ranging between 0.65m and 1.5m and with standard deviation ranging between 0.45m and 0.7m (see Figure 2.1).

Overstrop, et al. [1989] assumed an exponential distribution from the data observed in Stripa mine. Obtained mean fracture radius ranges between 1m and 2m. Kulatilake, et al. [1993] obtained the experimental data from the ventilation drift (granite rock) at the Stripa mine in Sweden. They claimed that a lognormal distribution is found to be unsuitable for describing the distribution of trace length. The trace length of fracture could be described by the gamma and exponential distributions. Mean and standard deviation of the observed joint trace length range between 1.01m and 1.64m, and between 0.31m and 1.47m, respectively. Kulatilake, et al. [1996] claimed that a gamma distribution is the best distribution for joint trace length and joint diameter for granite mass of a Presinian system in China. Observed mean values of joint trace length range between 1.67m and 2.55m. Observed mean values of joint diameter range between 0.48m and 34m.

Pusch [1990] gave the experimental values of the trace length at Finnsjön site (Gneissous grandiorite) and Stripa mine. For the Finnsjön site, 50% of all fracture has length shorter than 1m. 25% of all fracture varies from 1m to 3m. 3% of all fracture is longer than 7m. For the Stripa mine, 15% of all fracture is larger than 4m. 2% of all fracture is larger than 7m. Andersson, et al. [1991] observed the trace length of fractures varies from 0.1m to 12m at the 1m×48m cell in Finnsjön site.

In summary, the distribution of size of fractures is well characterized by the lognormal distribution [Baecher, et al., 1977; Long, 1985; Long, et al., 1987; Cacas et al., 1990(a); Hestir, et al., 1990; Odling, et al., 1991; Niemi, et al., 2000].

The normalized lognormal distribution is defined as

\[
f(\chi) = \frac{1}{\chi \alpha_\parallel \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\ln(\chi/\beta_\parallel)}{\alpha_\parallel} \right)^2 \right], \quad \alpha_\parallel > 0, \quad \beta_\parallel > 0, \quad \chi > 0, \quad (2.1)
\]

where \( \alpha_\parallel \) is the shape parameter and \( \beta_\parallel \) is the scale parameter. The scale parameter \( \beta_\parallel \) has the same unit as the variable \( \chi \). The shape parameter \( \alpha_\parallel \) is dimensionless.

The mean \( \mu \) of the distribution is defined as,

\[
\mu = \int_{\chi} \chi f(\chi) d\chi, \quad (2.2)
\]

and is calculated by substituting (2.1) into (2.2) as,

\[
\mu = \beta_\parallel \exp(\alpha_\parallel^2/2). \quad (2.3)
\]
Figure 2.1 Probability density functions of lognormal distributions for length of fracture segments for the crystalline rock at depth below than 150m based on literature review. Three different distributions, (\(\alpha_s=1.0, \beta_L=1.0m\)), (\(\alpha_s=0.1, \beta_L=1.0m\)), and (\(\alpha_s=0.1, \beta_L=3.0m\)), are described by the thick lines, and will be used in this study. An area under each curve is unity.

The variance \(\sigma^2\) is defined as,

\[
\sigma^2 = \int_0^\infty (\chi - \mu)^2 f(\chi)d\chi,
\]

and is calculated by substituting (2.1) and (2.3) into (2.4) as,

\[
\sigma^2 = \beta_L^2 \exp(\alpha_L^2)[\exp(\alpha_L^2) - 1].
\]

The scale parameter \(\beta_L\) can be written by rearranging (2.3) as

\[
\beta_L = \mu \exp(-\alpha_L^2 / 2). \tag{2.5a}
\]

By substituting (2.5a) into (2.5), the shape parameter \(\alpha_L\) is obtained in terms of \(\mu\) and \(\sigma\) as

\[
\alpha_L = \left\{ \ln\left[ \frac{\sigma^2}{\mu^2} + 1 \right] \right\}^{1/2}. \tag{2.5b}
\]
Thus, if $\mu$ and $\sigma$ are given, the shape parameter $\alpha_L$ and the scale parameter $\beta_L$ can be calculated as

$$
\alpha_L = \left( \ln \left( \frac{\sigma^2}{\mu} + 1 \right) \right)^{1/2}, \quad \text{and} \quad \beta_L = \mu \exp(-\alpha_L^2/2). \tag{2.6}
$$

In this dissertation, because a two-dimensional model is developed, length is represented as the size of a fracture hereafter. The shape ($\alpha_L$) and scale ($\beta_L$) parameters of the lognormal distribution of fracture length are assumed to be $\alpha_L = 0.1$ or 1.0 and $\beta_L = 1.0\text{m}$ or 3.0m for the water flow and particle transport analyses in this study. $\beta_L = 3.0\text{m}$ and $\alpha_L = 0.1$ is equivalent to mean ($\mu$) of 3.0m by (2.3) and standard deviation ($\sigma$) of 0.3m by (2.5).

Figure 2.1 shows the probability density functions of lognormal distributions for length of fracture segments based on the literature review for the crystalline rock at depth below 150m. In this study, three different distributions (thick lines) are selected based on the dimension (diameter of 10m) of the model space for the DFN, and will be used for the water flow and particle transport analyses.

### 2.2.2 Aperture

For aperture of fractures, two different types of apertures are used in the literatures: the mechanical aperture and the hydraulic aperture [National Research Council, 1996]. The mechanical aperture is defined as a distance between fracture walls. The hydraulic aperture is calculated by using a measured water flow rate, a pressure gradient, and the cubic law. The hydraulic aperture was observed to be approximately an order of magnitude smaller than the mechanical aperture [Long, et al., 1987; Chen, et al., 2000].

Bianchi, et al. [1968] observed that apertures in cores or well logs were distributed lognormally. Snow [1970] claimed that a lognormal distribution was found to describe the aperture distribution in various fractured rock. Bourke, et al. [1985] derived a lognormal distribution for the hydraulic aperture from permeability tests in granite. Long, et al. [1987] stated that the shape of aperture distributions was nearly lognormal for a granite rock at depth of 320m at Fanay-Augères in France for the nuclear waste storage research. Mechanical apertures were observed to be distributed lognormally with mean values ranging between 294$\mu$m and 312$\mu$m and standard deviation ranging between 146$\mu$m and 402$\mu$m (see Figure 2.2). Moreno, et al. [1988] assumed a lognormal distribution for aperture with a mean value ranging between 56.3$\mu$m and 145$\mu$m. Tsang, et al. [1988] used a lognormal distribution for the aperture with a mean value of 80$\mu$m and a standard deviation ranging between 18.7$\mu$m and 133$\mu$m as shown in Figure 2.2. Keller, et al. [1999] showed that apertures are distributed nearly lognormally for a natural fractured granite core. The arithmetic mean and the standard deviation are 825$\mu$m and 683$\mu$m, respectively. Geometric mean and standard deviation are 586$\mu$m and 864$\mu$m, respectively (see Figure 2.2).

Gentier [1986] indicated that apertures follow a gamma distribution for natural fracture in granite. Pyrak-nolte [1996] showed an approximately Gaussian distribution with mean values ranging between 40$\mu$m and 50$\mu$m and a maximum value up to 170$\mu$m for 4 intact bituminous coal cores from a coal mine and gas producing well in the San Juan Basin. Oron, et al. [1998] claimed that a “shifted” Gaussian distribution is appropriate for aperture because they claimed that the lognormal and gamma distributions have no zero aperture, while in fractures there must be contact point having zero aperture.

Abelin, et al. [1985] studied a single fracture in crystalline rock in the Stripa mine. Hydraulic apertures calculated from the water residence time and the flow rate of water range between 200$\mu$m and 300$\mu$m. Pusch [1990] gave the equivalent hydraulic aperture at 500m depth in the Stripa mine based on 169 packer-sealed borehole test. Apertures range between 10 $\mu$m and 200 $\mu$m. 2% of the apertures ranges between 100$\mu$m and 200$\mu$m. Larsson [1997] measured mechanical apertures for 8 subsections of a sample from Aspö Hard Rock Laboratory at 200m below sea level in Sweden. A total of 30000 aperture are measured for 8 sections with median values ranging between 317$\mu$m and 373$\mu$m. Mean and standard deviation values vary from 307$\mu$m and 384$\mu$m, and 133$\mu$m and 231$\mu$m, respectively. Chen, et al. [2000] obtained the mechanical aperture in a laboratory measurement for a granite sample from the subsurface at Olympic Dam (a mining site in Australia). Measured mechanical apertures varied from 20$\mu$m to 200$\mu$m.

In this study, apertures are sampled in two different ways. In the first way, the correlation between the length and the aperture is not considered. A value of aperture is sampled based on its own statistics independently. The probability density function for the aperture of fractures is assumed lognormal, based on the literature survey. The shape ($\alpha_L$) and scale ($\beta_L$) parameters of the lognormal distribution are assumed to be $\alpha_L = 0.833$ and $\beta_L = 7.07\times10^{-5}$ m (i.e. mean ($\mu$) and standard deviation ($\sigma$) of 100 $\mu$m). In the second way, a value of aperture is determined based on the observed correlation between the length and the aperture of the fracture after the value of length is sampled. A relationship between the length and aperture of fracture is given as [Ohno, et al., 1987],

$$\log_{10}(l) = 2.7 + 0.7 \cdot \log_{10}(b),$$  \hspace{1cm} (2.7)

where $l$ [m] is the fracture length and $b$ [m] is the aperture.

Numerical results obtained by these two sample methods are compared in Section 3.6.2.3. Figure 2.2 shows the probability density functions for aperture based on the literature review excepting Ohno, et al. [1987]. Similar to the lognormal distribution of length in Figure 2.1, the distributions described by the mean and standard deviation are shown in Figure 2.2. A distribution with $\alpha_L = 0.833$ and $\beta_L = 7.07\times10^{-5}$ m (thick line) in Figure 2.2 is selected as a typical distribution of aperture of the fracture segments, and will be used for the water flow and particle transport analyses in this study.
2.2.3 Orientation Angle

An orientation angle of a fracture is defined as the direction of a vector perpendicular to the fracture plane [Geier, et al., 1992], or as the angle between the borehole and the fracture pole [Baecher et al., 1977; Long, 1985].


Long, et al. [1982] assumed a normal distribution with mean values of 30° and 60° and variance of 5° and 10°, respectively. Hestir, et al. [1990] considered the uniform and normal distributions for the parameter studies to estimate permeability in fracture network. Kulatilake et al. [1996] claimed that the available theoretical probability distributions were found to be insufficient to represent the statistical distribution of orientation of fractures.

In summary, the orientation angle of fractures for a granite rock at depth below than 150m is well characterized by the Fisher distribution [Dverstrop, et al., 1989; Cacas, et al., 1990(a); Niemi, et al., 2000].

\[ f(\theta) = \frac{1}{2\pi}, \quad 0 \leq \theta \leq 2\pi. \quad (2.8) \]

Figure 2.3 shows the probability density function (2.8) for the orientation angle.

2.2.4 Location

Fracture location refers to the spatial coordinates of the center of a fracture [Geier, et al., 1992]. Long [1985] claimed based on field data that the best current estimate for the geometry of fracture location is randomly distributed in space. A Poisson process is applied to generate the center of fractures in space [Dverstorp, et al., 1989; Cacas, et al., 1990(a)]. Kulatilake, et al. [1993] assumed a uniform (random) distribution for location of fractures at the Stripa mine in Sweden.

\[ f(r) = \frac{2r}{k_1 - k_2}, \quad \frac{k_1}{k_2} \leq r \leq \frac{k_2}{k_1}. \]

Figure 2.4 shows the probability density function for location of the primary fractures.

In this study, for the location of fractures in the two-dimensional model space, two parameters \((r, \varphi)\) must be determined. \(r\) is defined as the distance between the one end of a fracture and an origin. \(\varphi\) is defined as the angle between the \(x\) axis and the line which connects the one end of a fracture with the origin. Two types of fractures are
considered. The primary fractures are defined as fractures that exist before the disturbance due to repository construction, and are assumed to distribute uniformly in the region between \( R_0 \) and \( R_2 \) (\( R_0 < R_2 \)), resulting in

\[
f(r) = \frac{2r}{(R_0^2 - R_2^2)}, \quad R_0 \leq r \leq R_2.
\]  

Figure 2.4 shows the probability density function (2.9) for location of the primary fractures.

The secondary fractures are defined as fractures that are added as a result of the repository construction, and are assumed to distribute exponentially [Pusch, et al., 1992; Gylling, et al., 1997],

\[
f(r) = e^{-(r-R_0)}, \quad r > R_0.
\]  

Figure 2.5 shows the probability density function (2.10) for location of the secondary fractures.

The angle distribution both for the primary and secondary fractures is assumed to be uniform,

\[
f(\varphi) = \frac{1}{2\pi}, \quad 0 \leq \varphi \leq 2\pi.
\]  

### 2.2.5 Linear Frequency, Spacing, and Number Density

The linear frequency of fractures, \( \lambda \), is defined as the number of fractures intersected per unit length of a line sample (i.e. a borehole or scan-line [Priest, et al., 1976]). Spacing is defined as the distance between fractures along a line, and can be obtained as the inverse of the fracture frequency [Geier, et al., 1992]. Number density of fractures, \( \lambda_A \), is defined as the number of fractures per unit area \( A \).

Priest, et al. [1976] and Hudson, et al. [1979] examined the distribution of a number of fractures with spacing along a scan-line. They concluded that the value of the spacing distributes exponentially. Baecher, et al. [1977] concluded by literature review that the spacing distributes exponentially or lognormally. Kulatilake, et al. [1993] concluded that the exponential function appears to be the most favored one to represent the statistical distribution of the fracture spacing, while in some cases, a lognormal distribution is selected as the best. Kulatilake, et al. [1996] used the exponential and gamma distributions for the fracture spacing for crystalline rock mass in China.

Hudson, et al. [1979] stated that by a set of scan-line measurements taken in various directions on a rock surface, the number density, \( \lambda_A \), is found to be a square of the linear frequency \( \lambda \), i.e.,

\[
\lambda_A = \lambda^2.
\]  

However, a counter example for (2.12) can easily be raised, where (2.12) is not valid. Lim, et al. [2001(b)] showed that the number density by (2.12) tends to overestimate the area number density for a case with long fracture segments, whereas a case with short fracture segments underestimates. It means that the length distribution of fracture segments should be considered for determining the area number density.

Hestir et al. [1990] gives a relationship between \( \lambda_A \) and \( \lambda \) for a two-dimensional Poisson network of line fracture segments with random orientations given by the probability density function \( f(\theta_o) \).

\[
\lambda = l_o \lambda_A E(\cos \theta_o),
\]  

where \( l_o \) [m] is the average fracture length, and \( \theta_o \) is the angle between the poles of the fractures and the reference line. \( E(\cos \theta_o) \) is the expected value of \( \cos \theta_o \), and is defined as

15
\[ E(\cos \theta_a) = \int_{\theta_a}^{\pi/2} \cos \theta_a f(\theta_a) d\theta_a . \] (2.14)

Since \( \theta_a \) varies between 0 and \( \pi/2 \), the probability density function \( f(\theta_a) \) for the orientation is

\[ f(\theta_a) = \frac{1}{\pi/2} = \frac{2}{\pi} , \quad 0 \leq \theta_a \leq \pi/2 . \] (2.15)

By substituting (2.15) into (2.14), \( E(\cos \theta_a) \) is calculated as

\[ E(\cos \theta_a) = \int_{0}^{\pi/2} \cos \theta_a \frac{2}{\pi} d\theta_a = \frac{2}{\pi} \int_{0}^{\pi/2} \cos \theta_a d\theta_a = \frac{2}{\pi} . \] (2.16)

By substituting (2.16) into (2.13), the relationship between \( \lambda_A \) and \( \lambda \) becomes

\[ \lambda_A = \frac{\pi \lambda}{2l_a} . \] (2.17)

The number density of fractures (\( \lambda_A \)) can be calculated by (2.17) if we know the linear frequency (\( \lambda \)) and the average length of the fracture segment (\( l_a \)).

Experimental data for the linear frequency of the fractures \( \lambda \) are shown in the first column in Table 2.2. The values for \( \lambda \) show variation originated from different experimental sets. The second and third columns show values of \( \lambda_A \) calculated by (2.17) with the values of \( \lambda \), in the first column and the average fracture length \( l_a \) for 1.0m and 3.0m, respectively. Using \( \lambda_A \) values, the total number of fractures in the NFR region with area of \( \pi(R_0^2 - R_0^2) \) is obtained for \( l_a \)=1.0m and 3.0m in the fourth and fifth columns, respectively. In this study, the number of the secondary fractures is assumed to be 30% of that of the total number of fractures [Gylling, 1997].

<table>
<thead>
<tr>
<th>Fracture frequency (measured) ( \lambda ) [1/m]</th>
<th>Fracture number density (calculated by (2.17)) ( \lambda_A ) [1/m²]</th>
<th>Total number of fractures (calculated) [fractures](^{*1})</th>
<th>Rock</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.2~12.8</td>
<td>1.9~20.1</td>
<td>0.6~6.7</td>
<td>142~1516</td>
</tr>
<tr>
<td>7.8</td>
<td>12.3</td>
<td>4.1</td>
<td>924</td>
</tr>
<tr>
<td>3.2~26.3</td>
<td>5.0~41.3</td>
<td>1.7~13.8</td>
<td>379~3115</td>
</tr>
<tr>
<td>2.64</td>
<td>4.1</td>
<td>1.4</td>
<td>313</td>
</tr>
<tr>
<td>2.0</td>
<td>3.1</td>
<td>1.0</td>
<td>237</td>
</tr>
<tr>
<td>8.7~53.8</td>
<td>13.7~84.5</td>
<td>4.6~28.2</td>
<td>1030~6372</td>
</tr>
<tr>
<td>23.8~37.0</td>
<td>37.4~58.1</td>
<td>12.5~19.4</td>
<td>2819~4382</td>
</tr>
<tr>
<td>0.6~6</td>
<td>0.9~9.4</td>
<td>0.3~3.1</td>
<td>71~711</td>
</tr>
<tr>
<td>0.2~2.0</td>
<td>0.3~3.1</td>
<td>0.1~1.0</td>
<td>24~237</td>
</tr>
<tr>
<td>10~20</td>
<td>15.7~31.4</td>
<td>5.2~10.5</td>
<td>1184~2369</td>
</tr>
<tr>
<td>0.06~1.8</td>
<td>0.1~2.8</td>
<td>0.03~0.9</td>
<td>7~213</td>
</tr>
<tr>
<td>0.2~4.2</td>
<td>0.3~6.6</td>
<td>0.1~2.2</td>
<td>24~497</td>
</tr>
<tr>
<td>5~22.5</td>
<td>7.9~35.3</td>
<td>2.6~11.8</td>
<td>592~2665</td>
</tr>
<tr>
<td>1~3</td>
<td>1.6~4.7</td>
<td>0.5~1.6</td>
<td>118~355</td>
</tr>
<tr>
<td>1.5~6.0</td>
<td>2.4~9.4</td>
<td>0.8~3.1</td>
<td>178~711</td>
</tr>
<tr>
<td>1.32</td>
<td>2.1</td>
<td>0.7</td>
<td>156</td>
</tr>
</tbody>
</table>


\* \( l_a=1.0m \) and \( l_a=3.0m \) are selected as mean fracture lengths in Section 2.2.1
2.3 Summary

In this study, the discrete fracture network is generated to determine water-flow paths in the NFR. The flow-bearing cluster is transformed into a heterogeneous continuum or a homogeneous continuum. The modeling approaches for the NFR will be compared in Chapter 3 for the groundwater flow rate and in Chapter 5 for the particle transport. For particle transport modeling, RWTM is selected because it is suitable to combine with a stochastic continuum (Chapter 5).

Based on the literature survey, statistical distributions of fracture geometry parameters are selected in the previous section, and summarized in Table 2.3. Parameters in Table 2.3 are used for the simulation of the water flow analysis in Chapter 3 and transport analysis in Chapter 5.

<table>
<thead>
<tr>
<th>Location</th>
<th>Fracture length</th>
<th>Aperture</th>
<th>Orientation</th>
</tr>
</thead>
<tbody>
<tr>
<td>r</td>
<td>φ</td>
<td>Dis</td>
<td>αL</td>
</tr>
<tr>
<td>Pri</td>
<td>Sec</td>
<td>Pri</td>
<td>Sec</td>
</tr>
<tr>
<td>Uni</td>
<td>Exp</td>
<td>Uni</td>
<td>Uni</td>
</tr>
</tbody>
</table>

Dis: Distribution; LN: Lognormal; Uni: Uniform; Exp: Exponential
Pri: Primary fractures; Sec: Secondary fractures; αL: Shape parameter; βL: Scale parameter
3. Water Flow Analysis in the Near Field of Geologic Repository

3.1 Introduction

In this chapter, a two-dimensional model for the groundwater flow is established for the one-waste canister configuration in the near field of a hypothetical water-saturated geologic repository.

A near-field model consists of an impermeable waste canister, a bentonite-filled buffer, and a near-field rock (NFR). The water flow path in the NFR is first represented by a Discrete-Fracture Network (DFN), which is generated based on the distribution functions of the fracture geometry parameters summarized in Section 2.3. The flow-bearing region in the DFN in the NFR is determined by checking the interconnectivity of the fractures, and is transformed into a heterogeneous continuum or a homogeneous continuum. The spatial distribution of the hydraulic potential is obtained by solving a steady-state potential equation numerically by a finite element method.

The objectives of this chapter are (1) to develop a water flow model incorporating the heterogeneity of the NFR with the one-waste canister configuration, (2) to investigate effects of the heterogeneity of the NFR on the groundwater flow rate, and (3) to investigate effects of the modeling approach for the NFR on the groundwater flow rate.

3.2 Model Space

A near-field model for the one-waste canister configuration is defined in a two-dimensional model space as shown in Figure 3.1. The outer circle with radius \( R_2 \) represents the model space boundary. The middle circle with radius \( R_0 \) represents the interface between the bentonite-filled buffer region and the NFR. The circle with radius \( R_1 \) represents the surface of the waste. The water-saturated buffer region between \( R_1 \) and \( R_0 \) is assumed to be homogeneous and isotropic. The hydraulic conductivity and the porosity in the buffer region are assumed to be uniform. The hydraulic conductivity for the buffer is assumed \( 2.3 \times 10^{-14} \) m/s [Verbeke, et al., 1997]. The porosity for the buffer is assumed 0.3 [PNC, 1992; Verbeke, et al., 1997].

![Figure 3.1 Model space](image)

The values of \( R_0 \), \( R_0 \), and \( R_2 \) have been determined as 0.35 m, 1.0 m, and 5.0 m, respectively, based on the previous studies [PNC, 1992; JNC, 2000 (Vol. 3, IV-134)].

3.3 Fracture Network Generation

A two-dimensional discrete fracture network is generated in the NFR region between \( R_0 \) and \( R_2 \) in Figure 3.1. In the 2-D model, a fracture segment is represented as a line element of length \( l \) and aperture \( b \) as shown in Figure 3.1. Discrete fractures are generated based on given statistics of the fracture geometry parameters in Table 2.3 in Section 2.3 by random sampling*. Each fracture segment is generated independently, and then superimposed until required number of fracture segments is generated in the model space between \( R_0 \) and \( R_2 \).

* Detail about the random sampling for a lognormal distribution is given in Appendix A.
3.3.1 Generation of Fracture Segments

Details about the generation of fracture segments are given below.

(1) Two random numbers ((r, \(\varphi\)) in Figure 3.2) for coordinates of one end of the fracture segment are generated between \(R_0\) and \(R_2\) based on the distribution functions.

For the primary fractures, one random number is generated for \(r\) based on the uniform distribution function (2.9) in the range between \(R_0\) and \(R_2\). For the secondary fractures, one random number is generated for \(r\) based on the exponential distribution function (2.10). For both primary and secondary fractures, one random number for angle \(\varphi\) is generated based on the uniform distribution (2.11) measured against the x-axis.

Figure 3.2 Determination of coordinates for one end of a fracture segment

(2) One random number for the length, \(l\), of the fracture segment is generated based on the lognormal distribution (2.1).

For the length, the different values of the scale (\(\beta_L\)) and shape (\(\alpha_L\)) parameters can be assigned for the primary and secondary fractures. The random sampling for the lognormal distribution is shown in Appendix A.

Figure 3.3 Determination of length (l) and aperture (b)

Figure 3.4 Determination of orientation (\(\Theta\))
Figure 3.5  Determination of the location \((r, \varphi)\), length \((l)\), and aperture \((b)\) of a second fracture segment

Figure 3.6  Possible two cases for two fractures

(3) One random number for the determination of the aperture, \(b\), of the fracture segment is generated based on the lognormal distribution \((2.1)\).

Figure 3.3 shows possible fracture segments with the assumption of isotropic fracture for the location of one end of the fracture \((r, \varphi)\), length \((l)\), and aperture \((b)\). In Figure 3.3, only 16 possible fracture segments are shown because of the limitation of graphical representation, but there are an infinite number of possible fracture segments.

(4) One random number for the determination of the orientation angle, \(\theta\), measured from the \(x\)-axis of the coordinate system is generated to select one fracture segment out of infinite possible fracture segments based on the uniform distribution \((2.8)\).

In Figure 3.4, a thick line with two end points represents a selected fracture segment for the location of one end of the fracture \((r, \varphi)\), length \((l)\), aperture \((b)\), and orientation \((\theta)\). Thin lines represent possible fracture segments.

Each fracture segment is generated independently by procedures (1) to (4), and then superimposed in the model space. Figure 3.5 shows the location, length, and aperture of a second fracture segment that is superimposed in the model space.

There are two possible cases depending on whether two fracture segments intersect or not. Figure 3.6 implies that isotropy of fracture orientation is an important assumption for determining intersection of fractures. If fractures are oriented anisotropically (especially if oriented in the same direction), the possibility for fractures to intersect is significantly decreased (see Appendix B). In this study, fracture intersection is crucial because only interconnected fractures form a path for water flow.
Table 3.1  Statistics of Fracture Geometry Parameters Used to Generate Figure 3.7

<table>
<thead>
<tr>
<th>Number of fractures</th>
<th>Fracture length</th>
<th>Aperture</th>
<th>Orientation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean [m]</td>
<td>SD [m]</td>
<td>Dis βL [m]</td>
</tr>
<tr>
<td>454</td>
<td>1.0</td>
<td>0.1</td>
<td>LN 1.0</td>
</tr>
</tbody>
</table>

Dis: Distribution; LN: Lognormal; SD: Standard Deviation; αL: Shape parameter; βL: Scale parameter

Figure 3.7 shows a realization of fracture network using parameters shown in Table 3.1. The values of the mean and the standard deviation both for the length and the aperture are obtained by (2.3) and (2.5) with the scale parameter (βL) and the shape parameter (αL) given in Table 3.1. The distributions of the length, aperture, and orientation of the secondary fractures are assumed to be same as those for the primary fractures. For each location of the fractures, the uniform distribution (2.9) and the exponential distribution (2.10) are assumed for the primary and secondary fractures, respectively.

Figure 3.8  Three realizations of fracture network by the same statistics.

Figure 3.8 shows three realizations of the fracture network based on parameters in Table 3.1. Three realizations (a), (b), and (c) show different fracture networks produced by different seeds because of random sampling of fracture parameters based on the distribution functions. A subroutine developed by Press, et al. [1992] is used as a random number generator. A different seed will result in a different random number sequence. Since the same seed will always return the same random sequence, a fracture network can be re-produced by assigning the same seed in the subroutine.
3.3.2 Flow-Bearing Cluster (FBC) of Fractures

There are two types of fracture clusters in a fracture network. In the first type, fracture clusters connect the outer boundary \( (r=R_2) \) of the model space with the interface between the buffer and the NFR \( (r=R_0) \). We call this type as a **Flow-Bearing Cluster (FBC)** of fractures. Clusters of the second type are those other than the FBC, called **Dead-End Clusters (DECs)** of fractures.

Figure 3.9 shows an example of fracture clusters. Fractures included in the FBC are represented by thick lines, whereas fractures included in the DECs are represented by thin lines. Note that the cluster designated as “B” in Figure 3.9 is also included in the FBC because a water flow path from the outer boundary exists through the buffer region.

In this study, it is assumed that the rock matrix is impermeable, and water can be supplied from the outer boundary of the model space to the EBS only through the FBC and the buffer region.

![Fracture clusters](image)

**Figure 3.9** Fracture clusters. Thick lines represent the FBC of the DFN, whereas the thin lines represent the DEC in the DFN.

3.3.3 Identification of FBC

After the generation of a fracture network (Figure 3.7), a FBC is identified by checking the interconnectivity of all fractures. Intersection of fractures is defined as:

1. two fracture segments cross each other with one common intersection point,
2. one end of the fracture segment lie on another segment,
3. two fracture segments overlap partly.

Figure 3.10 (a) shows the cases for intersection, and (b) shows the cases for no intersection. In Figure 3.10 (b), dashed lines represent the extensions of the fracture segments.

![Intersection cases](image)

(a) Intersection

(b) No intersection

**Figure 3.10** Intersection between two fracture segments. In (a), intersection is counted once.

*Here, it is implicitly assumed that water flows into and out of the model space through those fracture segments intersecting the outer boundary. Fracture segments which intersect with these are also assumed to bear water flow.*
Numerical schemes developed by O’Rourke [1993] are used in this study for determining whether two finite lines intersect or not. Input parameters for O’Rourke’s schemes are coordinates of 4 end points of two lines.

Figure 3.11  An example for the identification of the FBC in a fracture network.

To illustrate how to identify the FBC, an example is given in Figure 3.11, where ten fractures are included. The outer boundary is the outermost circle, and the interface is the middle circle.

The steps for identifying the FBC are as follows.
1. Identify fractures intersecting with the outer boundary (fractures 1, 2, and 9 in Figure 3.11).
2. Identify fractures intersecting with the interface (fractures 4, 5, 8, and 10 in Figure 3.11).
3. Select one among the fractures identified in procedure (1). Check all other fractures whether they intersect with the selected fracture or not. If intersection occurs, fix the intersecting fracture and check all other fractures except for those two fractures. Repeat this procedure until there is no more intersecting fractures.
4. Repeat (3) for all fractures intersecting the outer boundary identified by step (1). After at least one cluster of interconnected fractures is identified, step (3) is repeated for the fractures identified by step (2) to include fractures intersecting the interface.

Figure 3.12  FBC for the fracture network in Figure 3.11

To identify a FBC in Figure 3.11, let us start with fracture 1, and check the intersection with other fractures. Only fracture 3 intersects with fracture 1. Take fracture 3 and check the intersection with other fractures except for fractures 1 and 3. Only fracture 4 intersects with fracture 3. Fracture 4 intersects with the interface, and there are no more intersecting fractures with 4. Therefore, fractures 1, 3, and 4 are interconnected each other, and are parts of FBC. Repeat this procedure for other fractures identified in step (1). In this case, fractures 2 and 9. For fracture 2, there is no intersecting fracture with fracture 2. Also, fracture 2 does not intersect with the interface. Thus, fracture 2 is isolated, and is part of DEC. For fracture 9, only fracture 10 intersects with fracture 9, and fracture 10 intersects with the interface. Thus, fractures 9 and 10 are interconnected and are parts of FBC. After at least one cluster of interconnected fractures is identified, step (3) is repeated for the fractures identified by step (2) to include fractures intersecting the interface. Therefore, the FBC consists of fractures 1, 3, 4, 5, 6, 8, 9, and 10. Figure 3.12 shows the FBC. Thick lines represent fractures included in the FBC.
The FBC for the fracture network in Figure 3.7 is shown in Figure 3.13.

Figure 3.13  FBC for the fracture network in Figure 3.7.

3.4 Transformation of FBC into Equivalent Continuum

The FBC identified by inspecting the interconnectivity of the fractures in the NFR is transformed into an equivalent continuum in two different ways.

First, a transformation is applied locally to the FBC, which is called the local homogenization in this study. By the local homogenization, the FBC consisting of the discrete fractures is transformed into a heterogeneous continuum. Thus, the NFR is heterogeneous, and is divided by the flow-bearing region (i.e., heterogeneous continuum transformed from the FBC) and the water stagnant region.

In a second approach, a global transformation is applied to the FBC to cover the entire NFR, which is called the uniformization in this study. By the uniformization, the NFR is transformed into a homogeneous continuum. Thus, the entire NFR is homogeneous, and is a flow-bearing region.

3.4.1 Transformation of FBC into a Heterogeneous Continuum

In this section, a method of transformation of the FBC into a heterogeneous continuum by the local homogenization is developed.

First, the FBC is covered by many triangular elements. Then, inter-connected fracture segments included in the FBC in a small triangular area are transformed to a homogeneous, isotropic, porous medium. Single values of the porosity (Section 3.4.1.1) and hydraulic conductivity (Section 3.4.1.2) are obtained for that area. Because triangular elements contain different numbers of fractures with varying length and aperture, each element has different porosity and hydraulic conductivity. The heterogeneity of the FBC still remains after the transformation. Thus, the FBC is transformed into a heterogeneous continuum consisting of triangular elements which have different hydraulic properties.

By the local homogenization of the FBC, one obtains not only the small scale variability of the hydraulic conductivity and the porosity inside the FBC but also information about where localized flow channels exist in the FBC. All this information is incorporated and utilized in the flow analysis.

3.4.1.1 Equivalent porosity

The porosity is defined as the ratio of the pore volume to the total volume (pore + solid). To formulate the equivalent porosity for a triangular element, an example is considered in Figure 3.14. The figure shows four fracture segments with different lengths and apertures in a triangular element. In this example, fracture 4 is not included in the calculation of the porosity, because it is not included in the FBC. Only fractures 1, 2, and 3 are included in the FBC. Only the part of the fracture within the element is considered. \( \Delta_e \) is the area of the element \( e \). \( l_{e,1}, l_{e,2}, \text{ and } l_{e,3} \) are fracture lengths included in the element. \( b_{e,1}, b_{e,2}, \text{ and } b_{e,3} \) are fracture apertures.

With the assumption that the element has a unit depth normal to the plane of \( \Delta_e \), the equivalent porosity \( \varepsilon_e \) for element \( e \) can be written as

\[
\varepsilon_e = \frac{l_{e,1} b_{e,1} + l_{e,2} b_{e,2} + l_{e,3} b_{e,3}}{\Delta_e}.
\]  (3.1)
The generalized formula for the porosity $\varepsilon_e$ for element $e$ is

$$\varepsilon_e = \frac{\sum l_{i,e} b_{i,e}}{\Delta_e},$$

(3.2)

where $N_e$ denotes the number of fractures included in the FBC which pass through the element $e$.

### 3.4.1.2 Equivalent hydraulic conductivity

The hydraulic conductivity, $K$ [m/s], is a coefficient that depends on both medium and fluid properties. The relevant fluid properties are the density $\rho$ and the viscosity $\mu_w$. The relevant medium property is the permeability, $k$ [m$^2$]. For the equivalent permeability $k_e$ for element $e$, the Kozeny-Carman formula [Bear, 1979],

$$k_e = C \frac{\varepsilon_e^3}{(1-\varepsilon_e)^2 M_{s,e}},$$

(3.3)

is used in this study. The formula includes the equivalent porosity of the element $\varepsilon_e$ for the flow of water through the pores and the specific surface area of the element, $M_{s,e}$, which is defined as the pore surface area wet by the flowing water per unit volume of the porous medium [Bear, 1979]. Coefficient $C$ is a function of the shape of cross-sectional area normal to flow and the tortuosity [Carman, 1956]. The value of coefficient $C$ is less than unity, and is a space-dependent function because tortuosity, porosity, and the specific surface area vary within the FBC region. In this chapter, however, it is assumed that $C=1$. The coefficient $C$ will be discussed in Chapter 6 in detail.

$M_{s,e}$ is calculated by the ratio of the total surface area of intersecting fractures in element $e$ to the volume of solid in element $e$.

$$M_{s,e} = \frac{\sum l_{i,e} b_{i,e}}{[\Delta_e - \sum l_{i,e} b_{i,e}]} [m^2],$$

(3.4)

where $d$ is an arbitrary depth normal to the element and the fracture as shown in Figure 3.15.

If aperture $b_{i,e}$ is much smaller than $l_{i,e}$ or $d$, and $\varepsilon_e \ll \Delta_e$, (3.4) can be simplified as

$$M_{s,e} = \frac{\sum l_{i,e} b_{i,e}}{[\Delta_e]} [m^2].$$

(3.5)

The equivalent permeability, $k_e$, for element $e$ can be calculated by (3.3) with the equivalent porosity $\varepsilon_e$ by (3.2) and the specific surface area, $M_{s,e}$, by (3.5).

The equivalent hydraulic conductivity, $K_e$, for element $e$ is expressed as

* Detail about tortuosity is given in Chapter 6.
\[ K_x = \frac{k \rho g}{\mu_x}, \]  

where \( \rho \) is the density of water, \( g \) is the constant for gravity, and \( \mu_x \) is the viscosity of water.

3.4.2 Transformation of the FBC into a Homogeneous Continuum

In this section, a method of transformation of the FBC into a homogeneous continuum by the uniformization is developed.

By the uniformization, the entire NFR is transformed into a homogeneous continuum, and is a flow-bearing region. The uniformization gives a single value of hydraulic properties for the entire NFR, whereas the local homogenization shown in the previous section gives as many different values of hydraulic properties as the number of elements. The procedure for the uniformization consists of the following three steps.

1. A single value of uniformized porosity, \( \bar{\varepsilon} \), for the entire NFR is calculated by

\[ \bar{\varepsilon} = \frac{\sum N l_i b_i}{A}, \]  

where \( N \) is the number of fractures included in the FBC, and \( A \) is the area of the entire NFR region, given by \( A = \pi(R_2^2 - R_1^2) \).

2. A single value of the uniformized specific surface area \( \bar{M}_s \) for the entire NFR is calculated for \( b_i \) is much smaller than \( l_i \) or \( d \), and \( \bar{\varepsilon} << A \) as

\[ \bar{M}_s = \frac{\sum N (2l_i) b_i}{A} \text{ [m}^4]. \]  

3. By using \( \bar{\varepsilon} \) obtained by (3.7), and \( \bar{M}_s \) obtained by (3.8), a single value of uniformized permeability, \( \bar{k} \), for the entire NFR is calculated by Kozeny-Carman equation,

\[ \bar{k} = C \frac{\bar{\varepsilon}^3}{(1-\bar{\varepsilon})^2 \bar{M}_s^2}. \]  

where \( C \) is assumed to be 1.

With (3.9), the uniformized hydraulic conductivity \( \bar{K} \) for the entire NFR is calculated as

\[ \bar{K} = \frac{\bar{k} \rho g}{\mu_x}, \]  

where \( \rho \) is the density of water, \( g \) is the gravitational acceleration, and \( \mu_x \) is the viscosity of water.
3.5 Governing Equation and Side Conditions

Figure 3.16 shows the flowing-bearing domain (Ω), which covers the FBC and the buffer region. The governing equation of water flow in domain Ω can be obtained by the conservation of mass [Bear, 1979],

\[
\frac{\partial (\varrho \phi)}{\partial t} + \text{div}(\varrho \vec{q}) = 0, \quad \text{in } \Omega \tag{3.11}
\]

where \( \varrho [\text{kg/m}^3] \) is the density of water, and \( q_x \) and \( q_y \) are Darcy velocity components [m/s] in \( x \) and \( y \) directions, respectively. \( \varepsilon(x,y) \) is the porosity.

For the time-independent case,

\[
\frac{\partial (\varrho \phi)}{\partial t} = 0. \tag{3.13}
\]

For the incompressible case, \( \varrho \) is constant. With the constant \( \varrho \) and (3.13), the conservation equation (3.12) becomes

\[
\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0. \tag{3.14}
\]

For a steady flow in an anisotropic heterogeneous medium if principal directions are used as the coordinate system, Darcy’s law (3.15) and (3.16) applies [Bear, 1979].

\[
q_x = -K_x(x,y) \frac{\partial \phi}{\partial x}, \tag{3.15}
\]

\[
q_y = -K_y(x,y) \frac{\partial \phi}{\partial y}, \tag{3.16}
\]

where \( \phi(x,y) \) is the potential head [m], and \( K_x(x,y) \) and \( K_y(x,y) \) are the hydraulic conductivity [m/s] for two principal directions.

Substituting Equations (3.15) and (3.16) into (3.14) yields the governing equation for the steady-state flow in a heterogeneous anisotropic medium as...
\[
\frac{\partial}{\partial x} \left[ K_i(x, y) \frac{\partial \bar{\phi}}{\partial x} \right] + \frac{\partial}{\partial y} \left[ K_i(x, y) \frac{\partial \bar{\phi}}{\partial y} \right] = 0. \tag{3.17}
\]

The potential head \( \phi \) is to be found in a two-dimensional solution domain \( \Omega \) shown in Figure 3.16. Two different kinds of boundary conditions are considered. Along the \( C_i \) boundary (think lines on the outer boundary \( r=R_j \)) of the model space, the potential head is prescribed by

\[
\phi(x, y) = \phi_n \frac{1-(x/R_j)}{2}, \quad -R_j \leq x \leq R_j \text{ on } C_i,
\tag{3.18}
\]

where \( \phi_n = 1.0 \).m.

The Darcy velocity normal to the \( C_2 \) boundary (thick line on the surface of the metal canister \( r=R_j \)) is prescribed zero, or

\[
K_i(x, y) \frac{\partial \bar{\phi}}{\partial x} n_x + K_i(x, y) \frac{\partial \bar{\phi}}{\partial y} n_y = 0 \text{ on } C_2,
\tag{3.19}
\]

where \( n_x \) and \( n_y \) are the direction cosines of the outward normal vector \( \hat{n} \).

For the boundary of \( \Omega \) in the NFR except for \( C_i \) boundary as shown in Figure 3.16, the potential head is unknown and flux is prescribed as zero.

### 3.5.1 Solution for Governing Equation by Finite Element Method

To solve the governing equation (3.17), the finite element method is applied. Triangular elements* are used to discretize the domain. The method of weighted residuals is used for obtaining an approximate solution. The method of weighted residuals is summarized according to the reference [Huebner, 1975] hereafter.

If an approximated field variable \( \phi_{approx} \) is substituted, the left-hand side of the governing equation (3.17) is not equal to zero. This non-zero value is called residual, \( \mathfrak{R} \). Thus, we have

\[
\int_{\Omega} \mathfrak{R} W d\Omega = 0, \quad i = 1, 2, \ldots, m,
\tag{3.20}
\]

where \( W_i \) is a weight function. The domain \( \Omega \) is discretized into \( m \) nodes. By substituting (3.20) into (3.21),

\[
\int_{\Omega} \left[ \frac{\partial}{\partial x} \left( K_i(x, y) \frac{\partial \phi_{approx}}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_i(x, y) \frac{\partial \phi_{approx}}{\partial y} \right) \right] W_i d\Omega = 0, \quad i = 1, 2, \ldots, m.
\tag{3.22}
\]

The subscript “approx” is dropped. \( \phi \) is an approximate solution of the potential head, and is represented by

\[
\phi = \sum_{i=1}^{m} W_i \phi_i, \quad i = 1, 2, \ldots, m,
\tag{3.23}
\]

where \( \phi_i \) is an unknown nodal potential head at node \( i \).

Since there is no attempt to choose \( W_i \) so as to satisfy the boundary conditions, integration by parts is done, and yields

---

* These elements are the same as those considered in Section 3.4.1 for transformation (see Figure 3.14)
where variable \( s \) is the arc length of the outer boundary. The right-hand side integral represents the weighted integral of the Darcy normal velocity on \( C_j \).

\[
\int \left[ K_i(x, y) \frac{\partial W_i}{\partial x} + K_j(x, y) \frac{\partial W_j}{\partial y} \right] \, dx \, dy = \int_{C_i} \left[ K_i(x, y) \frac{\partial \phi}{\partial x} n_i + K_j(x, y) \frac{\partial \phi}{\partial y} n_j \right] W_i \, ds, \quad  \tag{3.24}
\]

Figure 3.17 Triangular element in the domain.

Equation (3.22) is for the entire domain \( \Omega \) (shown shaded in Figure 3.17). The governing equation (3.17) must be satisfied at any point in the domain \( \Omega \). Therefore, (3.24) is valid for any collection of points defining triangular elements in the whole domain \( \Omega \) [Huebner, 1975]. In Figure 3.17, an arbitrary triangular element \( e \) is shown with 3 nodes, 1, 2, and 3. Domain \( \Omega' \) represents the region within the triangular element \( e \). By applying (3.24) to element \( e \),

\[
\int \left[ K_i(x, y) \frac{\partial W_i}{\partial x} + K_j(x, y) \frac{\partial W_j}{\partial y} \right] \, dx \, dy = \int_{C_i} \left[ K_i(x, y) \frac{\partial \phi}{\partial x} n_i + K_j(x, y) \frac{\partial \phi}{\partial y} n_j \right] W_i \, ds, \quad x \in \Omega', \ y \in \Omega' \,
\tag{3.25}
\]

where the index \( i \) indicates the node included in element \( e \). The right-hand side of (3.25) has a non-zero value only if element \( e \) forms part of the \( C_j \) boundary.

Notice that, in this case, \( K_i(x, y) \) and \( K_j(x, y) \) are the hydraulic conductivities [m/s] in \( \Omega' \) in the principal directions. Following (3.23), \( \phi \) in (3.25) is written as

\[
\phi = \sum_{i=1}^{3} W_i \phi_i, \quad i = 1, 2, 3. \tag{3.26}
\]

The location of any point within the element, or on the element’s boundaries can be described as the natural coordinates \( L_1, L_2, \) and \( L_3 \). These coordinates range between zero and unity within the element [Huebner, 1975]. One particular coordinate has a unit value at one node of the element and zero value at the other node(s). Variation between nodes is assumed linear. The original Cartesian coordinates \( (x, y) \) of a point in the element are linearly related to the natural coordinates by the following equations [Huebner, 1975]:

\[
x = L_1 x_1 + L_2 x_2 + L_3 x_3, \tag{3.27}
\]

\[
y = L_1 y_1 + L_2 y_2 + L_3 y_3. \tag{3.28}
\]

Here, \( (x_1, y_1), (x_2, y_2), \) and \( (x_3, y_3) \) are the coordinates of nodes 1, 2, and 3 in element \( e \) (see Figure 3.18). The third condition requires the sum of the natural coordinates to be unity.

\[
L_1 + L_2 + L_3 = 1. \tag{3.29}
\]
Figure 3.18  Coordinates of three nodes in a triangular element by global coordinate system \((x, y)\).

The solutions of (3.27) and (3.28) yield the natural coordinates in terms of the Cartesian coordinates.

\[
L_1(x, y) = \frac{1}{2\Delta_e}(\alpha_{e1} + \beta_{e1} x + \gamma_{e1} y),
\]

(3.30)

\[
L_2(x, y) = \frac{1}{2\Delta_e}(\alpha_{e2} + \beta_{e2} x + \gamma_{e2} y),
\]

(3.31)

\[
L_3(x, y) = \frac{1}{2\Delta_e}(\alpha_{e3} + \beta_{e3} x + \gamma_{e3} y),
\]

(3.32)

where

\[
2\Delta_e = \left| \begin{array}{cc} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \end{array} \right| = 2 \times \text{(area of triangle 1-2-3)},
\]

(3.33)

and

\[
\alpha_{e,i} = x_i y_j - x_j y_i, \beta_{e,i} = y_j - y_i, \gamma_{e,i} = x_i - x_j, \text{ for } i = 1, 2, 3; j = 2, 3, 1; k = 3, 1, 2.
\]

(3.34)

Subscript \(e\) in (3.30)–(3.34) denotes element \(e\).

\(W_i\) is determined such that \(W_i = L_i\). The approximate potential head, \(\phi\), in element \(e\) can be evaluated by (3.26) as

\[
\phi = L_i \phi_i + L_2 \phi_2 + L_3 \phi_3.
\]

(3.35)

Substituting (3.30), (3.31), and (3.32) into (3.35) and differentiating it with respect to \(x\) and \(y\) yields

\[
\frac{\partial \phi}{\partial x} = \frac{1}{2\Delta_e} [\beta_e] [\phi] \text{ and } \frac{\partial \phi}{\partial y} = \frac{1}{2\Delta_e} [\gamma_e] [\phi]
\]

(3.36)

where \([\beta_e] = [\beta_{e1} \beta_{e2} \beta_{e3}], [\gamma_e] = [\gamma_{e1} \gamma_{e2} \gamma_{e3}],\)

\[
[\phi] = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix},
\]

(3.37)

and, \([\beta_e] [\phi]\) and \([\gamma_e] [\phi]\) are scalar product.

Differentiating (3.30), (3.31), and (3.32) with respect to \(x\) and \(y\) yields

\[
\frac{\partial L_i}{\partial x} = \frac{1}{2\Delta_e} \beta_{e,i} \text{ and } \frac{\partial L_i}{\partial y} = \frac{1}{2\Delta_e} \gamma_{e,i}.
\]

(3.38)

Substituting (3.36) and (3.38) into the left-hand side of (3.25) and noting that \(W_i = L_i\) yields
\[
\int_{\Omega} dxdy [K_e(x,y) \frac{\beta_e}{4\Delta_e} + (K_e(x,y) \frac{\gamma_e}{4\Delta_e})] \{\phi_e\} = \int_{\Omega} \left( K_e(x,y) \frac{\partial \phi}{\partial x} n_x + K_e(x,y) \frac{\partial \phi}{\partial y} n_y \right) ds, x \in \Omega^e, y \in \Omega^e, i = 1,2,3,
\]

(3.39)

where \(\beta_{e,i}, [\beta_e]\) and \(\gamma_{e,i}, [\gamma_e]\) are 3x3 matrix for the triangular element.

While \(K_e(x,y)\) and \(K_e(x,y)\) can vary within the element, two assumptions are introduced for simplicity. First, an isotropic medium is assumed for the entire domain \(\Omega\). The values of the hydraulic conductivity for the principal directions are identical, \(K_e(x,y) = K_e(x,y) = K_e(x,y)\) [Bear, 1979]. Second, by homogenization in each triangular element (Section 3.4.1), the hydraulic conductivity of element \(e\) is assumed to be a constant, everywhere in element \(e\), i.e., \(K(x,y) = K_e\) in \(\Omega^e\). The same assumptions are made for the porosity in element \(e\), i.e. \(e\) in \(\Omega^e\). Homogenized hydraulic properties can be different from element to element in domain \(\Omega\). Thus, heterogeneity of domain \(\Omega\) still remains.

Because \(\int_{\Omega} dxdy = \Delta_e\), equation (3.39) for the element is written in a matrix form as

\[
[\xi_e] \{\phi\} = \{Q\},
\]

(3.40)

where

\[
[\xi_e] = \frac{K_e}{4\Delta_e} \begin{bmatrix}
\beta_{e,1} \beta_{e,1} + \gamma_{e,1} \gamma_{e,1} & \beta_{e,1} \beta_{e,2} + \gamma_{e,1} \gamma_{e,2} & \beta_{e,1} \beta_{e,3} + \gamma_{e,1} \gamma_{e,3} \\
\beta_{e,2} \beta_{e,1} + \gamma_{e,2} \gamma_{e,1} & \beta_{e,2} \beta_{e,2} + \gamma_{e,2} \gamma_{e,2} & \beta_{e,2} \beta_{e,3} + \gamma_{e,2} \gamma_{e,3} \\
\beta_{e,3} \beta_{e,1} + \gamma_{e,3} \gamma_{e,1} & \beta_{e,3} \beta_{e,2} + \gamma_{e,3} \gamma_{e,2} & \beta_{e,3} \beta_{e,3} + \gamma_{e,3} \gamma_{e,3}
\end{bmatrix}, \quad \text{and}
\]

\[
\{Q\} = \int_{\Omega_e} K_e \left( \frac{\partial \phi}{\partial x} n_x + \frac{\partial \phi}{\partial y} n_y \right) ds, i = 1,2,3.
\]

(3.41)

Equations (3.40), (3.41), and (3.42) apply to the element \(e\). To formulate the problem for the whole domain \(\Omega\) including the FBC and the bentonite-filled buffer region, \(\Omega\) is discretized into triangular elements as shown in Figure 3.19, where a magnified triangular element with three nodes \(n1, n2, n3\) is also shown. If nodes 1, 2, and 3 in the natural coordinate system correspond to \(n1, n2, n3\) in the global numbering (see Appendix C), the finite-element solution for all elements with the total number of nodes, \(N_N\), and the total number of elements, \(N_E\), in the domain \(\Omega\) is written as

\[
[\xi] \{\phi\} = \{Q\},
\]

(3.43)

where

\[
[\xi] = \sum_{e=1}^{N_E} [\xi_e].
\]

(3.44)

If \(i=n1, n2\), or \(n3\) and \(j=n1, n2\), or \(n3\), then \(\xi_{(i,j)}\) are non zero. Otherwise, \(\xi_{(i,j)} = 0\). Thus, \(N_N \times N_N\) matrix \([\xi]\) is written as

\[
[\xi] = \begin{bmatrix}
0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & \xi_{(n1,n2)} & \xi_{(n1,n3)} & \xi_{(n1,a3)} & \cdots & \xi_{(n1,a4)} \\
0 & \cdots & 0 & \xi_{(n2,n1)} & \xi_{(n2,n2)} & \xi_{(n2,n3)} & \cdots & \xi_{(n2,a3)} \\
0 & \cdots & 0 & \xi_{(n3,n1)} & \xi_{(n3,n2)} & \xi_{(n3,n3)} & \cdots & \xi_{(n3,a3)} \\
0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0
\end{bmatrix}
\]

(3.45)

By (3.41),
\[
\begin{bmatrix}
0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
\end{bmatrix}
\]

where
\[
\beta_{n,i} = \gamma_{n,i} - \gamma_{n,3}, \quad \gamma_{n,i} = x_{n} - x_{n,i},
\]

\[
\begin{align*}
\phi &= \begin{bmatrix}
\phi_n \\
\vdots \\
\phi_{n_n}
\end{bmatrix}, \\
\{Q\} &= \begin{bmatrix}
Q_n \\
\vdots \\
Q_{n_n}
\end{bmatrix} = \sum_{i=1}^{n} \{Q_i\}, \\
\{Q_{n_i}\} &= \begin{bmatrix}
0 \\
\vdots \\
0
\end{bmatrix}
\end{align*}
\]

An example for assembling global matrix, (3.43), is given in Appendix C.

![Triangular elements covering the FBC and buffer region.](image)
3.5.2 Example for Results of Water Flow Analysis

After identifying a FBC (Figure 3.13) from a fracture network (Figure 3.7), the FBC in the NFR is transformed into a heterogeneous continuum by the local homogenization (Section 3.4.1), and a homogeneous continuum by the uniformization (Section 3.4.2). For the local homogenization, triangular finite-element meshes are generated over the FBC and the buffer region as shown in Figure 3.20. Hydraulic properties are obtained for each triangular element.

![Triangular mesh generation on the FBC (Figure 3.13) and the buffer region.](image)

A near-field model with a heterogeneous NFR by the local homogenization is described in this section. With obtained hydraulic properties and the prescribed boundary conditions (3.18) and (3.19), the values of potential head \( \phi \) at internal nodes in the FBC and at nodes in the buffer including the interface \((r=R_0)\) and the inner boundary \(C_2\) \((r=R_1)\) are calculated by solving the matrix equation (3.43) numerically. At nodes on the outer boundary \(C_1\), where the potential head is prescribed, the corresponding component of the vector, \( \{Q\} \), on the right side of (3.43) is calculated. The component, \( Q_i \) [m\(^3\)/m-yr], of the vector physically means the volume of water flowing across the outer boundary associated with node \( i \) normal to the boundary per unit time through unit depth normal to \( x-y \) plane. Positive \( Q_i \) means that the direction of flow at boundary node \( i \) is outward, whereas negative means inward.

To solve the matrix equation (3.43), the code developed by Huebner [1975] is used. Upon conversion from FORTRAN to C, some parts of the code have been modified. With the obtained numerical result for the potential head at nodes, the potential head can be numerically evaluated at any location in the FBC and the buffer by (3.23).

With these numerical results obtained by solving the matrix equation (3.43), four quantities of interest can be calculated: (1) the total discharge at the outer boundary, (2) the total discharge at the interface, (3) the residence time of water in the buffer region, and (4) the spatial distribution of Darcy velocity in the FBC.

The total discharge \( Q \) [m\(^3\)/yr], defined as the volumetric flow rate per unit depth normal to \( x-y \) plane, at the outer boundary \((r=R_2)\) is calculated by summing positive values of \( Q_i \) on the outer boundary. By the mass balance assumed for the establishment of the governing equation (3.17), the sum of negative values of \( Q_i \) should have the same magnitude with the sum of the positive values. This has been confirmed in the numerical examples shown below.

In the present study, because a steady state is assumed, total discharges into and out of the model space at the outer boundary should be equal to each other by mass balance. The values 996 kg/m\(^3\) for \( \rho \) and 0.799x10\(^{-3}\) N-s/m\(^2\) for \( \mu_0 \) are used for (3.6) and (3.10) by assuming that the system temperature is 30\(^\circ\)C. 9.8 m/s\(^2\) for \( g \) is used in (3.6) and (3.10). In order to demonstrate that numerical results satisfy the mass balance requirement, the FBC in Figure 3.13 is used as an example. The total discharges into and out of the model space are calculated as 2.69x10\(^2\) m\(^3\)/yr for the FBC in Figure 3.13. The difference between two quantities is of the order of 10\(^{-10}\) m\(^3\)/yr, which is 12 orders of magnitude smaller than 2.69x10\(^2\). For numerical results shown in this dissertation, it has been confirmed that mass balance is actually kept with a similar order of magnitude error.
Similar to the total discharge at the outer boundary, the total discharge at the interface \((r=R_0)\) is calculated by summing positive values of \(Q_i\) on the interface. \(Q_i\) at the nodes on the interface are calculated as follows. Because the values of the potential head at the interface \((r=R_0)\) are already obtained for the calculation of \(Q_i\) at the outer boundary, a similar matrix equation can be established for the buffer region with the hydraulic properties in the buffer region and the prescribed no flux boundary condition at the surface of the waste canister \((r = R_1)\). In the established matrix equation, the right-side vector, \([Q]\), contains unknown components, which are at the nodes on the interface. By solving this matrix equation numerically, the unknown \(Q_i\) at the nodes on the interface are calculated.

![Figure 3.21](image-url)  

**Figure 3.21**  
Darcy velocity for the FBC in Figure 3.13.

The residence time of water in the region of interest can be calculated by dividing the water volume \([\text{m}^3/\text{m}]\) of the region per unit depth by the total discharge \([\text{m}^3/\text{yr}]\) into and out of the region.

By (3.36), the gradient of the potential head in the \(x\)-direction and in the \(y\)-direction are obtained numerically for element \(e\). With the hydraulic conductivity \(K_e\) obtained by (3.6) and \((\partial \phi/\partial x)\) and \((\partial \phi/\partial y)\) by (3.36) for element \(e\), the Darcy velocity components \(q_{e,x}\) and \(q_{e,y}\) in \(x\) and \(y\) directions for element \(e\) are numerically calculated by (3.15) and (3.16), respectively. The Darcy velocity has a unit of \([\text{m}^3\text{ of water}/(\text{m}^2\text{ of medium} \cdot \text{time})]\), and is defined as the volume of water flowing per unit time through a unit cross-sectional area normal to the direction of flow.

Figure 3.21 shows a numerical result for Darcy velocity distribution obtained for the FBC in Figure 3.13. In this figure, Darcy velocity in the buffer region cannot be identified due to very small magnitude compared to that in the FBC \((i.e., \text{about 9 order difference})\). An arrow starts at the center of weight of each element. The length of an arrow indicates the magnitude of Darcy velocity, while the direction of the arrow indicates the flow direction at that point. The magnitude of the Darcy velocity is obtained by \(\sqrt{q_{e,x}^2 + q_{e,y}^2}\) for element \(e\). The flow direction at the center of weight for element \(e\) is obtained by \(\tan^{-1}(q_{e,y}/q_{e,x})\). For \(q_{e,x}>0\), the flow direction is \(\theta_{e,f}\) measured against the positive \(x\) axis, whereas the flow direction is \(\theta_{e,f}\) measured against the negative \(x\) axis for \(q_{e,x}<0\). Value of angle increases counter-clockwise from the axis.

To obtain the statistics of total discharges, calculations should be repeated for many realizations of fracture networks. Calculation time depends on the number of realizations, the number of fractures, the number of finite elements, and the user’s computing system.

A computer code, FFDF (Finite-element Flow and transport code for Discrete-Fracture networks), has been developed for the processes described in Section 3.3, Section 3.4, and Section 3.5. The code also includes statistical routines for many realizations. The features of FFDF are described in Appendix D.
3.5.3 Finite-Element Mesh Size

The size of finite-element mesh (i.e. triangular elements) should be determined by considering (1) the numerical errors due to finite element approximation, and (2) the size of the representative elementary volume (REV) [Bear, 1972] for the equivalent porous medium. From the viewpoint (1), numerical errors can be diminished by decreasing the size of elements, or by increasing the number of elements [Huebner, 1975]. From the viewpoint (2), elements must have sufficiently large volumes to define the REV. Two viewpoints (1) and (2) give opposite effects on numerical results.

A numerical experiment has been performed to determine proper size of elements by considering two viewpoints. Four different sizes of meshes are considered. Figure 3.22 shows the domain discretization by four different sizes of meshes for the same fracture network in Figure 3.13.

Figure 3.22 Domain discretization by four different sizes of mesh.
Table 3.2  Mesh Size Effect on Water Flow Calculation

<table>
<thead>
<tr>
<th>Case</th>
<th>Number of nodes*</th>
<th>Number of elements*</th>
<th>Total discharge at the outer boundary [m²/yr]</th>
<th>Normalized CPU time with 2 sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>68</td>
<td>110</td>
<td>2.65E+02</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>166</td>
<td>276</td>
<td>2.48E+02</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>477</td>
<td>805</td>
<td>2.69E+02</td>
<td>6</td>
</tr>
<tr>
<td>4</td>
<td>1471</td>
<td>2268</td>
<td>2.79E+02</td>
<td>73.5</td>
</tr>
</tbody>
</table>

*: Values for the NFR and the buffer regions

The values of total discharge at the outer boundary are calculated with four different sizes of finite-element meshes for the same fracture network. Numerical results are summarized in Table 3.2. A personal computer with Pentium III-500MHz and 128M-memory is used to measure CPU time.

The mesh size used in case 3 in Table 3.2 (Figure 3.22 (c)) can be selected because the CPU time increases significantly between cases 3 and 4 whereas relatively small difference in the numerical result for the total discharge at the outer boundary is observed.

Among four cases, case 3 in Table 3.2 is the best choice with respect to the viewpoint (1). Now, the viewpoint (2) is considered for the case 3. A hypothesis given by Matheron [1967] is adopted in this study. Matheron [1967] claimed that if global hydraulic conductivity \( K_{global} \) lies between arithmetic mean \( (K_a) \) and geometric mean \( (K_q) \) of the hydraulic conductivities measured in some small scale, i.e.,

\[
K_a \leq K_{global} \leq K_q ,\tag{3.51}
\]

then, the medium of the small scale can be treated as an equivalent continuum. Dagan [1986] and Cacas, et al., [1990(a)] used this hypothesis to determine the proper size of measurements for their models.

For case 3 in Table 3.2, \( K_{global} \) for the NFR is obtained as 1.37x10\(^{-5}\) m/s by (3.10) applying the uniformization (Section 3.4.2). \( K_a=9.66x10^{6} \) m/s and \( K_q= 5.55x10^{3} \) m/s for the NFR are also calculated from the values of the hydraulic conductivity for all triangular elements included in the FBC, which are obtained by (3.6) for each element applying the local homogenization (Section 3.4.1).

The results show that case 3 in Table 3.2 satisfy the inequality (3.51). Thus, triangular elements used in case 3 in Table 3.2 can be treated as an equivalent continuum, and will be used for water flow analysis in this chapter and particle transport analysis in Chapter 5.

3.6 Numerical Results

In this section, numerical explorations are made by FFDF to investigate: (1) fracture network generation and occurrence of FBC, (2) effects of the heterogeneity of NFR on water flow rate, and (3) effects of the modeling approach for NFR on water flow rate.

3.6.1 Fracture Network Generation and Occurrence of FBC

Three different sets of statistics of the fracture geometry parameters are considered for generation of fracture networks in the NFR as shown in Table 3.3 based on Table 2.3. The spatial distributions given in Table 2.3 are used for the location of fractures, i.e. \( (r,q) \) in Figure 3.2. The distributions of the length, aperture, and orientation of the secondary fractures are assumed to be same as those for the primary fractures. The number of the secondary fractures is assumed to be 30% of that of the total number of fractures [Gylling, 1997].

Table 3.3  Statistics of the Fracture Geometry Parameters for Three Curves in Figure 3.25.

<table>
<thead>
<tr>
<th>Case</th>
<th>Fracture length ( (l) )</th>
<th>Aperture ( (b) )</th>
<th>Orientation ( (\theta) )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean [m]</td>
<td>SD [m]</td>
<td>Dis</td>
</tr>
<tr>
<td>1</td>
<td>1.65</td>
<td>2.16</td>
<td>LN</td>
</tr>
<tr>
<td>2</td>
<td>3.02</td>
<td>0.30</td>
<td>LN</td>
</tr>
<tr>
<td>3</td>
<td>1.01</td>
<td>0.10</td>
<td>LN</td>
</tr>
</tbody>
</table>

Dis: Distribution; LN: Lognormal; SD: Standard deviation; \( \alpha_L \): Shape parameter; \( \beta_L \): Scale parameter
The connectivity is used as a measure to characterize the fractured media in this study. The connectivity is defined as the ratio of the total number of intersections to the total number of fractures in this study. For two intersected fractures, the connectivity is calculated as 0.5 in this study since the number of intersections is counted as 1, and the number of fractures is 2.

In Figure 3.23, the relationship between the connectivity and the number of fractures is illustrated for the statistics of fracture parameters of case 2 in Table 3.3. Three different realizations (I, II, and III) are shown in Figure 3.23. \( N_f \) represents the number of fractures at which the first FBC occurs. Figure 3.23 (a) and (b) show the relationship for two different ranges of the number of fractures from 0 to 30, and from 0 to 200, respectively.

Whenever a fracture is added in the model space, the connectivity is calculated, and percolation, \( \text{i.e.} \), occurrence of the first FBC, is checked. It is shown in Figure 3.23 that the number of fractures for the first FBC to occur is quite different from realization to realization. In realization I, the first intersection occurs when the fifth fracture is added. Thus, the connectivity is zero until the 5th fracture is added. It increases to 0.2 (=1 intersection/5 fractures) at the addition of the 5th fracture. The connectivity between the 6th and 8th fractures decreases, because the added fractures do not intersect others. The connectivity increases to 4/9 at the addition of the 9th fracture because it intersects with 3 exiting fractures. For three realizations, the first FBC occurs at the 5th, 26th, and 56th fractures, respectively, and the corresponding values of connectivity are 0.2, 0.88, and 1.71, respectively. The connectivity at which the FBC occurs for the first time is called the threshold connectivity in this study.

Figure 3.24 (a), (b), and (c) show the frequency of the threshold connectivity for cases 1, 2 and 3 in Table 3.3, respectively. 500 realizations have been made for each case shown in Table 3.3. In Figure 3.24 (a), the threshold connectivity is observed to be zero for 19 out of 500 realizations. This means that the percolation occurs without intersection of fractures. In this zero threshold connectivity case, only one fracture connects the outer boundary with the interface without any intersection with other fractures.

Cumulative distribution functions (CDFs) of the threshold connectivity for three cases in Table 3.3 are shown in Figure 3.25. Case 1 is characterized as short fractures with a large standard deviation. Long fractures can be generated due to the large standard deviation. For case 2, long fractures with the small standard deviation are assumed. So, fractures have length close to the mean length. For case 3, short fractures with the small standard deviation are assumed. Fractures are short and close to mean length due to the small standard deviation.

Due to the 19 realizations, for which the threshold connectivity was observed to be zero in Figure 3.24 (a), CDF of case 1 is 0.038 at the zero connectivity. At the threshold connectivity of 1.2, CDF becomes unity. It means that FBC must exist if the connectivity is greater than 1.2 for 500 realizations. For case 2, because long fractures (~3.0 m) are generated, percolation occurs at smaller connectivity than for case 3 where short fractures are generated. CDF reaches unity at connectivity of 1.7 and 2.2 for cases 2 and 3, respectively.
Figure 3.24  Frequency for the threshold connectivity for three cases in Table 3.3

Figure 3.25  CDF for FBC occurrence. Labels 1, 2, and 3 indicate the cases shown in Table 3.3

3.6.2  Effects of Heterogeneity of NFR on Flow Rate

Nine cases shown in Table 3.4 have been selected to represent the heterogeneity of NFR based on the CDF of the threshold connectivity in Figure 3.25. Three cases are set for each curve in Figure 3.25. For example, cases A, B, and C are determined by the curve 1 in Figure 3.25. The values of connectivity are set as 1.2, 3.0, and 6.0, respectively. Because at the connectivity of 1.2, the probability that the FBC occurs is 1 in cases A, B, and C, a FBC will be generated.

For one realization, fractures are generated based on statistical distributions of the fracture geometry parameters. Whenever a fracture is added in the model space, the connectivity is calculated by FFDF code. Fractures are added until the predetermined connectivity (i.e. 1.2 for case A) is reached. Then, total discharges $Q$ [m$^3$/yr] at the outer boundary ($r=R_2$) and at the interface ($r=R_0$) are calculated by FFDF code.

<table>
<thead>
<tr>
<th>Case in Table 3.3</th>
<th>Case</th>
<th>Connectivity</th>
<th>Length ($l$)</th>
<th>Orientation ($\theta$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Mean [m]</td>
<td>SD [m]</td>
<td>$\beta_L$ [m]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>A</td>
<td>1.2</td>
<td>1.65</td>
<td>2.16</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>3.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>6.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>D</td>
<td>1.7</td>
<td>3.02</td>
<td>0.30</td>
</tr>
<tr>
<td></td>
<td>E</td>
<td>3.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>F</td>
<td>6.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>G</td>
<td>2.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H</td>
<td>3.0</td>
<td>1.01</td>
<td>0.10</td>
</tr>
<tr>
<td></td>
<td>I</td>
<td>6.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Dis: Distribution; LN: Lognormal; SD: Standard deviation
3.6.2.1 Determination of the number of realizations

Because a statistical approach has been applied, numerical results should be expressed not by a single number but by a range of values. In order to determine the number of realizations for statistically meaningful results, the total discharges at the outer boundary and at the interface have been calculated for five different numbers of realizations $N_r$=20, 50, 100, 500, and 1000.

Table 3.5 Statistical Results of Total Discharges at the Outer Boundary and at the Interface for a Model with a Heterogeneous NFR for Different Number of Realizations for Case E in Table 3.4.

<table>
<thead>
<tr>
<th>$N_r$</th>
<th>Total discharge at the outer boundary [m²/yr]</th>
<th>Total discharge at the interface [m²/yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean Standard deviation</td>
<td>Mean Standard deviation</td>
</tr>
<tr>
<td>20</td>
<td>7.15E+02 1.22E+03</td>
<td>3.35E-07 1.62E-07</td>
</tr>
<tr>
<td>50</td>
<td>6.09E+02 9.80E+02</td>
<td>4.88E-07 2.28E-07</td>
</tr>
<tr>
<td>100</td>
<td>3.88E+02 2.80E+02</td>
<td>4.19E-07 1.92E-07</td>
</tr>
<tr>
<td>500</td>
<td>5.84E+02 9.97E+02</td>
<td>4.19E-07 2.13E-07</td>
</tr>
<tr>
<td>1000</td>
<td>4.65E+02 5.59E+02</td>
<td>4.12E-07 1.99E-07</td>
</tr>
</tbody>
</table>

Table 3.5 shows the total discharges at the outer boundary and at the interface for five different numbers of realizations for case E in Table 3.4. The differences of the total discharges at the outer boundary and at the interface for 5 different numbers of realizations are not significant. In this study, the number of realizations for the water flow and particle transport analyses is selected as 100.

3.6.2.2 Effect of Length distribution

To investigate effects of the heterogeneity of the NFR, water flow analysis has been performed for 100 realizations for selected 9 cases shown in Table 3.4 for a model with a heterogeneous NFR by the local homogenization. In this section, aperture of a fracture segment is generated based on the given lognormal distribution as shown in Table 3.3.

Figure 3.26 (a), (b), and (c) show the CDFs of the total discharge at the outer boundary for cases A, B, and C, cases D, E, and F, and cases G, H, and I, respectively. Figure 3.27 shows a generated network, FBC, triangular mesh generation over the FBC and buffer, and Darcy velocity distribution for a realization which gives the most probable total discharge of water (indicated by dots in Figure 3.26) for each case.

![CDF of total discharge at the outer boundary for a model with a heterogeneous NFR by the local homogenization for 9 cases in Table 3.4.](image)

For case A in Figure 3.26 (a), the total discharge at the outer boundary ranges widely from $6.53\times10^0$ to $2.97\times10^3$ [m²/yr] because of irregular shape of FBC due to the large standard deviation of the fracture length. As shown in Figure 3.27, the network is sparse because the connectivity is as small as 1.2. By increasing the connectivity to 3.0 (Case B) and to 6.0 (Case C) with the same fracture length distribution, the network becomes better connected and covers a greater area of the model space. As shown in Figure 3.26 (a), the total discharges for case B and C are distributed more narrowly than that of case A. Figure 3.26 (a) also shows that the network with a greater connectivity has a greater total discharge because a larger amount of water can flow through a medium with more fractures. Same trends are observed for other cases in Figure 3.26 (b) and (c).

Let us compare cases C, F, and I with the connectivity 6.0 in Figure 3.26. Due to the large standard deviation of the length distribution for case C, the smaller number of fractures is required to obtain the connectivity of 6.0. Total discharges at the outer boundary for case C are smaller than those of case I because the network for case I
contains more fractures than those of case C. Due to the small standard deviation of the length distribution for case I, the network consists of short fractures of nearly equal length. The total discharge at the outer boundary for case I is distributed more narrowly between 1.13×10^3 m^3/yr and 3.03×10^3 m^3/yr. This is confirmed by the steeper slope for case I than that for case C in Figure 3.26 (a) and (c).

Due to the small standard deviation (or shape factor) of the length distributions both for cases F and I, the networks consist of nearly equal length fractures. More fractures are required to obtain the connectivity of 6.0 for case I than case F due to a smaller mean length for case I. As a result, total discharges for case I are larger than that of case F due to the fact that the network contains more fractures for case I than for case F. The total discharges at the outer boundary for case I range more narrowly than those of case F. A steeper slope for case I is also observed than that for case F in Figure 3.26 (b) and (c).

### Table 3.6 Statistical Results of Total Discharges for 100 Realizations at the Outer Boundary and at the Interface for a Model with a Heterogeneous NFR by the Local Homogenization for 9 cases

<table>
<thead>
<tr>
<th>Case</th>
<th>Mean discharge at the outer boundary [m^3/yr]</th>
<th>Mean discharge at the interface [m^3/yr]</th>
<th>Mean water mean residence time in buffer [yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1.65E+02</td>
<td>3.85E+02</td>
<td>2.07E+06</td>
</tr>
<tr>
<td>B</td>
<td>7.48E+02</td>
<td>5.00E+02</td>
<td>2.27E+06</td>
</tr>
<tr>
<td>C</td>
<td>1.34E+03</td>
<td>1.55E+03</td>
<td>2.54E+06</td>
</tr>
<tr>
<td>D</td>
<td>1.10E+02</td>
<td>1.31E+02</td>
<td>2.36E+06</td>
</tr>
<tr>
<td>E</td>
<td>3.12E+02</td>
<td>2.80E+02</td>
<td>1.98E+06</td>
</tr>
<tr>
<td>F</td>
<td>8.33E+02</td>
<td>7.96E+02</td>
<td>2.32E+06</td>
</tr>
<tr>
<td>G</td>
<td>2.95E+02</td>
<td>2.50E+02</td>
<td>4.07E+06</td>
</tr>
<tr>
<td>H</td>
<td>6.76E+02</td>
<td>5.32E+02</td>
<td>3.01E+06</td>
</tr>
<tr>
<td>I</td>
<td>1.58E+03</td>
<td>3.49E+02</td>
<td>3.54E+06</td>
</tr>
</tbody>
</table>

Table 3.6 shows the results of the total discharges at the outer boundary and at the interface for a model with a heterogeneous NFR for 100 realizations for 9 cases. The median, mean and standard deviation are given in Table 3.6.

The total discharges at the interface are about 9 orders of magnitude smaller than those at the outer boundary (Table 3.6). It means that the water flow in the buffer region is very slow. This is due to the assumed small hydraulic conductivity (2.3×10^-14 m/s) for the buffer.

To confirm the slow water flow in the buffer, the water residence time in the buffer is calculated as follows. The volume of the pores in the cylindrical buffer per unit height with the outer radius R_0 of 1 m, the inner radius of 0.35 m, and the porosity of 0.3 is calculated as 0.83 m^3. The total volumetric water flow rate [m^3/yr] through the buffer is calculated by multiplying the total discharge Q [m^3/yr] at R_0 by unit depth, 1 [m]. The residence time is obtained by dividing 0.83 m^3 by the volumetric flow rate Q · 1 [m^3/yr]. The results are shown in the right-most column of Table 3.6.

In Figure 3.28, the relationship between the total discharge at the outer boundary for a model with a heterogeneous NFR by the local homogenization and the connectivity is shown, based on the numerical results for the nine cases. Mark ■ in Figure 3.28 represents the median of the total discharges at the outer boundary for 100 realizations. An error bar for the 90% confidence interval is shown. The lower limits and the upper limits are the values at the cumulative probability of 0.05 and 0.95, respectively, in Figure 3.26 (a), (b) and (c). Observations from Figure 3.28 are as follows.

First, compare three cases with the same length statistics shown in Table 3.3, i.e., compare cases A, B with C, cases D, E, with F, and cases G, H, with I. As the connectivity increases, the total discharge increases because water can flow through more fractures. For the same length statistics, a greater connectivity is achieved by adding more fractures.

Second, the error bar of total discharges at the outer boundary decreases, as the connectivity increases. With more fractures, the FBC becomes more homogeneous, resulting in a narrower distribution of the total discharge.

Third, case E has a wider error bar of the total discharge than those of cases B and H. Although case E has the same connectivity as case B and H, the number of fractures to obtain the connectivity of 3.0 is smaller than others due to the generation of longer fractures. Because the FBC consists of long fractures, areas where no fractures exist occur inside the FBC. Due to these areas for case E, the medium is more heterogeneous than others with the same connectivity. Therefore, the error bar is wider than that of others. Same observation can be made for case F in comparison with cases C and I.

40
Figure 3.27 Fracture networks, FBCs, and Finite element mesh, and Darcy velocity distribution for a selected realization for 9 cases.
3.6.2.3 Effects of Aperture Correlation

Aperture of a fracture segment is generated based on the given lognormal distribution in the previous section. In this section, aperture is determined based on the relationship (2.7) between the length and aperture [Ohno, et al., 1987] after the value for the length is sampled. Other parameters and distributions are kept the same as shown in Tables 3.4. Cases A and B in Table 3.4 have been selected because fracture length has a wide variation due to the greater standard deviation (2.16 m) than those assumed in cases D, E, F, G, H, and I.

Table 3.7 Statistical Results of Total Discharges for 100 Realizations at the Outer Boundary and at the Interface for a Model with a Heterogeneous NFR by the Local Homogenization for Correlated Aperture Cases

<table>
<thead>
<tr>
<th>Case</th>
<th>Total discharge at the outer boundary [m²/yr]</th>
<th>Total discharge at the interface [m²/yr]</th>
<th>Water mean residence time in buffer [yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Median</td>
<td>Mean</td>
<td>Standard deviation</td>
</tr>
<tr>
<td>A</td>
<td>5.24E+05 (1.65E+02)</td>
<td>4.81E+06 (2.56E+02)</td>
<td>2.15E+07 (3.85E+02)</td>
</tr>
<tr>
<td>B</td>
<td>1.61E+06 (7.48E+02)</td>
<td>4.07E+06 (8.87E+02)</td>
<td>7.88E+06 (5.00E+02)</td>
</tr>
</tbody>
</table>

The values in parentheses are for uncorrelated case, same as in Table 3.6.

Figure 3.28 Total discharges at the outer boundary by the local homogenization for 9 cases with 90% confidence intervals

(a) Case A (correlated and uncorrelated aperture)  (b) Case B (correlated and uncorrelated aperture)

Figure 3.29 CDF of total discharge at the outer boundary for a model with a heterogeneous NFR for cases A and B (correlated and uncorrelated)
Table 3.8  Total Discharges of a Particular Realization for Cases A and B with the Correlated Aperture in Figure 3.30 (b) and (d)

<table>
<thead>
<tr>
<th>Case</th>
<th>Total discharge at $r=R_2$ [m$^3$/yr]</th>
<th>Total discharge at $r=R_0$ [m$^3$/yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1.63E+05</td>
<td>5.13E-07</td>
</tr>
<tr>
<td>B</td>
<td>3.22E+06</td>
<td>8.16E-07</td>
</tr>
</tbody>
</table>

Figure 3.30  Darcy velocity distributions in the model space both for correlated and uncorrelated cases

Total discharges for a model with a heterogeneous NFR for the cases with aperture-length correlation are shown in Table 3.7. Figure 3.29 shows the CDF of the total discharge at the outer boundary for a model with a heterogeneous NFR by the local homogenization both for the cases with or without the length-aperture correlation for cases A and B.

In Figure 3.29, two distinct differences are observed. First, the total discharge at the outer boundary for the correlated case is greater by about 3 to 4 orders of magnitude than those for the uncorrelated case. This difference can be explained as follows. About 1~2 orders of magnitude wider values of aperture can be generated by the correlated case, resulting in about one order greater porosities than those of the uncorrelated case. According to $(3.3)$, the permeability $k$ is proportional to $k\cdot\varepsilon^3/M_s^2$. Because $M_s$ in $(3.5)$ is independent of the aperture, permeability is proportional to the porosity cubed. Thus, about 1 order of magnitude greater porosity results in about 3 orders of magnitude greater permeability (or hydraulic conductivity), and thus total discharges.

Second, the range of total discharge distribution for the correlated case is wider than that for the uncorrelated case. Because long fractures have greater apertures in the correlated case, water flows mainly through a few long fractures, whereas water flow in the uncorrelated case is more averaged over the FBC. Due to this difference, the
flow becomes more heterogeneous for the correlated case. Thus, total discharges at the outer boundary for the correlated case are distributed more widely than those of the uncorrelated case.

Figure 3.30 depicts the Darcy velocity distributions both for the correlated and uncorrelated cases for a particular realization for cases A and B shown in Figure 3.27. Table 3.8 shows the total discharges of a particular realization for cases A and B with the correlated aperture in Figure 3.30 (b) and (d).

3.6.3 Effect of Modeling Approach for NFR on Flow Rate

In this section, to investigate effects of the modeling approach for the NFR, water flow analysis has been performed for a model with a homogenized NFR by the uniformization. Aperture of a fracture segment is generated based on the given lognormal distribution as shown in Table 3.3.

Table 3.9 Total Discharges at the Outer Boundary for a Model with a Heterogeneous NFR and a Model with a Homogenized NFR for 100 Realizations for 9 cases

<table>
<thead>
<tr>
<th>Case</th>
<th>Total discharge at the outer boundary for a model with a heterogeneous NFR by the local homogenization [m²/yr] (Same as values in Table 3.6)</th>
<th>Total discharge at the outer boundary for a model with a homogenized NFR by the uniformization [m²/yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Median</td>
<td>Mean</td>
</tr>
<tr>
<td>A</td>
<td>1.65E+02</td>
<td>2.56E+02</td>
</tr>
<tr>
<td>B</td>
<td>7.48E+02</td>
<td>8.87E+02</td>
</tr>
<tr>
<td>C</td>
<td>1.34E+03</td>
<td>1.52E+03</td>
</tr>
<tr>
<td>D</td>
<td>1.10E+02</td>
<td>1.95E+02</td>
</tr>
<tr>
<td>E</td>
<td>3.12E+02</td>
<td>3.88E+02</td>
</tr>
<tr>
<td>F</td>
<td>8.33E+02</td>
<td>1.02E+03</td>
</tr>
<tr>
<td>G</td>
<td>2.95E+02</td>
<td>3.58E+02</td>
</tr>
<tr>
<td>H</td>
<td>6.76E+02</td>
<td>8.08E+02</td>
</tr>
<tr>
<td>I</td>
<td>1.58E+03</td>
<td>1.65E+03</td>
</tr>
</tbody>
</table>

Total discharges at the outer boundary for a model with a homogenized NFR by the uniformization have been calculated for 100 realizations for nine cases in Table 3.4. Table 3.9 shows the total discharges at the outer boundary both for a model with a heterogeneous NFR by the local homogenization and for a model with a homogenized NFR by the uniformization for 100 realizations for 9 cases.

Figure 3.31 Comparison of the 90% confidence intervals of total discharges at the outer boundary between a model with a homogenized NFR by the uniformization (thick lines) and a model with a heterogeneous NFR by the local homogenization (thin lines) for 9 cases.
Figure 3.31 shows the comparison of the 90% confidence intervals of total discharges at the outer boundary between a model with a homogenized NFR (thick lines) and a model with a heterogeneous NFR (thin lines) for 9 cases. Symbols ♦ and ▲ represent the median of the total discharges at the outer boundary for 100 realizations for each case for a heterogeneous NFR and for a homogenized NFR, respectively. Characteristics for each case for a homogenized NFR shown in Figure 3.31 are similar to those for a heterogeneous NFR as shown in Figure 3.28. Observations from the comparison of the Figure 3.31 with Figure 3.28 are as follows.

First, the total discharge at the outer boundary for a homogenized NFR distributes more narrowly than those for a heterogeneous NFR. This is because hydraulic properties for a heterogeneous NFR are spatially distributed over the FBC in the domain whereas they are single values over the entire NFR for a homogenized NFR after transformation by the uniformization.

Second, the ranges of the total discharge distributions for each case for a homogenized NFR are within the ranges obtained for a heterogeneous NFR. The median values are very close to each other.

### 3.7 Conclusions

A two-dimensional near-field model incorporating the heterogeneity of the near-field rock (NFR) for the groundwater flow for the one-waste canister configuration has been developed for the time-independent, incompressible Darcy’s flow through a fracture network. A flow-bearing cluster (FBC) of fractures is extracted from the discrete fracture network (DFN) by checking the interconnectivity of fractures. The FBC is transformed into a heterogeneous continuum by the local homogenization and a homogeneous continuum by the uniformization. The Kozeny-Carman equation is used to calculate the permeability for a transformed continuum. A finite element solution has been derived for the spatial distribution of the hydraulic potential in the FBC. A computer code, FFDF, has been developed.

Relationship between the threshold connectivity and the number of fractures has been numerically explored. For a given set of distribution functions for fracture geometry parameters, a threshold connectivity beyond which a fracture network in NFR always contains at least one FBC has been determined. The FBC is considered to be more heterogeneous if the value of the connectivity is closer to the threshold connectivity. As the connectivity increases, the FBC becomes less heterogeneous.

Effects of the heterogeneity of the NFR have been investigated by performing the water flow analysis for different sets of statistics of fracture geometry parameters.

Numerical results show that:

- A network with a greater connectivity exhibits a greater total discharge because a larger amount of water can flow through the medium with more fractures (see Figure 3.28).
- The total discharge at the outer boundary ranges more narrowly as the connectivity of the network increases (see Figure 3.28).
- For two networks with the same connectivity, the total discharge ranges more widely with the network consisting of long fractures than with the network consisting of short fractures (see Figure 3.28).
- The residence time of water in the buffer region is extremely long due to the assumed low hydraulic conductivity for the bentonite ($K=2.3\times10^{-14}\text{m/s}$), compared with that in NFR (see Table 3.6).

Effects of modeling approaches for the NFR are investigated by comparing the groundwater flow rates between the model with a heterogeneous NFR by local homogenization and the model with a homogenized NFR by uniformization.

Numerical results show that:

- The total discharge at the outer boundary obtained for a homogenized NFR distributes more narrowly than that obtained for a heterogeneous NFR (see Figure 3.31).
- The homogenized NFR does not necessarily overestimate the total discharge of water (see Figure 3.31).
- The median values of the total discharges obtained for the homogenized NFR and the heterogeneous NFR are close to each other (see Figure 3.31).

For the NFR hosting a geologic repository, a small connectivity (or, highly heterogeneous rock) is desirable. For highly heterogeneous fractured rock, the homogenized NFR cannot reproduce high and low tails of the flow rate distribution, and does not necessarily overestimate the water flow rate. Thus, the homogeneous medium by the uniformization may not be an appropriate approach to simulate the water flow in highly fractured rock.

### 3.8 Limitations

The current model for the water flow analysis has following limitations:
- A two-dimensional analysis tends to underestimate the permeability because fractures not connected to the network in the plane of analysis may be connected in the third dimension [Long, 1985].
- Processes affecting the EBS by groundwater (i.e. corrosion, bentonite swelling, heat generated by waste) are neglected.
- Effects of multiple canisters [Ahn et al., 1998; Kawasaki, et al., 2001] are not considered.
- Coefficient $C$ in the Kozeny-Carman equation including tortuosity correction is neglected by assuming $C=1$. Coefficient $C$ will be discussed in Chapter 6 in detail.
4. Mathematical Model for Water Flow Analysis in the Near Field

4.1 Introduction

This chapter establishes a mathematical model to partially verify the flow model developed in Chapter 3. A mathematical model consists of an impermeable waste canister, a homogeneous buffer, and a homogenized NFR by the uniformization (Section 3.4.2).

An analytical solution of the steady-state potential distribution is formulated for the mathematical model. With analytically obtained potential distribution in the model space, a distribution of the stream functions can be obtained analytically. Then, the water flow rate through the model space is calculated from the distribution of stream functions and hydraulic conductivity of the region of interest. The comparisons of the results obtained by numerical model with those obtained by analytical solutions have been made for some specific cases.

The objectives of this chapter are (1) to formulate analytical solutions of the potential distribution and stream functions for the mathematical model, and (2) to verify partially a numerical model developed in Chapter 3 by the mathematical model.

4.2 Mathematical Problem and Solution of Potential Equation

The model space ($\Omega=\Omega_1+\Omega_2$) in Figure 4.1 consists of two homogeneous sub-domains, $\Omega_1$ with $K_1=\text{const}$, and $\Omega_2$ with $K_2=\text{const}$. The variables used for obtaining the analytical solutions for the potential head and the stream functions are dimensionless, $[\phi_1, \phi_2, \psi_1, \psi_2, r, \theta, R_0, R_1, R_2, K_1, K_2]=1$. The potential head is prescribed arbitrarily as $f(\theta)$ at $r=R_2$. The flux is prescribed zero at $r=R_1$.

![Figure 4.1 Model space for the mathematical model.](image)

$\phi$ satisfying $\nabla^2\phi=0$ in $\Omega$ cannot be solved because $K$ is discontinuous along $r=R_0$. Therefore, the problem is decomposed into two sub-problems, denoting the potential in $\Omega_1$ by $\phi_1$, and in $\Omega_2$ by $\phi_2$. Simultaneous solutions are then sought for $\phi_1$ and $\phi_2$, satisfying the considered partial differential equation in their respective sub-domains, and specified boundary conditions at $r=R_1$ (for $\phi_1$), and $r=R_2$ (for $\phi_2$) [Bear, 1979].

Governing equations are

$$\nabla^2\phi_1 = r \frac{\partial}{\partial r} \left( r \frac{\partial \phi_1}{\partial r} \right) + \frac{\partial^2 \phi_1}{\partial \theta^2} = 0, \text{ in } \Omega_1 \ (R_1 < r < R_2, \ 0 < \theta < 2\pi), \quad (4.1)$$

and

$$\nabla^2\phi_2 = r \frac{\partial}{\partial r} \left( r \frac{\partial \phi_2}{\partial r} \right) + \frac{\partial^2 \phi_2}{\partial \theta^2} = 0, \text{ in } \Omega_2 \ (R_0 < r < R_1, \ 0 < \theta < 2\pi). \quad (4.2)$$
The forms of the solutions for (4.1) and (4.2) are highly dependent on that of \( f(\theta) \), which is any periodic, piecewise continuous, and piecewise differentiable function [Hildebrand, 1950]. For example, if \( f(\theta) \) is just a constant, then the solution should be angle \((\theta)\) independent. If \( f(\theta) \) is the function of cosine, then the solution is also responded with the function of cosine.

The potential head, \( \phi \), has been prescribed at \( r=R_2 \) arbitrarily as

\[
\phi_j(R_j, \theta) = f(\theta), \quad 0 \leq \theta < 2\pi. \tag{4.3}
\]

No flux boundary is assumed at \( r=R_1 \),

\[
\frac{\partial \phi}{\partial r} = 0, \quad \text{at} \quad r = R_1, \quad 0 \leq \theta < 2\pi. \tag{4.4}
\]

At the interface \((r=R_0)\), the elevation head and pressure head are the same when a point on the interface is approached from both sides [Bear, 1979].

\[
\phi_j(R_0, \theta) = \phi_i(R_0, \theta), \quad \text{at} \quad 0 \leq \theta < 2\pi. \tag{4.5}
\]

Continuity of flux across the interface is expressed through the components of the specific discharge normal \((r \text{ direction in polar coordinates)}\) to the interface [Bear, 1979].

\[
K_i \frac{\partial \phi_i}{\partial r} = K_j \frac{\partial \phi_j}{\partial r}, \quad \text{at} \quad r = R_0, \quad 0 \leq \theta < 2\pi. \tag{4.6}
\]

General solutions for (4.1) and (4.2) are shown in (4.7) and (4.8), respectively [Hildebrand, 1950].

\[
\phi_1(r, \theta) = \left[ (A_0 + B_0 \ln r) \cdot (C_0 + D_0 \theta) \right] + \sum_{n=1}^{\infty} \left[ (a_n r^n + b_n r^{-n}) \cos n\theta + (c_n r^n + d_n r^{-n}) \sin n\theta \right], \tag{4.7}
\]

\[
R_i \leq r \leq R_0, \quad 0 \leq \theta < 2\pi , \quad n=1, 2, 3, \ldots , \quad A_0, B_0, C_0, D_0 \text{ are constant},
\]

\[
\phi_2(r, \theta) = \left[ (E_0 + F_0 \ln r) \cdot (G_0 + H_0 \theta) \right] + \sum_{n=1}^{\infty} \left[ (e_n r^n + f_n r^{-n}) \cos n\theta + (g_n r^n + h_n r^{-n}) \sin n\theta \right], \tag{4.8}
\]

\[
R_0 \leq r \leq R_j, \quad 0 \leq \theta < 2\pi , \quad n=1, 2, 3, \ldots , \quad E_0, F_0, G_0, H_0 \text{ are constant}.
\]

In order that \( \phi(r,\theta) \) be single-valued in the domain, the following must be taken [Hildebrand, 1950],

\[
D_0 = H_0 = 0. \tag{4.9}
\]

If \( D_0 \) and \( H_0 \) are not equal to zero, there are no unique solution because \( \phi \) gives different values for \( \theta=2\pi n + \theta_0 \), where \( \theta_0 \) is an arbitrary angle between 0 and \( 2\pi \), and \( n \) is the integer.

Substituting (4.9) into (4.7), (4.8) gives

\[
\phi_1(r, \theta) = \left[ a_0 + b_0 \ln r \right] + \sum_{n=1}^{\infty} \left[ (a_n r^n + b_n r^{-n}) \cos n\theta + (c_n r^n + d_n r^{-n}) \sin n\theta \right], \tag{4.10}
\]

\[
R_i \leq r \leq R_0, \quad 0 \leq \theta < 2\pi , \quad n=1, 2, 3, \ldots, \quad a_0 = A_0 C_0, \quad b_0 = B_0 C_0,
\]

\[
\phi_2(r, \theta) = \left[ e_0 + f_0 \ln r \right] + \sum_{n=1}^{\infty} \left[ (e_n r^n + f_n r^{-n}) \cos n\theta + (g_n r^n + h_n r^{-n}) \sin n\theta \right], \tag{4.11}
\]

\[
R_0 \leq r \leq R_j, \quad 0 \leq \theta < 2\pi , \quad n=1, 2, 3, \ldots , \quad e_0 = E_0 G_0, \quad f_0 = F_0 G_0.
\]

Using the BC (4.3),

\[
f(\theta) = \left[ e_0 + f_0 \ln R_j \right] + \sum_{n=1}^{\infty} \left[ (e_n R_j^n + f_n R_j^{-n}) \cos n\theta + (g_n R_j^n + h_n R_j^{-n}) \sin n\theta \right], \quad 0 \leq \theta < 2\pi \tag{4.12}
\]

Using the BC (4.4),
\[ 0 = \left( \frac{b_o}{R_i} \right) + \sum_{n=1}^{\infty} n \left[ (a_n R_i^{n+1} - b_n R_i^{-n}) \cos n\theta + (c_n R_i^{n+1} - d_n R_i^{-n}) \sin n\theta \right], \quad 0 \leq \theta < 2\pi \quad (4.13) \]

Using the BC (4.5),
\[ \left[ a_o + b_o \ln R_o \right] + \sum_{n=1}^{\infty} n \left[ (a_n R_o^{n+1} + b_n R_o^{-n}) \cos n\theta + (c_n R_o^{n+1} + d_n R_o^{-n}) \sin n\theta \right] = \left[ e_o + f_o \ln R_o \right] + \sum_{n=1}^{\infty} n \left[ (e_n R_o^{n+1} + f_n R_o^{-n}) \cos n\theta + (g_n R_o^{n+1} + h_n R_o^{-n}) \sin n\theta \right], \quad 0 \leq \theta < 2\pi \quad (4.14) \]

Using the BC (4.6),
\[ K_o \left[ \frac{b_o}{R_o} \right] + \sum_{n=1}^{\infty} n \left[ (a_n R_o^{n+1} - b_n R_o^{-n}) \cos n\theta + (c_n R_o^{n+1} - d_n R_o^{-n}) \sin n\theta \right] = K_o \left[ \frac{f_o}{R_o} \right] + \sum_{n=1}^{\infty} n \left[ (e_n R_o^{n+1} - f_n R_o^{-n}) \cos n\theta + (g_n R_o^{n+1} - h_n R_o^{-n}) \sin n\theta \right], \quad 0 \leq \theta < 2\pi. \quad (4.15) \]

Equating three coefficients, \( \frac{b_o}{R_i} \), \( (a_n R_i^{n+1} - b_n R_i^{-n}) \), and \( (c_n R_i^{n+1} - d_n R_i^{-n}) \), of constant, \( \sin n\theta \), \( \cos n\theta \), respectively, of right-hand side and zero of left-hand side in (4.13) give (4.16), (4.17), and (4.18) for \( R_i \neq 0 \).

\[ b_o = 0, \quad (4.16) \]
\[ b_o = a_o R_i^{2n}, \quad (4.17) \]
\[ d_o = c_o R_i^{2n}. \quad (4.18) \]

Equating two coefficients of \( \sin n\theta \), \( \cos n\theta \), of left-hand side and right-hand side in (4.14) gives (4.19), (4.20), and (4.21), respectively.

\[ a_o = e_o + f_o \ln R_o, \quad R_o \neq 0, \quad (4.19) \]
\[ f_o = b_o + R_o^{2n} (a_o - e_o), \quad (4.20) \]
\[ h_o = d_o + R_o^{2n} (c_o - g_o). \quad (4.21) \]

Equating three coefficients of constant, \( \sin n\theta \), \( \cos n\theta \), of left-hand side and right-hand side in (4.15) gives (4.22), (4.23), and (4.24), respectively.

\[ f_o = 0, \quad (4.22) \]
\[ R_o^{2n} (K_o a_o - K_o e_o) = K_o h_o - K_o f_o, \quad (4.23) \]
\[ R_o^{2n} (K_o c_o - K_o g_o) = K_o d_o - K_o h_o. \quad (4.24) \]

(4.12) and trigonometric series with Fourier coefficients gives [Hildebrand, 1950]
\[ (e_o + f_o \ln R_o) = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) d\theta, \quad (4.25) \]
\[ (e_o R_o^{n} + f_o R_o^{-n}) = \frac{1}{\pi} \int_0^{2\pi} f(\theta) \cos n\theta \, d\theta, \quad (4.26) \]
\[ (g_o R_o^{n} + h_o R_o^{-n}) = \frac{1}{\pi} \int_0^{2\pi} f(\theta) \sin n\theta \, d\theta. \quad (4.27) \]
Now, there are 12 unknowns \( (a_0, b_0, e_0, f_0, a_n, b_n, c_n, d_n, e_n, f_n, g_n, \text{ and } h_n) \) and 12 equations. To simplify the equations, substituting (4.22) into (4.19) and (4.25) gives, respectively,

\[
a_n = e_0, \quad (4.28)
\]

\[
e_n = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) d\theta, \quad (4.29)
\]

where \( e_0 \) is obtained by integrating \( f(\theta) \) with respect to \( \theta \) from 0 to \( 2\pi \) and dividing by \( 2\pi \).

12 equations are summarized as follows.

\[
b_0 = 0, \quad (4.16)
\]

\[
b_n = a_n R_1^{2n}, \quad (4.17)
\]

\[
d_n = c_n R_1^{2n}, \quad (4.18)
\]

\[
f_n = b_n + R_0^{2n}(a_n - e_n), \quad (4.20)
\]

\[
h_n = d_n + R_0^{2n}(c_n - g_n), \quad (4.21)
\]

\[
f_0 = 0, \quad (4.22)
\]

\[
R_0^{2n}(K_a - K_e) = K_b f - K_f, \quad (4.23)
\]

\[
R_0^{2n}(K_c - K_g) = K_d h - K_h, \quad (4.24)
\]

\[
(e_n R_1^n + f_n R_1^{-n}) = \frac{1}{\pi} \int_0^{2\pi} f(\theta) \cos n\theta d\theta, \quad (4.26)
\]

\[
(g_n R_1^n + h_n R_1^{-n}) = \frac{1}{\pi} \int_0^{2\pi} f(\theta) \sin n\theta d\theta, \quad (4.27)
\]

\[
a_n = e_n, \quad (4.28)
\]

\[
e_n = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) d\theta. \quad (4.29)
\]

To obtain \( e_n \) from (4.26), \( f_n \) should be replaced by the form of \( e_n \). For this, substitution of (4.17) into (4.20) gives,

\[
f_n = a_n R_1^{2n} + R_0^{2n}(a_n - e_n). \quad (4.30)
\]

Substitution of (4.17) and (4.30) into (4.23) gives relationship between \( a_n \) and \( e_n \).

\[
e_n = \frac{\kappa}{2R_0^{2n}} a_n, \quad (4.31)
\]

where

\[
\kappa = \frac{K_2}{K_1} R_0^{2n} + R_0^{2n} + \frac{K_1 - K_2}{K_1} R_1^{2n}, \quad (4.32)
\]

According to the geometry of the model in Figure 4.1, \( R_0 \) is larger than \( R_1 \). Thus variable \( \kappa \) in (4.32) is always larger than zero.

Substitution of (4.31) into (4.30) gives \( f_n \) that is the only function of \( e_n \).
\[ f_n = \left( \frac{2R_n}{\kappa} - (R_n^{(\sigma)} + R_n^{(\tau)}) \right) e_n, \quad \kappa \neq 0. \] (4.33)

Substitution of (4.33) into (4.26) gives \( e_n \)

\[ e_n = \frac{1}{\sigma} \int_0^{\frac{\pi}{2}} f(\theta) \cos n\theta \, d\theta, \quad \sigma \neq 0, \] (4.34)

where

\[ \sigma = R_n^* + \frac{\left( \frac{2R_n}{\kappa} - (R_n^{(\sigma)} + R_n^{(\tau)}) \right)}{R_n^*}, \quad \kappa \neq 0, \] (4.35)

In this case, \( \kappa \) and \( \sigma \) always larger than zero since \( R_2 > R_0 > R_1 > 0 \) as shown in Figure 4.1. \( e_n \) is obtained by integrating \( f(\theta) \cos n\theta \) with respect to \( \theta \) from 0 to \( 2\pi \) and dividing by \( \sigma \).

To obtain the solution for \( g_n \) from (4.27), the same procedures ((4.30)~(4.35)) are applied. Substituting (4.18) into (4.21) gives

\[ h_n = c_n R_n^{2\sigma} + R_n^{2\sigma} (c_n - g_n). \] (4.36)

Substitution of (4.18) and (4.36) into (4.24) gives relationship between \( g_n \) and \( c_n \).

\[ g_n = \frac{K_1 R_n^{2\sigma} + R_n^{2\sigma} + \frac{K_2 - K_1}{K_2} R_n^{2\sigma}}{2K_2 R_n^{2\sigma}} c_n = \frac{\kappa}{2K_2} c_n, \quad R_n \neq 0, \] (4.37)

where

\[ \kappa = \frac{K_1}{K_2} R_n^{2\sigma} + R_n^{2\sigma} + \frac{K_2 - K_1}{K_2} R_n^{2\sigma}, \quad K_n \neq 0. \] (4.38)

Substitution of (4.37) into (4.36) gives \( h_n \) that is the only function of \( g_n \).

\[ h_n = \left( \frac{2R_n^{2\sigma}}{\kappa} - (R_n^{(\sigma)} + R_n^{(\tau)}) \right) g_n, \quad \kappa \neq 0. \] (4.39)

Substitution of (4.39) into (4.27) gives \( g_n \).

\[ g_n = \frac{1}{\pi} \int_0^{\frac{\pi}{2}} f(\theta) \sin n\theta \, d\theta, \quad \sigma \neq 0, \] (4.40)

where

\[ \sigma = R_2^{2\sigma} + \frac{\left( \frac{2R_0^{2\sigma}}{\kappa} - (R_0^{(\sigma)} + R_0^{(\tau)}) \right)}{R_2^{2\sigma}}, \quad \kappa \neq 0, \quad R_2 \neq 0. \] (4.41)

\( g_n \) is obtained by integrating \( f(\theta) \sin n\theta \) with respect to \( \theta \) from 0 to \( 2\pi \) and dividing by \( \sigma \).

Now, the obtained analytical solution is summarized as follow. The verification of the solution is given in Section 4.5.

\[ \phi_i (r, \theta) = a_i + \sum_{s=1}^{n} \left[ \left( a_s r^n + b_s r^m \right) \cos n\theta + (c_s r^n + d_s r^m) \sin n\theta \right], \quad R_i \leq r \leq R_0, \quad 0 \leq \theta < 2\pi, \quad n = 1, 2, 3, \ldots, \] (4.42)

\[ \phi_s (r, \theta) = e_s + \sum_{s=1}^{n} \left[ (e_s r^n + f_s r^m) \cos n\theta + (g_s r^n + h_s r^m) \sin n\theta \right], \quad R_0 \leq r \leq R_s, \quad 0 \leq \theta < 2\pi, \quad n = 1, 2, 3, \ldots, \] (4.43)

where

\[ a_0 = \frac{1}{2\pi} \int_0^{\frac{\pi}{2}} f(\theta) d\theta, \] (4.44)
\[ a_n = \left( \frac{2 \Re}{\kappa} \right) \frac{1}{\pi} \int_0^{2\pi} f(\theta) \cos n\theta \, d\theta, \quad \kappa \neq 0, \ \varpi \neq 0, \quad (4.45) \]

\[ b_n = \Re \left( \frac{2 \Re}{\kappa} \right) \frac{1}{\pi} \int_0^{2\pi} f(\theta) \cos n\theta \, d\theta, \quad \kappa \neq 0, \ \varpi \neq 0, \quad (4.46) \]

\[ c_n = \left( \frac{2 \Re}{\kappa} \right) \frac{1}{\pi} \int_0^{2\pi} f(\theta) \sin n\theta \, d\theta, \quad \kappa \neq 0, \ \varpi \neq 0, \quad (4.47) \]

\[ d_n = \Re \left( \frac{2 \Re}{\kappa} \right) \frac{1}{\pi} \int_0^{2\pi} f(\theta) \sin n\theta \, d\theta, \quad \kappa \neq 0, \ \varpi \neq 0, \quad (4.48) \]

\[ e_n = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) \, d\theta, \quad (4.49) \]

\[ f_n = \left( \frac{2 \Re}{\kappa} \right) (R_1^{2n} + R_0^{2n}) - \Re \left( \frac{2 \Re}{\kappa} \right) \frac{1}{\pi} \int_0^{2\pi} f(\theta) \cos n\theta \, d\theta, \quad \kappa \neq 0, \ \varpi \neq 0, \quad (4.51) \]

\[ g_n = \frac{1}{\pi} \int_0^{2\pi} f(\theta) \sin n\theta \, d\theta, \quad \varpi \neq 0, \quad (4.52) \]

\[ h_n = \left( \frac{2 \Re}{\kappa} \right) (R_1^{2n} + R_0^{2n}) - \Re \left( \frac{2 \Re}{\kappa} \right) \frac{1}{\pi} \int_0^{2\pi} f(\theta) \sin n\theta \, d\theta, \quad \kappa \neq 0, \ \varpi \neq 0, \quad (4.53) \]

\[ \kappa = \frac{K_1}{K_2} R_0^{2n} + \frac{K_2 - K_1}{K_2} R_1^{2n}, \quad K_2 \neq 0, \quad (4.54) \]

\[ \varpi = R_0^{2n} - \frac{2 \Re}{\kappa} \frac{R_0^{2n} + R_1^{2n} - R_0^{2n}}{R_1^{2n}}, \quad \kappa \neq 0, \ R_2 \neq 0, \quad (4.55) \]

where \( R_1 > R_2 > R_0 > 0 \).

### 4.3 Stream Functions

From the obtained potential functions \((\phi_i)\), the stream functions \((\psi_i)\) can be determined by

\[ \frac{\partial \phi_i}{\partial r} = \frac{1}{r} \frac{\partial \psi_i}{\partial \theta}, \quad \frac{1}{r} \frac{\partial \phi_i}{\partial \theta} = -\frac{\partial \psi_i}{\partial r}, \quad i = 1, 2, \quad (4.56) \]

where \(i=1\) represents the region 1 \((R_1 < r < R_0)\), and \(i=2\) represents the region 2 \((R_0 < r < R_2)\). Thus, from (4.42) and (4.56), the stream function \(\psi_i\) in the region \((R_1 < r < R_0)\) can be obtained as follows.

Differentiating (4.42) with respect to \(r\) and \(\theta\), and relating to (4.56) yields

\[ \frac{\partial \psi_1}{\partial \theta} = \frac{r}{r} \frac{\partial \phi_1}{\partial r} = \sum_{n=1}^{\infty} n \left( [a_r^+ r^+ b^+ r^{-}] \cos n\theta + (c_r^+ r^+ d^+ r^{-}) \sin n\theta \right), \quad (4.57) \]

\[ \frac{\partial \psi_1}{\partial r} = -\frac{1}{r} \frac{\partial \phi_1}{\partial \theta} = \sum_{n=1}^{\infty} n \left( [a_r^+ r^+ b^+ r^{-}] \sin n\theta - (c_r^+ r^+ d^+ r^{-}) \cos n\theta \right). \quad (4.58) \]

Integrating (4.57) with respect to \(\theta\) gives
\[ \psi_i = \sum_{n=1}^{\infty} \left[ (a_n r^n - b_n r^{-n}) \sin n\theta - (c_n r^n - d_n r^{-n}) \cos n\theta \right] + \eta(r), \quad (4.59) \]

where \( \eta(r) \) is the arbitrary function of \( r \).

To determine \( \eta(r) \), differentiating (4.59) with respect to \( r \) yields

\[ \frac{d\psi_i}{dr} = \sum_{n=1}^{\infty} n \left[ (a_n r^{n-1} + b_n r^{-n+1}) \sin n\theta - (c_n r^{n-1} + d_n r^{-n+1}) \cos n\theta \right] + \frac{d\eta(r)}{dr}. \quad (4.60) \]

Comparison of (4.58) with (4.60) gives

\[ \frac{d\eta(r)}{dr} = 0, \quad \text{or} \quad \eta(r) = C_i. \quad (4.61) \]

Therefore, from (4.59) and (4.61),

\[ \psi_i(r, \theta) = \sum_{n=1}^{\infty} \left[ (a_n r^n - b_n r^{-n}) \sin n\theta - (c_n r^n - d_n r^{-n}) \cos n\theta \right] + C_i, \quad (4.62) \]

for \( R_i \leq r \leq R_j, 0 \leq \theta < 2\pi, \ n = 1, 2, 3, \ldots \)

\( C_j \) is constant.

Following the above procedure, the stream function in region 2 \((R_0 < r < R_2)\), is

\[ \psi_i(r, \theta) = \sum_{n=1}^{\infty} \left[ (e_n r^n - f_n r^{-n}) \sin n\theta - (g_n r^n - h_n r^{-n}) \cos n\theta \right] + C_i, \quad (4.63) \]

for \( R_i < r \leq R_j, 0 \leq \theta < 2\pi, \ n = 1, 2, 3, \ldots \)

\( C_2 \) is constant.

The constants \( C_i=C_i=0 \) in (4.62) and (4.63) are taken since difference between two stream-lines gives physically meaningful result. Thus, stream functions become

\[ \psi_i(r, \theta) = \sum_{n=1}^{\infty} \left[ (a_n r^n - b_n r^{-n}) \sin n\theta - (c_n r^n - d_n r^{-n}) \cos n\theta \right], \quad (4.64) \]

\( R_i \leq r \leq R_j, 0 \leq \theta < 2\pi, \ n = 1, 2, 3, \ldots \)

\[ \psi_2(r, \theta) = \sum_{n=1}^{\infty} \left[ (e_n r^n - f_n r^{-n}) \sin n\theta - (g_n r^n - h_n r^{-n}) \cos n\theta \right], \quad (4.65) \]

\( R_i < r \leq R_j, 0 \leq \theta < 2\pi, \ n = 1, 2, 3, \ldots \)

While variables have been assumed to be dimensionless to obtain the analytical solutions, they actually have dimensions as shown in Table 4.1. For the graphical representation, special cases with \( f(\theta)=\phi_0 \cos \theta \) for \( n=1 \) are assumed as shown in Table 4.1, where \( \phi_0 \) [m] is the unit potential head.

### Table 4.1 Input Parameters for Graphical Representation of Analytical Solution.

<table>
<thead>
<tr>
<th>Case</th>
<th>( K_1 ) [m/s]</th>
<th>( K_2 ) [m/s]</th>
<th>( K_1/K_2 )</th>
<th>( R_i ) [m]</th>
<th>( R_j ) [m]</th>
<th>( f(\theta) ) [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1.0</td>
<td>0.35</td>
<td>1.0</td>
<td>5.0 ( \phi_0 \cos \theta )</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td>1</td>
<td>10.0</td>
<td>0.35</td>
<td>1.0</td>
<td>5.0 ( \phi_0 \cos \theta )</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>10</td>
<td>0.1</td>
<td>0.35</td>
<td>1.0</td>
<td>5.0 ( \phi_0 \cos \theta )</td>
</tr>
</tbody>
</table>

The analytical solutions of the potential functions ((4.42) and (4.43)), and stream functions ((4.64) and (4.65)) for 3 cases in Table 4.1 are

\[ \phi_i(r, \theta) = \left[ a_n r + \frac{b_n}{r} \right] \cos \theta, \quad R_i \leq r \leq R_j, 0 \leq \theta < 2\pi, \quad (4.66) \]
\[ \phi_i(r, \theta) = \left[ e_i + \frac{f_i}{r} \right] \cos \theta, \ R_i \leq r \leq R_i, \ 0 \leq \theta < 2\pi, \]  
\[ \psi_i(r, \theta) = \left[ a_i r - \frac{b_i}{r} \right] \sin \theta, \ R_i \leq r \leq R_i, \ 0 \leq \theta < 2\pi. \]  
\[ \psi_i(r, \theta) = \left[ e_i r - \frac{f_i}{r} \right] \sin \theta, \ R_i \leq r \leq R_i, \ 0 \leq \theta < 2\pi. \]  

Coefficients in (4.66~4.69) are calculated by (4.44~4.55) using the parameters in Table 4.1, and are shown in Table 4.2. Other coefficients \((a_0, b_0, c_0, d_0, g_0, \text{and} h_0)\) are equal to zero for the parameters in Table 4.1.

### Table 4.2 Numerical Values of Coefficients in Analytical Solution.

<table>
<thead>
<tr>
<th>Case</th>
<th>(a_i)</th>
<th>(b_i [m^2])</th>
<th>(e_i)</th>
<th>(f_i [m^2])</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.199025</td>
<td>0.024381</td>
<td>0.199025</td>
<td>0.024381</td>
</tr>
<tr>
<td>2</td>
<td>0.041704</td>
<td>0.005109</td>
<td>0.206383</td>
<td>-0.15957</td>
</tr>
<tr>
<td>3</td>
<td>0.319581</td>
<td>0.039149</td>
<td>0.193386</td>
<td>0.165343</td>
</tr>
</tbody>
</table>

Figure 4.2 shows the potential and stream functions for 3 cases. In Figure 4.2, vertical lines represent equipotential lines and horizontal lines represent the streamlines. If physical property \(K\) is considered as the hydraulic conductivity \([m/s]\), then (1) case 1 represents one homogeneous medium with \(K_1=K_2\), (2) case 2 represents that region 1 is more permeable than region 2 \((K_1>K_2)\), and (3) case 3 represents that region 1 is less permeable than region 2 \((K_1<K_2)\).

![Potential and stream functions for 3 cases.](image)

**Figure 4.2** Potential and stream functions for 3 cases.

### 4.4 Comparison between the Analytical and Numerical Solutions

For the purpose of comparison between the analytical solution ((4.42) and (4.43)) and the numerical solution by FFDF code for a model with a homogenized NFR, special cases for \(f(\theta)=\phi_0(1-\cos\theta)/2\) are considered, where \(\phi_0=1 [m]\). Assumed values for each variable are shown in Table 4.3.

Figure 4.3 (a), (b), and (c) show the domain discretization for a model with a homogenized NFR by 144, 280, and 560 points, respectively. The size of mesh used in case (c) in Figure 4.3 is the same as that used in water flow analysis in Chapter 3.

Here, only two analytical solutions for all cases exist. One is for \(K_1/K_2=1\) \((K_1=1.0 \text{ m/s and } K_2=1.0 \text{ m/s})\) and the other is for \(K_1/K_2=0.1\) \((K_1=0.1 \text{ m/s and } K_2=1.0 \text{ m/s})\). Other parameters \((R_i, R_o, R_2, \text{and} f(\theta))\) are assumed to be identical for all cases. Analytical solutions for cases 1, 3, and 5 are obtained by (4.42) and (4.43) as
Figure 4.3  Domain discretization for numerical solution by FFDF
\[
\phi_1(r, \theta) = 0.5 - 0.09951 r + \frac{0.01219}{r} \cos \theta, R_i \leq r \leq R_o, 0 \leq \theta < 2\pi, \quad (4.70)
\]
\[
\phi_2(r, \theta) = 0.5 - 0.09951 r + \frac{0.01219}{r} \cos \theta, R_i \leq r \leq R_o, 0 \leq \theta < 2\pi. \quad (4.71)
\]

(4.70) and (4.71) are identical because \(K_1\) is equal to \(K_2\). Analytical solutions for cases 2, 4, and 6 are

\[
\phi_1(r, \theta) = 0.5 - 0.15979 r + \frac{0.01957}{r} \cos \theta, R_i \leq r \leq R_o, 0 \leq \theta < 2\pi, \quad (4.72)
\]
\[
\phi_2(r, \theta) = 0.5 - 0.09669 r + \frac{0.08267}{r} \cos \theta, R_i \leq r \leq R_o, 0 \leq \theta < 2\pi. \quad (4.73)
\]

For all cases, the absolute difference is estimated as

\[
\xi_\phi = |\phi_{\text{anal}} - \phi_{\text{nume}}|. \quad (4.74)
\]

where \(\phi_{\text{anal}}\) is the potential obtained from the analytical solution, and \(\phi_{\text{nume}}\) is the potential obtained numerically by FFDF.

Figure 4.4 shows the values of potential obtained by the analytical solution (line) and those obtained numerically by FFDF (dot) at all 144 points for case 1. In this case, the average difference, which is obtained by averaging differences by (4.74) arithmetically for 144 points, is \(1.06 \times 10^{-3}\). The upper bound of difference, which is the maximum difference for 144 points, is \(8.66 \times 10^{-4}\). The lower bound of difference, which is minimum difference for 144 points, is zero. Figure 4.5 shows the results for case 3. In this case, the average difference for 280 points is \(7.31 \times 10^{-4}\). The upper and lower bounds of difference are \(6.66 \times 10^{-4}\) and zero, respectively. Figure 4.6 shows the results for case 5. In this case, the average difference for 560 points is \(6.78 \times 10^{-4}\). The upper and the lower bounds of difference are \(5.80 \times 10^{-4}\) and zero, respectively. For \(K_1\)/\(K_2\) equal to 0.1 (cases 2, 4, and 6), results are shown in Figure 4.7, Figure 4.8, and Figure 4.9 for cases 2, 4, and 6, respectively.

Table 4.4 and Table 4.5 show the summary of difference for \(K_1\)/\(K_2\)=1 and \(K_1\)/\(K_2\)=0.1. According to these tables, difference between the analytical solution and the numerical solution decreases as the number of points increases (Figure 4.10). For all cases, the differences for the analytical and numerical solutions by (4.74) at all points are less than \(1.88 \times 10^{-5}\). Differences for \(K_1\)/\(K_2\)=0.1 are larger than those for \(K_1\)/\(K_2\)=1.0 because of different physical properties between two regions for \(K_1\)/\(K_2\)=0.1. Although differences for \(K_1\)/\(K_2\)=0.1 are larger than that for \(K_1\)/\(K_2\)=1.0, agreement between the analytical solution and the numerical solution for both cases is good enough \((\xi_\phi < 1.88 \times 10^{-5})\).

**Table 4.3 Input Parameters for Comparison**

<table>
<thead>
<tr>
<th>Case</th>
<th>Points</th>
<th>(K_1)/(K_2)</th>
<th>(R_i) [m]</th>
<th>(R_o) [m]</th>
<th>(R_j) [m]</th>
<th>(f(0)) [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>144</td>
<td>1.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>280</td>
<td>0.1</td>
<td>0.35</td>
<td>1.0</td>
<td>5.0</td>
<td>(\phi_i(1-\cos\theta)/2)</td>
</tr>
<tr>
<td>3</td>
<td>560</td>
<td>0.1</td>
<td>1.0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Table 4.4 Difference for \(K_1\)/\(K_2\)=1**

<table>
<thead>
<tr>
<th>Case</th>
<th>Average (\xi_\phi)</th>
<th>Upper bound of (\xi_\phi)</th>
<th>Lower bound of (\xi_\phi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.06E-03</td>
<td>8.66E-03</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>7.31E-04</td>
<td>6.66E-03</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>6.78E-04</td>
<td>5.80E-03</td>
<td>0</td>
</tr>
</tbody>
</table>

**Table 4.5 Difference for \(K_1\)/\(K_2\)=0.1**

<table>
<thead>
<tr>
<th>Case</th>
<th>Average (\xi_\phi)</th>
<th>Upper bound of (\xi_\phi)</th>
<th>Lower bound of (\xi_\phi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3.46E-03</td>
<td>1.88E-02</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>1.75E-03</td>
<td>1.18E-02</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>1.17E-03</td>
<td>9.84E-03</td>
<td>0</td>
</tr>
</tbody>
</table>
Figure 4.4 Analytical vs. numerical for (case 1: \(K_1/K_2=1\) and 144 points).

Figure 4.5 Analytical vs. numerical for (case 3: \(K_1/K_2=1\) and 280 points).

Figure 4.6 Analytical vs. numerical for (case 5: \(K_1/K_2=1\) and 560 points).
Figure 4.7 Analytical vs Numerical for (case 2: $K_1/K_2=0.1$ and 144 points).

Figure 4.8 Analytical vs Numerical for (case 4: $K_1/K_2=0.1$ and 280 points).

Figure 4.9 Analytical vs. numerical for (case 6: $K_1/K_2=0.1$ and 560 points).
Figure 4.10  Average difference and number of points.

Table 4.6 shows the comparison of the total discharge \( [m^3 \cdot \text{water/m-\text{medium-s}}] \) at the outer boundary and the interface between the analytical solution and the numerical solution. Total discharge (in terms of volume of water per unit width normal to the \( r-\theta \) plane per unit time) between two streamlines is equal to the difference in the stream functions corresponding to these lines [Bear, 1979]. The stream functions at regions 1 and 2 for \( K_1/K_2=1.0 \) are obtained by using the potential functions ((4.70) and (4.71)) and the relationship between the potential function and the stream function (4.56) as

\[
\psi_r(r, \theta) = \left[ -0.09951 r + \frac{0.01219}{r} \right] \sin \theta, R_1 \leq r \leq R_2, 0 \leq \theta < 2\pi .
\]  

(4.75)

and

\[
\psi_z(r, \theta) = \left[ -0.09951 r + \frac{0.01219}{r} \right] \sin \theta, R_1 \leq r \leq R_2, 0 \leq \theta < 2\pi .
\]

(4.76)

For \( K_1/K_2=0.1 \), the stream functions are obtained by (4.72), (4.73), and (4.56) as

\[
\psi_r(r, \theta) = \left[ -0.15979 r + \frac{0.01957}{r} \right] \sin \theta, R_1 \leq r \leq R_2, 0 \leq \theta < 2\pi .
\]

(4.77)

and

\[
\psi_z(r, \theta) = \left[ -0.09669 r + \frac{0.08267}{r} \right] \sin \theta, R_1 \leq r \leq R_2, 0 \leq \theta < 2\pi .
\]

(4.78)

The total discharge at the outer boundary \( (r=R_2) \) can be analytically evaluated by (4.76) for cases 1, 3, and 5 and (4.78) for cases 2, 4, and 6. The total discharge at the interface \( (r=R_0) \) can be analytically evaluated by (4.75) for cases 1, 3, and 5 and (4.77) for cases 2, 4, and 6. For example, the total discharge at the outer boundary for case 1, 3, and 5, the maximum (at \( r=R_2=5, \theta=3\pi/2 \)) and minimum (at \( r=R_1=5, \theta=\pi/2 \)) values of the stream function are calculated by (4.76) as 0.495 m and -0.495 m, respectively. Thus, the total discharge at the outer boundary for cases 1, 3, and 5 is obtained by subtracting the minimum value (-0.495 m) from the maximum value (0.495 m) and multiplying the resultant (0.99 m) by the hydraulic conductivity \( K_2=1.0 \) m/s, resulting in 0.99 [m^3/s].

Table 4.6  Comparison of Total Discharge at the Outer Boundary and at the Interface.

<table>
<thead>
<tr>
<th>Case</th>
<th>Total discharge at ( r=R_2 ) [m^3/s] (Analytical)</th>
<th>Total discharge at ( r=R_2 ) [m^3/s] (Numerical)</th>
<th>% Difference</th>
<th>Total discharge at ( r=R_0 ) [m^3/s] (Analytical)</th>
<th>Total discharge at ( r=R_0 ) [m^3/s] (Numerical)</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>9.90E-01</td>
<td>9.25E-01</td>
<td>6.59</td>
<td>1.75E-01</td>
<td>1.64E-01</td>
<td>5.98</td>
</tr>
<tr>
<td>3</td>
<td>9.67E-01</td>
<td>9.67E-01</td>
<td>2.36</td>
<td>1.72E-01</td>
<td>1.72E-01</td>
<td>1.57</td>
</tr>
<tr>
<td>5</td>
<td>9.85E-01</td>
<td>9.85E-01</td>
<td>0.54</td>
<td>1.75E-01</td>
<td>1.75E-01</td>
<td>0.26</td>
</tr>
<tr>
<td>2</td>
<td>8.76E-01</td>
<td>8.76E-01</td>
<td>6.24</td>
<td>2.51E-02</td>
<td>2.51E-02</td>
<td>10.04</td>
</tr>
<tr>
<td>4</td>
<td>9.13E-01</td>
<td>9.13E-01</td>
<td>2.21</td>
<td>2.71E-02</td>
<td>2.71E-02</td>
<td>3.47</td>
</tr>
<tr>
<td>6</td>
<td>9.29E-01</td>
<td>9.29E-01</td>
<td>0.48</td>
<td>2.79E-02</td>
<td>2.79E-02</td>
<td>0.55</td>
</tr>
</tbody>
</table>
According to Table 4.6, a difference between the total discharges obtained analytically and numerically is decreased as the number of point increases. For each case in Table 4.6, the amount of water enters from the outer region to the inner region in terms of percentage can be calculated as the ratio of the total discharge at the interface \( (r=R_0) \) to the total discharge at the outer boundary \( (r=R_2) \). For cases 5 and 6, the ratios of amount of water flowing into the inner region from the outer region are 18% and 3%, respectively. The higher ratio (18%) for case 5 \( (K_1/K_2=1) \) than that (3%) for case 6 \( (K_1/K_2=0.1) \) is expected result since \( K_2<K_1 \) for case 6. Cases 1, 3, and 5 \( (K_1/K_2=1) \) have same trend of water flow as shown in Figure 4.2 (a). Figure 4.2 (c) shows the trend of water flow for cases 2, 4, and 6 \( (K_1/K_2=0.1) \).

### 4.5 Verification of Analytical Solution for Potential

#### 4.5.1 Governing Equations

To verify the analytical solution for potential, the analytical solutions ((4.42) and (4.43)) should satisfy the governing equations \( (4.1) \) and \( (4.2) \). According to the obtained solutions, \( a_n \), to \( h_n \) including \( \kappa \) and \( \omega \) ((4.44) to (4.55)) are constant.

Substitution of (4.42) into the first term \( r \frac{\partial}{\partial r}(r \frac{\partial \phi(r, \theta)}{\partial r}) \) and the second term \( \frac{\partial^2 \phi(r, \theta)}{\partial \theta^2} \) in (4.1) yield the same magnitude but opposite sign as shown in (4.79) and (4.80), respectively.

\[
\begin{align*}
    r \frac{\partial}{\partial r}(r \frac{\partial \phi(r, \theta)}{\partial r}) &= n^2 \left[ \sum_{n=1}^{\infty} \left( a_n r^n + b_n r^{-n} \right) \cos n \theta + (c_n r^n + d_n r^{-n}) \sin n \theta \right] , \\
    \frac{\partial^2 \phi(r, \theta)}{\partial \theta^2} &= -n^2 \left[ \sum_{n=1}^{\infty} \left( a_n r^n + b_n r^{-n} \right) \cos n \theta + (c_n r^n + d_n r^{-n}) \sin n \theta \right] .
\end{align*}
\]  

(4.79) \quad (4.80)

Substitution of (4.79) and (4.80) into (4.1) gives zero.

\[
\nabla^2 \phi = r \frac{\partial}{\partial r}(r \frac{\partial \phi}{\partial r}) + \frac{\partial^2 \phi}{\partial \theta^2} = 0.
\]

(4.81)

Therefore, the solution of the \( \phi_1 \), (4.42), satisfies the governing equation (4.1). Similarly, the solution for \( \phi_2 \), (4.43), also satisfies the governing equation (4.2).

#### 4.5.2 Boundary Conditions

The boundary condition (BC) prescribed at \( r=R_2 \) is \( \phi_2(R_2, \theta) = f(\theta) \) as shown in (4.3). Substituting \( r=R_2 \) into (4.43) gives

\[
\phi_2(R_2, \theta) = a_n + \sum_{n=1}^{\infty} \left[ (e_n r_n^+ + f_n r_n^-) \cos n \theta + (g_n r_n^+ + h_n r_n^-) \sin n \theta \right] .
\]

(4.82)

Equation (4.12) for \( f(\theta) \) with \( f_0=0 \) (4.22) gives

\[
f(\theta) = e_n + \sum_{n=1}^{\infty} \left( e_n r_n^+ + f_n r_n^- \right) \cos n \theta + (g_n r_n^+ + h_n r_n^- \sin n \theta \right], \quad 0 \leq \theta < 2\pi.
\]

(4.83)

Since the right side of (4.82) is equal to the right side of (4.83), the solution satisfies the BC (4.3).

The boundary condition prescribed as \( r=R_1 \) is \( \partial \phi_1 / \partial r = 0 \) as shown in (4.4). Substituting \( r=R_1 \) into (4.42) gives

\[
\phi_1(R_1, \theta) = a_n + \sum_{n=1}^{\infty} \left[ a_n r_n^+ + b_n r_n^- \cos n \theta + (c_n r_n^+ + d_n r_n^-) \sin n \theta \right] .
\]

(4.84)

Differentiating the right-hand side of (4.84) with respect to \( r \) gives zero because the right-hand side of (4.84) is independent of \( r \). Therefore, the solution satisfies BC (4.4).
The boundary condition prescribed as \( r=R_0 \) is \( \phi_1(R_0, \theta) = \phi_2(R_0, \theta) \) as shown in (4.5). Substituting \( r=R_0 \) into (4.42), (4.43) gives

\[
\phi_1(R_0, \theta) = a_0 + \sum_{n=1}^{\infty} \left[ (a_n R_n + b_n R_n^{-1}) \cos n\theta + (c_n R_n + d_n R_n^{-1}) \sin n\theta \right],
\]

(4.85)

\[
\phi_2(R_0, \theta) = e_0 + \sum_{n=1}^{\infty} \left[ (e_n R_n + f_n R_n^{-1}) \cos n\theta + (g_n R_n + h_n R_n^{-1}) \sin n\theta \right].
\]

(4.86)

Substituting (4.44) – (4.55) into (4.85) and (4.86) respectively gives

\[
\phi_1(R_0, \theta) = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) d\theta + \sum_{n=1}^{\infty} \left[ \left( \frac{2R_n}{\kappa \Omega \pi} \right)^2 \int_0^{2\pi} f(\theta) \cos n\theta d\theta \right] (R_{2n} - R_{2n}^{-1}) \cos n\theta
\]

\[
+ \sum_{n=1}^{\infty} \left[ \left( \frac{2R_n}{\kappa \Omega \pi} \right)^2 \int_0^{2\pi} f(\theta) \sin n\theta d\theta \right] (R_{2n} + R_{2n}^{-1}) \sin n\theta
\]

(4.87)

\[
\phi_2(R_0, \theta) = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) d\theta + \sum_{n=1}^{\infty} \left[ \left( \frac{2R_n}{\kappa \Omega \pi} \right)^2 \int_0^{2\pi} f(\theta) \cos n\theta d\theta \right] (R_{2n} + R_{2n}^{-1}) \cos n\theta
\]

\[
+ \sum_{n=1}^{\infty} \left[ \left( \frac{2R_n}{\kappa \Omega \pi} \right)^2 \int_0^{2\pi} f(\theta) \sin n\theta d\theta \right] (R_{2n} - R_{2n}^{-1}) \sin n\theta
\]

(4.88)

The solutions satisfy BC (4.5) because the right-hand side of (4.87) and (4.88) are identical.

Continuity of flux prescribed at \( r=R_0 \) is \( K_1 [\hat{\phi}_1 / \hat{r}] = K_2 [\hat{\phi}_2 / \hat{r}] \) as shown in (4.6). At \( r=R_0 \), the left-hand side of the BC (4.6) becomes

\[
K_1 \frac{\partial \hat{\phi}_1(R_0, \theta)}{\partial r} = K_n \sum_{n=1}^{\infty} \left[ (a_n R_n - b_n R_n^{-1}) \cos n\theta + (c_n R_n - d_n R_n^{-1}) \sin n\theta \right]
\]

(4.89)

At \( r=R_0 \), the right-hand side of BC (4.6) becomes

\[
K_2 \frac{\partial \hat{\phi}_2(R_0, \theta)}{\partial r} = K_n \sum_{n=1}^{\infty} \left[ (e_n R_n - f_n R_n^{-1}) \cos n\theta + (g_n R_n - h_n R_n^{-1}) \sin n\theta \right]
\]

(4.90)

Substituting (4.44) – (4.55) into the (4.89) and (4.90) gives, respectively,

\[
K_1 \frac{\partial \hat{\phi}_1(R_0, \theta)}{\partial r} = K_n R_0 \sum_{n=1}^{\infty} \left[ \left( \frac{1}{\sin \pi} \right)^2 \int_0^{2\pi} f(\theta) \cos n\theta d\theta \right] \left( \frac{2R_n^3}{\kappa} - R_{2n}^3 \frac{2R_n}{\kappa} \right) \cos n\theta
\]

\[
+ K_n R_0 \sum_{n=1}^{\infty} \left[ \left( \frac{1}{\sin \pi} \right)^2 \int_0^{2\pi} f(\theta) \sin n\theta d\theta \right] \left( \frac{2R_n^3}{\kappa} - R_{2n}^3 \frac{2R_n}{\kappa} \right) \sin n\theta
\]

(4.91)

\[
K_2 \frac{\partial \hat{\phi}_2(R_0, \theta)}{\partial r} = K_n R_0 \sum_{n=1}^{\infty} \left[ \left( \frac{1}{\sin \pi} \right)^2 \int_0^{2\pi} f(\theta) \cos n\theta d\theta \right] \left( 2R_n - R_{2n} \frac{2R_n}{\kappa} \right) \cos n\theta
\]

\[
+ K_n R_0 \sum_{n=1}^{\infty} \left[ \left( \frac{1}{\sin \pi} \right)^2 \int_0^{2\pi} f(\theta) \sin n\theta d\theta \right] \left( 2R_n - R_{2n} \frac{2R_n}{\kappa} \right) \sin n\theta
\]

(4.92)

If (4.93) is satisfied, (4.91) is identical to (4.92), and then the solution satisfies BC (4.6).

\[
K_1 \left[ \frac{2R_n^3}{\kappa} - R_{2n}^3 \frac{2R_n}{\kappa} \right] = K_2 \left[ 2R_n - R_{2n} \frac{2R_n}{\kappa} \right].
\]

(4.93)
where \[ \kappa = \frac{K_1}{K_2} R_n^{2n} + R_n^{2n} + \frac{K_1 - K_2}{K_2} R_i^{2n}, \quad K_i \neq 0. \]

The left-hand side of (4.93) gives
\[ 2K_i R_n^{2n} - 2K_i R_i^{2n} R_n^{2n}. \quad (4.94) \]

The right-hand side of (4.93) gives
\[ 2K_i R_n^{2n} - 2K_i R_i^{2n} R_i^{2n}. \quad (4.95) \]

Since (4.94) and (4.95) are identical, so are (4.91) and (4.92). Therefore, the solution satisfies BC (4.6).

Because the solutions of the \( \phi_1 \) and \( \phi_2 \), i.e. (4.42) and (4.43), respectively, satisfy governing equations, (4.1) and (4.2), and the boundary conditions, (4.3), (4.4), (4.5), and (4.6), they are correct.

### 4.6 Conclusions

Numerical solution obtained by the numerical model with a homogenized NFR by the uniformization, developed in Chapter 3, is bench-marked against an analytical solution.

For the size of mesh in Figure 4.3 (c) used for water flow analysis in Chapter 3, the numerical results for the values of hydraulic potential differ from those by analytical solution by an average difference less than 1.17\times10^{-3}. The numerical results for the total discharges at the outer boundary and the interface differ from those obtained by analytical solutions by a relative difference less than 0.55\%.
5. Transport Analysis in the Near Field of Geologic Repository

5.1 Introduction

In this chapter, a near-field model for the particle transport simulation is developed based on the flow model, which is developed in Chapter 3.

Particle transport is modeled by a Random-Walk Tracking Method (RWTM) [Tompson, et al., 1987], which is based on the spatial distribution of the flow obtained by the water flow analysis in Chapter 3. Particle movement over discrete time steps is governed by a random walk algorithm for the advection and the molecular diffusion. The residence time of particles is obtained by observing tracks of each particle. The mass absorption rate at the outer boundary is also obtained by counting the number of particles being absorbed at the boundary per unit time.

The objectives of this chapter are (1) to develop a model for particle transport simulation based on the flow model developed in Chapter 3, (2) to investigate effects of the heterogeneity of the NFR on the particle transport, and (3) to investigate effects of the modeling approach for the NFR on the particle transport.

In this chapter, first, the RWTM by Tompson, et al., [1987] for the particle transport simulation in the continuum is discussed. This discussion was initiated by Chambré [2002]. The development shown in Section 5.2 is based on the discussions with Chambré [2002].

5.2 Review of Tompson’s Treatment

5.2.1 Tompson’s Model

Tompson, et al. [1987] developed the transport model by using a Random-Walk Tracking Method (RWTM) to investigate the solute movement through large, three dimensional heterogeneous flow systems in saturated and unsaturated porous media. In order to obtain the mass distribution of a large number of particles corresponding to that given by the transient transport equation, the step equation, which governs the particle movements over discrete time steps, is obtained by adopting the Ito assumption; i.e. a particle movement at the next time step is governed by the properties of the current time step before movement. The step equations are obtained by using an analogy between the Ito-Fokker-Planck equation [Haken, 1983] and the transient advection-dispersion equation, such that the Ito-Fokker-Planck equation with the step equation is equivalent to the transient transport equation.

For a two-dimensional (x, y) saturated flow system, the step equation for the time-dependent, space-dependent water velocity and constant molecular diffusion coefficient without mechanical dispersion in a time interval $\tau$ was given by Tompson, et al. [1987] as follows:

\[
\begin{align*}
    x(t + \tau) &= x(t) + v_x(\bar{X}(t)) \tau + Z_x \sqrt{2D\tau}, \\
    y(t + \tau) &= y(t) + v_y(\bar{X}(t)) \tau + Z_y \sqrt{2D\tau},
\end{align*}
\]

(5.1)

where $x$ and $y$ are random variables, and $t$ and $\tau$ are deterministic parameters. $\bar{X}(t)$ is a position vector of a particle at time $t$, and $v_x(\bar{X}(t))$ and $v_y(\bar{X}(t))$ are the components of the water pore velocity vector at time $t$ in $x$ and $y$ directions, respectively. $D$ is the diffusion coefficient (including medium tortuosity), and is constant in time and space in (5.1). $\bar{Z}_x$ and $\bar{Z}_y$ are independent random numbers at time $t$ satisfying the moments, $\langle \bar{Z}_x \rangle = 0$, $\langle \bar{Z}_y^2 \rangle = 1$, and $\langle \bar{Z}_x^2 \rangle = 0$, $\langle \bar{Z}_y^2 \rangle = 1$, respectively. The brackets $\langle \cdot \rangle$ denote the average value of $\cdot$. $\bar{Z}_x \sqrt{2D\tau}$ and $\bar{Z}_y \sqrt{2D\tau}$ denote the normalized random displacements in $x$ and $y$ directions, respectively.

---

* It is only necessary for $Z$ to have the statistical qualities such as $\langle Z \rangle = 0$ and $\langle Z^2 \rangle = 1$. Thus, many kinds of distributions might be implemented. A normal distribution with mean of 0 and variance of 1 is one possible distribution for $Z$ satisfying two statistical qualities [Tompson et al., 1987].

** It was defined by Tompson et al., [1987] without detailed explanation. The term “normalized random displacement” can be interpreted as a normalized random displacement by the standard deviation of the displacement (see Section 5.2.4).
For the random displacement terms in the step equation (5.1), Tompson, et al. [1987] did not derive the random terms, \( Z_1 \sqrt{\tau} \) and \( Z_2 \sqrt{\tau} \), analytically but assumed a priori some probability distributions without any justification. Thus, a mathematical basis of the step equation needs to be studied.

In the following, a step equation is determined analytically for a case with constant velocity and diffusivity. It reveals some restrictions on the step equation used by Tompson, et al., [1987].

### 5.2.2 Random Movement including Advection

In the flowing water with a constant water velocity, \( v_n \), in the \( x \)-coordinate, movements of particles are determined by the two force components, a deterministic force and a statistical random force. Gravity is neglected. In this section, advection and molecular diffusion refer to the deterministic force and the statistical random force, respectively.

The mathematical framework for Brownian motion set up by Einstein [1905]* is used in the following and summarized below. However, Einstein [1905] did not deal with the problem including the advection in his study.

Since a displacement in \( x \)-coordinate by advection in time \( \tau \) is \( v_x \tau \), a new random variable \( X'(t) \) is defined as

\[
x'(t) = x(t) - v_x \tau,
\]

where \( x(t) \) is a random variable, and \( \tau \) and \( v_x \) are deterministic parameters.

To derive a step equation by using the theory of Brownian movement for a given special case, \( x'(t) \) is first considered, and then \( x(t) \) is obtained by changing the variable using (5.2).

A displacement in \( x \)-coordinate by the statistical random force in time interval \( \tau \) can be obtained by the theory [Einstein, 1905]. Three assumptions are made. (1) Each particle executes a movement which is independent of all other particles. (2) The movements of one and the same particle after different intervals of time (\( \tau \)) must be considered as mutually independent processes, so long as these intervals of times being chosen are not too small. (3) The time interval \( \tau \) is to be very small compared with the observed interval of time \( t \), but, nevertheless, of such a magnitude that the movements executed by a particle in two consecutive intervals of time \( \tau \) are to be considered as mutually independent phenomena. In Section 5.2, \( \tau \) is assumed to be constant, and the observation time \( t \) after \( m \) steps of time interval \( \tau \) is \( mt \), i.e. \( t=mt \).

In an interval of time \( \tau \), the \( x \)-coordinate of the single particle will increase by \( \Delta \), where \( \Delta \) has a different value (positive or negative) for each particle. Let \( \phi(\Delta) \) be a probability of a particle to be displaced between \( \Delta \) to \( \Delta+\Delta \) at an interval \( \tau \). The distribution function \( \phi(\Delta) \) is normalized as,

\[
\int_{\Delta=-\infty}^{\Delta=\infty} \phi(\Delta)d\Delta = 1, \tag{5.3}
\]

\( \phi \) only differs from zero for very small values of \( \Delta \) and fulfills the condition such that the probabilities at \( \Delta \) and \(-\Delta \) are same.

\[
\phi(\Delta)=\phi(-\Delta). \tag{5.4}
\]

Let \( f(x',t)dx' \) be the number of particles located between \( x' \) and \( x'+dx' \) at time \( t \). Then, the number of particles located between \( x' \) and \( x'+dx' \) at the time \( t+\tau \), i.e. \( f(x',t+\tau)dx' \), can be calculated from the number of particles at time \( t \) as follows. For a certain position \( x' \), \( f(x'+\Delta,t) \) denotes the number of particles located at \( x'+\Delta \) at time \( t \). By the definition of \( \phi(\Delta) \), \( f(x'+\Delta,t)\phi(\Delta) \) denotes the number of particles displaced from \( x'+\Delta \) at time \( t \) to \( x' \) in a time interval \( \tau \). Since \( \Delta \) varies from \(-\infty \) to \( \infty \), the total number of particles displaced from any position at time \( t \) to \( x' \) by displacement \( \Delta \) in \( \tau \), i.e. \( f(x',t+\tau) \), is obtained by integrating \( f(x'+\Delta,t)\phi(\Delta) \) with respect to \( \Delta \). Thus, \( f(x',t+\tau)dx' \) is obtained as

\[
f(x',t+\tau)dx' = dx'\int_{\Delta=-\infty}^{\Delta=\infty} f(x'+\Delta,t)\phi(\Delta)d\Delta. \tag{5.5}
\]

Since \( \tau \) is assumed to be very small compared with \( t \), \( f(x',t+\tau) \) can be expanded in power of \( \tau \) to the first order of \( \tau \) as

* Einstein [1926] is used as a reference for Einstein [1905].
\[ f(x', t + \tau) = f(x', t) + \tau \frac{\partial f(x', t)}{\partial t}. \]  

(5.6)

Further, \( f(x' + \Delta t) \) can be expanded in power of \( \Delta \) to the second order of \( \Delta \) as

\[ f(x' + \Delta t) = f(x', t) + \Delta \frac{\partial f(x', t)}{\partial x'} + \frac{\Delta^2}{2} \frac{\partial^2 f(x', t)}{\partial x'^2}. \]  

(5.7)

Substituting (5.6) and (5.7) into (5.5) yields

\[ f(x', t + \tau) + \tau \frac{\partial f(x', t)}{\partial t} = f(x', t) + \Delta \frac{\partial f(x', t)}{\partial x'} + \frac{\Delta^2}{2} \frac{\partial^2 f(x', t)}{\partial x'^2} \int_{x' - \Delta}^{x' + \Delta} \phi(\Delta) d\Delta. \]

(5.8)

(5.8) can be written as

\[ \tau \frac{\partial f(x', t)}{\partial t} = \frac{1}{2} \frac{\partial^2 f}{\partial x'^2} \int_{-\infty}^{\infty} \Delta \phi(\Delta) d\Delta, \]

(5.9)

because \( \int_{-\infty}^{\infty} \phi(\Delta) d\Delta = 1 \) by (5.3), and \( \int_{-\infty}^{\infty} \Delta \phi(\Delta) d\Delta = 0 \) by (5.4).

Let

\[ \frac{1}{2} \int_{-\infty}^{\infty} \Delta \phi(\Delta) d\Delta = D \cdot \tau, \]

(5.11)

where \( D \) is a constant.

Substituting (5.11) into (5.9) yields

\[ \frac{\partial f(x', t)}{\partial t} = D \frac{\partial^2 f(x', t)}{\partial x'^2}. \]

(5.12)

If (5.12) is considered as the one-dimensional transport equation for diffusion, then \( D \) can be interpreted as the diffusion coefficient.

Consider the case, where \( N_0 \) particles are inserted instantaneously at \( x = 0 \) initially \((t = 0)\) into an infinite one-dimensional medium:

\[ f(x', t = 0) = N_0 \, \delta(x'), \quad -\infty < x' < \infty, \]

(5.13)

where

\[ \delta(x') = \begin{cases} \infty, & x' = 0, \\ 0, & x' \neq 0. \end{cases} \]

At \( x = \pm \infty \), there are no particles, i.e.,

\[ f(x' = \pm \infty, t) = 0, \quad t \geq 0. \]

(5.14)

The solution for the diffusion equation (5.12) subject to the side conditions (5.13) and (5.14) is given by (5.15).

\[ f(x', t) = \frac{N_0}{\sqrt{4\pi D t}} e^{-\frac{x'^2}{4D t}}, \quad t \geq 0, -\infty < x' < \infty. \]

(5.15)

It should be remarked that (5.15) is specifically applicable to an infinite medium in view of the boundary condition (5.14).

\( f(x', t) \) in (5.15) denotes the profile of particle distribution in position and time. Furthermore, \( f(x', t) \) can be interpreted as the probability that the particle displaced in the time \( t \) to a region between \( x' \) and \( x' + dx' \) since the relative frequency of the displacements experienced in successive intervals of time for a single particle will likewise be given by \( f(x', t) \) in (5.15) \([\textit{Einstein}, 1926, \text{notes (10) by \text{Fürth}}]\). Thus, the probability, \( w(x', t) \), that the particle has been displaced in the time \( t \) to a region between \( x' \) and \( x' + dx' \) can be written as

\[ w(x', t) = \frac{N_0}{\sqrt{4\pi D t}} e^{-\frac{x'^2}{4D t}} dx'. \]
\[
\frac{w(x', t)}{N_0} = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x'^2}{4Dt}}, t \geq 0, -\infty < x' < \infty ,
\]
(5.16)

where \(x'\) is a random variable, and \(t\) is a deterministic parameter.

The average displacement \(< x'(t) >\) by diffusion of a particle in time \(t\) from the initial (i.e. \(t=0\)) position is defined as

\[
<x'(t) >= \int_{-\infty}^{\infty} x'w(x', t)dx', t \geq 0 .
\]
(5.17)

Substituting (5.16) into the right-hand side of (5.17) yields

\[
\int_{-\infty}^{\infty} x'w(x', t)dx' = \int_{-\infty}^{\infty} \frac{x'}{\sqrt{4\pi D}} e^{-\frac{x'^2}{4Dt}} dx', t \geq 0 .
\]
(5.18)

By setting \(x'^2/4Dt = r^2\), the right-hand side of (5.18) becomes zero.

\[
\int_{-\infty}^{\infty} \frac{x'}{\sqrt{4\pi Dt}} e^{-\frac{x'^2}{4Dt}} dx' = \frac{\sqrt{4Dt}}{\sqrt{\pi}} \int_{-\infty}^{\infty} re^{-r^2} dr = 0, t \geq 0 .
\]
(5.19)

Thus,

\[
<x'(t) >= 0, t \geq 0 ,
\]
(5.20)

where (5.20) is an application of the second equation of (5.10), i.e. \(<\Delta>=0\).

The average square displacement \(< x'^2(t) >\) by diffusion of a particle in time \(t\) from the initial position is defined as

\[
<x'^2(t) >= \int_{-\infty}^{\infty} x'^2w(x', t)dx', t \geq 0 .
\]
(5.21)

Substituting (5.16) into the right-hand side of (5.21) yields

\[
\int_{-\infty}^{\infty} x'^2w(x', t)dx' = \int_{-\infty}^{\infty} \frac{x'^2}{\sqrt{4\pi D}} e^{-\frac{x'^2}{4Dt}} dx', t \geq 0 .
\]
(5.22)

By setting \(x'^2/4Dt = r^2\), the right-hand side of (5.22) becomes

\[
\int_{-\infty}^{\infty} \frac{x'^2}{\sqrt{4\pi Dt}} e^{-\frac{x'^2}{4Dt}} dx' = \frac{4Dt}{\sqrt{\pi}} \int_{-\infty}^{\infty} r^2 e^{-r^2} dr = \frac{4Dt}{\sqrt{\pi}} \cdot \frac{\sqrt{\pi}}{2} = 2Dt, t \geq 0 .
\]
(5.23)

Thus,

\[
<x'^2(t) >= 2Dt, t \geq 0 ,
\]
(5.24)

where (5.24) is an application of (5.11), i.e. \(<\Delta'^2>=2Dt\).

In summary, \(< x'(t) >\) and \(< x'^2(t) >\) are obtained as

\[
<x'(t) >= 0, t \geq 0 ,
\]
(5.20)

\[
<x'^2(t) >= 2Dt, t \geq 0 .
\]
(5.24)

By the relationship between \(x'(t)\) and \(x(t)\) as defined in (5.2), \(w(x,t), <x(t)>, \text{ and } <x(t)^2>\) can be obtained from \(w(x',t)\) in (5.16), \(<x'(t)\>\) in (5.20), and \(<x'(t)^2>\) in (5.24), respectively.

Because \(w(x,t)dx=w(x',t)dx'\) and \(dx=dx'\) from (5.2), the probability, \(w(x,t)\), that the particle has been displaced in the time \(t\) to a region between \(x\) and \(x+dx\), can be obtained from \(w(x',t)\) by substituting (5.2) into (5.16) as
where \( x \) is a random variable, and \( v_s \) and \( t \) are deterministic parameters.

\(<x(t)>\) denotes the average displacement by diffusion and advection of a particle in time \( t \) from the initial position, and \(<x(t)'>\) denotes the average square displacement by diffusion and advection of a particle in time \( t \) from the initial position. \(<x(t)>\) and \(<x(t)'\) can be obtained by substituting (5.2) into (5.20) and (5.24), respectively, as follows.

Substituting (5.2) into the left-hand side of (5.20) yields
\[
<x(t) - v_t t \geq 0, t \geq 0.
\]

(5.26)

The left-hand side of (5.26) can be calculated as
\[
<x(t) - v_t t > = <x(t) - v_t t > = <x(t) > - v_t t, t \geq 0.
\]

(5.27)

By (5.27) and (5.26), \(<x(t)>\) is obtained as
\[
<x(t) = v_t t, t \geq 0.
\]

(5.28)

where (5.28) shows that the random movement being averaged is deterministic.

Substituting (5.2) into left-hand side of (5.24) yields
\[
<(x(t) - v_t t)^2 \geq 2Dt, t \geq 0.
\]

(5.29)

The left-hand side of (5.29) can be calculated as
\[
<(x(t) - v_t t)^2 \geq (x(t)^2 > <2x(t)v_t t > + (v_t t)^2 > = (x(t)^2 > - 2v_t t <x(t) + (v_t t)^2.
\]

(5.30)

By (5.29) and (5.30),
\[
<x(t)^2 > - 2v_t t <x(t) + (v_t t)^2 = 2Dt
\]

(5.31)

Substituting (5.28) into (5.31) yields
\[
<x(t)^2 = (v_t t)^2 + 2Dt, t \geq 0.
\]

(5.32)

As shown in (5.32), the mean of random variable \( x(t)^2 \) is given by the sum of two deterministic terms, \((v_t t)^2 \) and \( 2Dt \).

(5.28) and (5.32) are the basic relations between \(<x(t)>\) and \( t \), and between \(<x(t)^2>\) and \( t \), respectively. Using (5.28) and (5.32), the variance of \( x(t), i.e. Var(x(t)) \), can be calculated as follow. \( Var(x(t)) \) is defined as
\[
Var(x(t)) = <x(t)^2 > - <x(t)>^2, t \geq 0.
\]

(5.33)

\( Var(x(t)) \) is obtained by substituting (5.28) and (5.32) into the right-hand side of (5.33) as,
\[
Var(x(t)) = 2Dt, t \geq 0.
\]

(5.34)

5.2.3 Derivation of (5.28) and (5.32) from Step Equation for Constant Velocity and Diffusivity in an Infinite One-Dimensional Medium

The step equation in \( x \)-axis given by Tompson et al. [1987] for constant \( v_t \) and \( D \) can be written as
\[
x(t + \tau) - x(t) = v_t \tau + Z \sqrt{2Dt},
\]

(5.35)

where \( x(t + \tau) \) and \( x(t) \) are random variables, \( \tau \) and \( \tau \) are deterministic parameters. \( Z \) is an independent random variable satisfying the two properties [Tompson et al., 1987]
\[ < Z > = 0, \quad (5.36) \]

and
\[ < Z^2 > = 1. \quad (5.37) \]

The step equation for each time interval, i.e. \( t = 0, \tau, 2\tau, \ldots, (m-1)\tau \), can be written by (5.35) as
\[
x(\tau) - x(0) = v_0 \tau + Z_1 \sqrt{2D\tau} \\
x(2\tau) - x(\tau) = v_0 \tau + Z_2 \sqrt{2D\tau} \\
\vdots \\
x((m-1)\tau) - x((m-2)\tau) = v_0 \tau + Z_m \sqrt{2D\tau} \\
x(m\tau) - x((m-1)\tau) = v_0 \tau + Z_m \sqrt{2D\tau}
\]

(5.38)

where \( \tau \) is a constant, \( Z_i \) denotes a realization of the random variable \( Z \) for \( i = 1, 2, \ldots, m \).

A location of a particle in the \( x \)-coordinate at time \( t \), which denotes \( m \) steps of interval \( \tau \) (i.e. \( t = m\tau \)), \( x(t) \), can be obtained for \( x(0) = 0 \) by summing the \( m \) equations in (5.38) as
\[
x(t) = v_0 t + \sqrt{2D\tau} \sum_{i=1}^{m} Z_i. \quad (5.39)
\]

By taking average of (5.39), the average displacement of a particle in time \( t \) from the initial position, \( < x(t) > \), is expressed as
\[
< x(t) >= v_0 t + \sqrt{2D\tau} < \sum_{i=1}^{m} Z_i >
\]
\[
= v_0 t + \sqrt{2D\tau} \sum_{i=1}^{m} < Z_i >. \quad (5.40)
\]

Since
\[
< \sum_{i=1}^{m} Z_i > = \sum_{i=1}^{m} < Z_i >, \quad (5.41)
\]

(5.41) is given by the rule of addition of means [Pitman, 1993].

By (5.36), (5.40) becomes
\[
< x(t) >= v_0 t. \quad (5.42)
\]

(5.42) is the same as (5.28). Thus, the analytically obtained relation between \( < x(t) > \) and \( t \), i.e. \( < x(t) >= v_0 t \), has been derived from the step equation (5.35).

Similar to the above procedures for \( < x(t) > \), the average square displacement of a particle in time \( t \) from the initial position, \( < x(t)^2 > \), is obtained by taking average of square of (5.39) as
\[
< x(t)^2 >= (v_0 t + \sqrt{2D\tau} \sum_{i=1}^{m} Z_i)^2. \quad (5.43)
\]

(5.43) is expressed as
\[
< x(t)^2 >= (v_0 t)^2 + 2D\tau \left( \sum_{i=1}^{m} Z_i \right)^2 + 2v_0 t \sqrt{2D\tau} \sum_{i=1}^{m} Z_i. \quad (5.44)
\]

Since \( v_0, D, \) and \( \tau \) are constant, (5.44) can be written using (5.41) as
\[
< x(t)^2 >= (v_0 t)^2 + 2D\tau \left( \sum_{i=1}^{m} Z_i \right)^2 + 2v_0 t \sqrt{2D\tau} \sum_{i=1}^{m} < Z_i >. \quad (5.45)
\]

Since \( Z_i \) denotes a realization of the random variable \( Z \) for \( i = 1, 2, \ldots, m \), and \( Z_i \) is assumed to be independent [Tompson et al., 1987], (5.45) can be written as
\[
<x(t)^2> = (v_i t)^2 + 2Dt \sum_{j=1}^{m} <Z_j^2> + 2v_i t \sqrt{2Dt} \sum_{j=1}^{m} <Z_j>,
\]  
(5.46)

where
\[
<(\sum_{j=1}^{m} Z_j)^2> = \sum_{j=1}^{m} <Z_j^2>,
\]
(5.47)

where (5.47) denotes the rule of addition of variances [Pitman, 1993] for \(<Z> = 0>.

By (5.36), (5.46) becomes
\[
<x(t)^2> = (v_i t)^2 + 2Dt \sum_{j=1}^{m} <Z_j^2>.
\]
(5.48)

Since \(<Z^2> = 1> as given in (5.37), (5.48) can be written using \(t = m \tau> as
\[
<x(t)^2> = (v_i t)^2 + 2Dt.
\]
(5.49)

where
\[
\sum_{j=1}^{m} <Z_j^2> = \sum_{j=1}^{m} 1 = m.
\]
(5.50)

(5.49) is the same as (5.32). Thus, the analytically obtained relation between \(<x(t)^2> > t>,
\]
i.e. \(<x(t)^2> = (v_i t)^2 + 2Dt>, has been derived from the step equation (5.35).

In summary, the two analytical formulae, \(<x(t) = v_i t> and \(<x(t)^2> = (v_i t)^2 + 2Dt>, have been derived from the

step equation (5.35) for constant \(v_i> and \(D> given by Tompson et al. [1987].

5.2.4 Derivation of Step Equation from (5.28) and (5.32) for Constant Velocity and Diffusivity in an Infinite One-Dimensional Medium

The moments of random variable \(x(t)> are obtained analytically in the Section 5.2.2 as
\[
<x(t) = v_i t>, t \geq 0,
\]
(5.28)
\[
<x(t)^2> = (v_i t)^2 + 2Dt, t \geq 0,
\]
(5.32)
\[
Var(x(t)) = 2Dt, t \geq 0,
\]
(5.34)

where \(x(t)> is a random variable, \(t> is deterministic parameter. (5.34) is obtained from the (5.28) and (5.32) as shown in (5.33).

Since the position of a particle at time \(t + \tau>, i.e. \(x(t + \tau), is determined by the displacement of the particle in a

time interval \(\tau>, i.e. \(\hat{\Delta}, from that of particle at time \(t>, i.e. \(x(t), a random variable \(x(t + \tau) is defined as
\[
x(t + \tau) = x(t) + \hat{\Delta},
\]
(5.51)

where \(x(t)> and \(\hat{\Delta}> are independent random variables.

Since \(t> and \(\tau> are deterministic parameters, the mean and variance of \(x(t + \tau) are obtained by substituting \(t = t + \tau>

into (5.28) and (5.34), respectively, as
\[
<x(t + \tau) = v_i [t + \tau],
\]
(5.52)
\[
Var(x(t + \tau)) = 2D [t + \tau].
\]
(5.53)

Substituting (5.51) into the left-hand side of (5.52) yields
\[
<x(t) + \hat{\Delta} = v_i [t + \tau].
\]
(5.54)

By the rule of addition of means [Pitman, 1993], (5.54) can be written as
\[< x(t) > + < \hat{\Delta} > = v_x [t + \tau ] , \]

or

\[< \hat{\Delta} >= v_x [t + \tau ] - < x(t) > . \]  \hspace{1cm} (5.55)

The mean of \( \hat{\Delta} \) is obtained by substituting (5.28) into (5.55) as

\[< \hat{\Delta} >= v_x \tau . \]  \hspace{1cm} (5.56)

Substituting (5.51) into the left-hand side of (5.53) yields

\[Var(x(t) + \hat{\Delta}) = 2D[t + \tau ] . \]  \hspace{1cm} (5.57)

If \( x(t) \) and \( \hat{\Delta} \) are assumed to be independent random variables, (5.57) can be written by using rule of addition of variances [Pitman, 1993] as

\[Var(x(t)) + Var(\hat{\Delta}) = 2D[t + \tau ], \]

or

\[Var(\hat{\Delta}) = 2D[t + \tau ] - Var(x(t)). \]  \hspace{1cm} (5.58)

The variance of \( \hat{\Delta} \) is obtained by substituting (5.34) into (5.58) as

\[Var(\hat{\Delta}) = 2D\tau . \]  \hspace{1cm} (5.59)

The random variable \( \hat{\Delta} \) denotes the displacement of a particle in a time interval \( \tau \), and has the mean \( v_x \tau \) and variance \( 2D\tau \). From a given random variable \( \hat{\Delta} \), a new random variable \( \Delta' \) can be obtained by the transformation [Kreyszig, 1993] as

\[\Delta' = a\hat{\Delta} + b, \quad a \neq 0, \]  \hspace{1cm} (5.60)

where \( a \) and \( b \) are constant.

In the particular case where \( a = 1/\sqrt{Var(\hat{\Delta})} \) and \( b = -< \hat{\Delta} >/\sqrt{Var(\hat{\Delta})} \), the random variable \( \Delta' \) is defined as \( Z \),

\[Z = \Delta' = \hat{\Delta} - < \hat{\Delta} >/\sqrt{Var(\hat{\Delta})} , \]  \hspace{1cm} (5.61)

and is called the standardized random variable [Kreyszig, 1993] because \( Z \) has mean 0 and variance 1, i.e. \( < Z > = 0 \) and \( < Z^2 > = 1 \).

(5.61) can be written in terms of \( \hat{\Delta} \) as

\[\hat{\Delta} = < \hat{\Delta} > + Z\sqrt{Var(\hat{\Delta})} . \]  \hspace{1cm} (5.62)

Substituting (5.56) and (5.59) into (5.62) yields

\[\hat{\Delta} = v_x \tau + Z\sqrt{2D\tau} , \]  \hspace{1cm} (5.63)

where \( < Z > = 0 \) and \( < Z^2 > = 1 \).

Substituting (5.63) into the second term of right-hand side of (5.51) yields

\[x(t + \tau) = x(t) + v_x \tau + Z\sqrt{2D\tau} , \]  \hspace{1cm} (5.64)

where \( < Z > = 0 \) and \( < Z^2 > = 1 \).

In summary, the step equation (5.64) in \( x \)-axis for constant \( v_x \) and \( D \) has been derived from the analytical formulae \( < x(t) >= v_x t \) in (5.28) and \( < x(t)^2 >= (v_x t)^2 + 2Dt \) in (5.32).
In view of results of Section 5.2.3 and Section 5.2.4, the relations \(< x(t) >= v_t t \) in (5.28) and \(< x(t)^2 >= (v_t)^2 + 2Dt \) in (5.32) form necessary and sufficient conditions of the step equation [Tompson et al., 1987] with constant \( v_t \) to be valid.

5.2.5 Numerical Simulation by Step Equation for Constant Velocity and Diffusivity in an Infinite One-Dimensional Medium

In this section, it is investigated numerically if the resulting distributions of a large number of particles moved by the step equation (5.35) are equivalent to those obtained analytically by (5.25), where \( w(x,t) \) in (5.25) denotes the probability density function of the random variable \( x(t)^* \). For the analytical solution, equations (5.28) and (5.32) are used to check the agreement.

\[
< x(t) >= v_t t, \quad t \geq 0, \tag{5.28}
\]

\[
< x(t)^2 >= (v_t)^2 + 2Dt, \quad t \geq 0, \tag{5.32}
\]

and

\[
x(t + \tau) - x(t) = v_t \tau + Z \sqrt{2Dt}, \quad \tau \geq 0, \tag{5.35}
\]

where \( Z \) is assumed to be an independent random number \({}^*\) with mean of zero and variance of 1, \( D \) [m\(^2\)/yr] is a diffusion coefficient, and is constant in space and in time.

Initially, a single particle is located at \( x=0 \). The particle moves according to (5.35) for each time interval \( \tau \) to a given observation time \( t=mt \). Particle movements for each time interval depend only on the current time, and are not affected by the history of the current time. To generate the random number \( Z \) in (5.35) numerically, the probability density function (PDF) is required. Since only moments of \( Z \) are given by Tompson et al. [1987], in this numerical simulation, a normal distribution with mean 0 and variance 1 is assumed for the PDF of \( Z \).

Since \( t=mt \), the location of the particle \( j \) at time \( t \), i.e. \( x_j(t) \), can be expressed by summing (5.35) for \( t=0, \tau, 2\tau, \ldots, (m-1)\tau \) as shown in (5.39) as

\[
x_j(t) = \left[ v_t t + \sqrt{2Dt} \sum_{i=1}^{m} Z_i \right]. \tag{5.65}
\]

Repeat the above simulation \( N \) times to simulate random walk of \( N \) particles. Since movements of \( N \) particles are independent of other particles, an average displacement of a particle in time \( t \) from the initial position, \(< x(t) >_{num} \), is obtained numerically by averaging arithmetically \( x_j(t) \) over \( N \) as

\[
< x(t) >_{num} = \frac{1}{N} \sum_{j=1}^{N} \left[ v_t t + \sqrt{2Dt} \sum_{i=1}^{m} Z_i \right]. \tag{5.66}
\]

An average square displacement of a particle in time \( t \) from the initial position, \( < x(t)^2 >_{num} \), is obtained numerically by averaging arithmetically \( x_j(t)^2 \) over \( N \) as

\[
< x(t)^2 >_{num} = \frac{1}{N} \sum_{j=1}^{N} \left[ (v_t t + \sqrt{2Dt} \sum_{i=1}^{m} Z_i)^2 \right]. \tag{5.67}
\]

For the numerical simulation, 3 cases are considered as shown in Table 5.1. For all cases, the value for the diffusion coefficient in free water, \( D=0.032\) [m\(^2\)/yr], is used. In case 1, molecular diffusion is the dominant mechanism for transport \( (P_s < 1 \) [Bear, 1972]). In case 2, advection and molecular diffusion are competitive mechanisms \( (0.4 < P_s < 5 \) [Bear, 1972]). In case 3, advection is the dominant mechanism \( (P_s > 2 \sim 10 \) [Tompson et al., 1987]).

\* In the Appendix E, it is shown analytically that the step equation (5.35) satisfies the transport equation by checking if the probability density function, \( w(x,t) \) in (5.25), satisfies the transient transport equation. Also, two dimensional problem of random walk including advection in the \( x-y \) coordinate system is considered in this appendix.

\*\* See Appendix A for random sampling for (log) normal distribution.
Table 5.1  Input data for numerical simulation for 3 cases

<table>
<thead>
<tr>
<th>Cases</th>
<th>( v_x ) [m/yr]</th>
<th>( D ) [m(^2)/yr]</th>
<th>( P_x = v_x L/D ), For ( L=1)m</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.00032</td>
<td>0.032</td>
<td>0.01</td>
</tr>
<tr>
<td>2</td>
<td>0.032</td>
<td>0.032</td>
<td>1.0</td>
</tr>
<tr>
<td>3</td>
<td>3.2</td>
<td>0.032</td>
<td>100.0</td>
</tr>
</tbody>
</table>

Table 5.2  Comparison of \( <x(t)> \) (Analytical and Numerical)

<table>
<thead>
<tr>
<th>( t )</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( &lt;x(t)&gt; )</td>
<td>( &lt;x(t)&gt; )</td>
<td>( &lt;x(t)&gt; )</td>
</tr>
<tr>
<td>10</td>
<td>0.0032</td>
<td>0.0030</td>
<td>6.6</td>
</tr>
<tr>
<td>50</td>
<td>0.016</td>
<td>0.0163</td>
<td>1.9</td>
</tr>
<tr>
<td>100</td>
<td>0.032</td>
<td>0.0325</td>
<td>1.7</td>
</tr>
</tbody>
</table>

\( \xi_1=100\times \| <x(t)>-<x(t)>_{num} / <x(t)> \| \)

Table 5.3  Comparison of \( <x(t)^2> \) (Analytical and Numerical)

<table>
<thead>
<tr>
<th>( t )</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( &lt;x(t)^2&gt; )</td>
<td>( &lt;x(t)^2&gt; )</td>
<td>( &lt;x(t)^2&gt; )</td>
</tr>
<tr>
<td>10</td>
<td>0.640</td>
<td>0.640</td>
<td>4.5E-2</td>
</tr>
<tr>
<td>50</td>
<td>3.200</td>
<td>3.202</td>
<td>4.0E-2</td>
</tr>
<tr>
<td>100</td>
<td>6.401</td>
<td>6.399</td>
<td>2.5E-2</td>
</tr>
</tbody>
</table>

\( \xi_2=100\times \| <x(t)^2>-<x(t)^2>_{num} / <x(t)^2> \| \)

Figure 5.1  Probability density function of \( x(t) \) for 3 cases

For all cases, \( t=1 \) [yr] and \( N=10^7 \) are used. For each case, values of \( <x(t)>_{num} \) and \( <x(t)^2>_{num} \) are obtained numerically by (5.66) and (5.67), respectively, for \( t=10, 50, \) and 100 [yr].

Figure 5.1 shows the numerically obtained probability density function of \( x(t) \) for 3 cases. Table 5.2 and Table 5.3 show the comparisons between \( <x(t)> \) by (5.28) and \( <x(t)>_{num} \) by (5.66), and \( <x(t)^2> \) by (5.32) and \( <x(t)^2>_{num} \) by (5.67), respectively. In Table 5.2, \( \xi_1 \) is defined in the footnote of the table, and denotes the percent difference between \( <x(t)> \) by (5.28) and \( <x(t)>_{num} \) by (5.66). In Table 5.3, \( \xi_2 \) is defined in the footnote of the table, and denotes the percent difference between \( <x(t)^2> \) by (5.32) and \( <x(t)^2>_{num} \) by (5.67).

In Figure 5.1, corresponding values of \( x \)-coordinate to the peaks of each curve denote the mean values of \( x(t) \) for time \( t \). For Case 1 in Figure 5.1(a), since the molecular diffusion is the dominant transport mechanism, the

\* \( \xi_1 \) and \( \xi_2 \) in Tables 5.2 and 5.3 are calculated based on the values of \( <x(t)>_{num} \) and \( <x(t)^2>_{num} \) before truncation.
numerically obtained mean values for different times are close to zero as shown in Table 5.2. Particle displacement from the mean values is primarily determined by $Dt$ as given in (5.34). For case 3 in Figure 5.1(c), since the advection is dominant, the mean values for different times are apart by $v_x t$ as given in (5.28), and particles are displaced around the mean values. For case 2, since the advection and the molecular diffusion are competitive mechanisms, behavior of the particle movements is in between two cases 1 and 3.

There is a difference between numerically obtained distributions in Figure 5.1 and analytical formula (5.25). (5.25) predicts that with a very short time period after $t=0$, some particles can move very fast and exist at $|x| > 0$. In numerical simulation, however, a random number is hardly generated in the “tail” part of the distribution. Thus, numerical simulation cannot generate the analytical formula perfectly. As shown in Table 5.2 and Table 5.3, because numerically calculated $<Z>_\text{num}$ and $<Z^2>_{\text{num}}$ are not 0 and 1, respectively, the percent differences, i.e. $\xi_1$ and $\xi_2$, between analytical solutions and numerical solutions are observed.

For the comparison of $<x(t)>$ as shown in Table 5.2, the percent difference $\xi_1$ is relatively large for case 1 at $t=10 \text{ yr}$, i.e. $\xi_1=6.6\%$, and it decreases as $v_x$ increases or as $t$ increases. For case 1, relatively large differences occur because the molecular diffusion (i.e. statistical random term), which causes the statistical error, is dominant. For case 3, however, the differences are negligibly small since the advection (i.e. deterministic term) is dominant. For case 2, where the advection and molecular diffusion are competing mechanisms for transport, percent differences are negligibly small, and lie in between two extreme cases 1 and 3.

For the comparison of $<x(t)^2>$ as shown in Table 5.3, percent differences $\xi_2$ have similar trends as $\xi_1$, and are negligibly small for all cases.

The differences $\xi_1$ and $\xi_2$ can be diminished either by generating better random number $Z$ (e.g. $<Z>_{\text{num}}=0$, and $<Z^2>_{\text{num}}=1$), or by increasing the number of realizations, i.e. $N$. However, increasing $N$ does not show the same degree as an improvement of results because the numerical fluctuation is proportional to the square root of $N$ [Kienzelbach, 1988].

As shown in Table 5.2 and Table 5.3, the values of $<x(t)>_{\text{num}}$ and $<x(t)^2>_{\text{num}}$ obtained numerically by the step equation (5.35) for constant $v_x$ and $D$ and those obtained analytically by (5.28) and (5.32), respectively, agree well with negligibly small differences. Thus, the analytical formulae (5.28) and (5.32) support the step equation (5.35) for constant $v_x$.

### 5.2.6 Discussion

The step equation for constant velocity and diffusivity given by Tompsoon et al. [1987] has a structure of a particular form of the transformation of random variable $Z$. The standardized random variable $Z$ is useful for the normal distribution. In the step equation, however, $<Z>=0$ and $<Z^2>=1$ have no special meaning because the probability density function of $Z$ is not determined. This implies that the step equation is not unique, and is a particular form of the transformation of the random variable $\hat{X}$, which denotes the displacement of particles in a time interval $\tau$.

In Section 5.2, a mathematical basis of the step equation has been developed for constant velocity and diffusivity. Based on the theory of the Brownian movement [Einstein, 1905], the analytical formulae $<x(t)>$ and $<x(t)^2>$ have been derived (Section 5.2.2). It has been shown numerically that the analytical formulae support the numerical solution obtained by the step equation with negligibly small differences (Section 5.2.5). It has been shown analytically that the analytical formulae $<x(t)>$ and $<x(t)^2>$ are derived from the step equation for constant velocity and diffusivity (Section 5.2.3), and that the step equation for constant velocity and diffusivity is derived from the

---

* $<Z>=0$ and $<Z^2>=1$ are applied in (5.35).
** The standardized random variable $Z$ is practically useful for normal distribution because the exponential term in the probability density function of the normal distribution cannot be integrated by one of the methods of calculus [Kreyszig, 1993]. Thus, by defining $Z=(X-\mu)/\sigma$ where $\mu$ and $\sigma$ are mean and standard deviation of $X$, respectively, the distribution function of $X$ can be calculated using the tabulated values for distribution function of the $Z$ with mean 0 and standard deviation 1, i.e. $<Z>=0$ and $<Z^2>=1$ [Kreyszig, 1993].
*** There are infinitely many possibilities for defining a new random variable for given $X$, e.g. $Z=(X-\mu)/\sigma$, $Z_\sigma=(X-\mu)/3\sigma$, etc. For $Z_\sigma$, two moments are $<Z_\sigma>=0$ and $<Z_\sigma^2>=1/4$. Thus, $X$ can be written in terms of not only $Z$ but also $Z_\sigma$, etc. as $X = \mu + Z_\sigma$, $X = \mu + 2Z_\sigma$, or $X = 2\mu + Z_\sigma^2$, etc.
analytical formulae $<x(t)>$ and $<x(t)^2>$ (Section 5.2.4). Therefore, the analytical formulae are both necessary and sufficient conditions for the step equation for constant velocity and diffusivity.

### 5.3 Governing Equation and Side Conditions

To obtain the step equation (5.1), Tompson et al., [1987] did not take into account the boundary conditions, and implicitly assumed an infinite domain. As shown in Section 5.2, it is essential to know about the domain for random walks for determining the step equation. Particularly, the size of the medium and the boundary conditions must be known to determine a proper step equation. For example, to derive the step equation (5.35) in this study, following conditions are used. (i) Instantaneous source input, (ii) infinite medium boundary condition, (iii) space independent water velocity and diffusivity, and (iv) one dimensional domain. If a certain condition in (i)–(iv) is changed, the step equation should be changed accordingly. Thus, rigorously speaking, the step equation (5.35) obtained for an infinite domain with constant $v$ and $D$ is not applicable to a heterogeneous, finite medium. For more rigorous treatment, a proper step equation should be obtained.

In this study, the step equation (5.35) is applied without any justification to each finite triangular element with constant velocity and diffusivity. Since movements of particles in $x$-coordinate are independent of those in $y$-coordinate, the step equation in $y$-coordinate can be obtained similar to the step equation in $x$-coordinate as shown in (5.68).

Particle movement over discrete time steps is governed by the following random walk algorithms, which are incorporated in the FFDF code, for the advection and the molecular diffusion for the bentonite-filled buffer, FBC, and non-FBC regions,

\[
\begin{align*}
  x(t+\tau) &= x(t) + v_{e,x} \cdot \tau + Z_e \sqrt{2D \tau}, \\
  y(t+\tau) &= y(t) + v_{e,y} \cdot \tau + Z_e \sqrt{2D \tau},
\end{align*}
\]  

(5.68)

where $D = \begin{cases} 
  D_s, & \text{for buffer} \\
  D_f, & \text{for FBC} \\
  D_n, & \text{for Non-FBC}
\end{cases}$

where $x(t+\tau)$ is the location of a particle in $x$ direction at time $t+\tau$, $Z_e$ and $Z_n$ are assumed to be normally distributed independent random numbers at time $t$ with mean of zero and variance of 1. $v_{e,x}$ and $v_{e,y}$ are the uniform water velocities in element $e$ for the buffer and FBC regions in $x$ and $y$ directions, respectively, and are obtained from the water flow analysis as $v_{e,x} = q_{e,x}/\epsilon_e$ and $v_{e,y} = q_{e,y}/\epsilon_e$, where $q_{e,x}$ and $q_{e,y}$ are the Darcy velocity components in element $e$ in $x$ and $y$ directions, respectively. $\epsilon_e$ is the porosity in element $e$. In the Non-FBC region in the NFR, $v_{e,x}$ and $v_{e,y}$ are assumed to be zero. $D_b$, $D_f$, and $D_n$ are the effective molecular diffusion coefficient including tortuosity for the bentonite-filled buffer region, the FBC region, and the non-FBC regions, respectively. $D_b$, $D_f$, and $D_n$ are assumed to be constant in time and space over the whole buffer, FBC, and non-FBC regions, respectively.

As an initial (source) condition, instantaneous input source condition is applied on the surface of the canister. To simulate this condition, $N_b$ particles are initially located uniformly around the surface of the waste canister with a small distance away from it for each realization of DFN and the resulting water flow velocity profile. Because $N_b$ different realizations will be simulated for water flow velocity distributions (or DFN) for a given set of statistics, the movements of total of $N_b \cdot N_e$ particles are considered for the particle transport analysis.

Two boundary conditions are prescribed in this analysis. An absorbing boundary condition is prescribed at the outer boundary ($r=R_2$). A reflecting boundary condition is prescribed at the surface of the waste canister ($r=R_1$). A particle can move into any region (the bentonite-filled buffer, FBC, and non-FBC) before being absorbed at the outer boundary.

* The homogeneous isotropic bentonite-filled buffer is considered. The bentonite swelling by water uptake is neglected.

** Whenever a particle arrives at the boundary, it is not considered any more.
5.3.1 Example for results of particle transport analysis

Particle movement over the discrete time steps is governed by random walk algorithm (5.68). The uniform water velocities \( v_{e,x} \) and \( v_{e,y} \) in element \( e \) in \( x \) and \( y \) directions are obtained from the Darcy velocity components \( q_{e,x} \) and \( q_{e,y} \) and porosity \( \epsilon_0 \) as \( v_{e,x} = q_{e,x}/\epsilon_0 \) and \( v_{e,y} = q_{e,y}/\epsilon_0 \). In the Non-FBC region, \( v_{e,x} \) and \( v_{e,y} \) are assumed to be zero. The effective molecular diffusion coefficient including tortuosity for the bentonite-filled buffer (\( D_b \)), FBC (\( D_f \)), and non-FBC (\( D_n \)) regions are prescribed in this particular example as \( D_b = 3.2 \times 10^{-3} \text{[m}^2\text{/yr]} \), and \( D_f = D_n = 2.1 \times 10^4 \text{[m}^2\text{/yr]} \) [PNC, 1992; Ahn, 1999].

Time step \( \tau \) in (5.68) should be determined properly based on the hydraulic and transport properties for each region. For the diffusion dominant regions, such as the buffer and the non-FBC regions, the time step is determined by \( (\sqrt{D \cdot \tau / L_e}) = \omega_0 \), where \( D = D_b \) for the buffer, and \( D = D_n \) for the non-FBC region. The characteristic length \( L_e \) is \( R_p - R_i \) (i.e. thickness of the buffer) for the buffer and is assumed to be \( (R_2 - R_0)/H \) (i.e. size of a mesh in radial direction) for the non-FBC region. \( H \) is the number of nodes in the radial direction between the interface \( (r=R_0) \) and the outer boundary \( (r=R_2) \). For example, \( H = 11 \) for the 3rd figures from the top for each case in Figure 5.2. \( \omega_0 \) represents that particles pass through an element with \( 1/\omega_0 \) step to make sure that the element is sampled. These time steps for the buffer and non-FBC regions are unchanged while a particle is in those regions for all realizations.

Due to ranging water velocity and molecular diffusion coefficient, a time step for the FBC region should be determined for each element for each realization both by water velocity as \( \tau = \frac{v_L}{L_e} \) and by molecular diffusion as \( \tau = \frac{D_x \cdot \tau}{L_e} = \omega_0 \), where \( v_L = \sqrt{v_{e,x}^2 + v_{e,y}^2} \), \( L_e \) is assumed to be \( (R_2 - R_0)/H \). Smaller between time step obtained by water velocity and time step obtained by diffusivity is used for each element to make sure that particles experience at least \( 1/\omega_0 \) time steps in that element. In this study, \( \omega_0 = 0.05 \) and \( H = 11 \) are prescribed to determine the time step \( \tau \).

As the initial (source) condition, an instantaneous input source condition is applied on the surface of the canister. 100 particles are initially located uniformly a small distance (0.01m) away from the canister for each realization of water flow velocity profile as shown in Figure 5.2 (a). The Darcy velocity profile shown in Figure 3.21 is considered in this example.

Two boundary conditions are prescribed. An absorbing boundary condition at the outer boundary \( (r=R_2=5m) \) and a reflecting boundary condition at the surface of the waste canister \( (r=R_p=0.35m) \). For the purpose of numerical calculation, actual absorbing boundary condition is prescribed not at \( r=R_2 \) but at \( r=R_2' \). Imaginary absorbing boundary is considered at \( r=R_2' \) with radius of 4.98m to avoid the numerical error due to gap regions, which are created by triangular element discretization in a circular domain, and are neither FBC nor Non-FBC regions.

Figure 5.2 (a), (b), and (c) show the location of the particles for particular time steps of zero, 10, and 200. The physical time for a particle in the model can be obtained by multiplying the number of time step and the magnitude of each time step of the particle. In Figure 5.2 (b), because all 100 particles remain in the buffer region, physical time for all particles is the same, and is calculated as \( 10 \times \tau \). In Figure 5.2 (c), however, each particle has its own time history because time step for each particle is different depending on its location, i.e. buffer, non-FBC, and elements in FBC.

The residence time is obtained for all particles by observing the detailed tracks of each particle. Figure 5.3 shows the tracks of all particles until they are absorbed at the imaginary absorbing boundary \( (r=R_2') \). Particles can move anywhere in the buffer region because the molecular diffusion is dominant \( (P_c < 10^5) \) mechanism in the buffer. Particles move along the streamlines in the FBC region since the advection is dominant \( (P_c < 10^5) \).

Sharp changes are observed in the tracks of particles in Figure 5.3 due to the uniform water velocity for each element but different from element to element. More significant sharp changes are observed in the regions close to non-FBC region and close to the outer boundary. Figure 5.4 (a), (b), and (c) show the tracks of all particles for the same input data as Figure 5.2 and Figure 5.3 except for the higher diffusion coefficient as \( D_f = D_n = 2.1 \times 10^2 \text{[m}^2\text{/yr]} \) (a), \( D_f = D_n = 2.1 \times 10^4 \text{[m}^2\text{/yr]} \) (b), and \( D_f = 2.1 \times 10^4 \text{[m}^2\text{/yr]} \) (c), respectively. In Figure 5.4 (c), the diffusion is important transport mechanism as well as the advection whereas the advection is dominant in Figure 5.4 (a).

* Detail about the imaginary absorbing boundary is given in Appendix F
Figure 5.2 Particle transport for different time steps 0, 10τ, and 200τ, for water velocity in Figure 3.21

Figure 5.3 Tracks of all particles for water velocity in Figure 3.21

Figure 5.4 Tracks of all particles for water velocity in Figure 3.21 for higher diffusion coefficients in the NFR (FBC and non-FBC) region than Figure 5.3.

5.4 Numerical results

Particle transport analysis has been performed on top of the flow model for 100 realizations for 9 cases shown in Table 3.4.

Effective molecular diffusion coefficient including tortuosity for the bentonite-filled buffer, FBC, and non-FBC regions, are prescribed as $D_b=3.2\times10^{-3}$, $D_f=3.2\times10^{-2}$, and $D_n=2.1\times10^{-4} \text{ m}^2/\text{yr}$, respectively [Neretnieks, 1980; PNC, 1992; Ahn, 1999]. $\omega_0=0.05$ and H=11 are also used.
In this section, numerical explorations are made by FFDF to investigate effects of the heterogeneity of the NFR and effects of the modeling approach for the NFR on (1) the residence time of particles, and (2) the mass absorption rate at the outer boundary.

5.4.1 Effects of Heterogeneity of NFR and Modeling Approach for NFR on Residence Time

The residence time, which is defined as the time for a particle to take until it arrives at the (imaginary) absorbing outer boundary \( r=\frac{R}{2} \), is obtained by observing the detailed tracks of each particle.

5.4.1.1 Effects of Length Distribution

Figure 5.5 shows the CDFs of the residence times of \( 10^4 \) particles for a heterogeneous NFR for 9 cases based on the water velocity profiles obtained in Section 3.6.2.2. Figure 5.5 (a), (e), and (i) show the CDFs of the residence times for the entire model space for cases A, B, and C, cases D, E, and F, and cases G, H, and I, respectively. The residence time for the entire model space is simply denoted as the residence time in this study.

Figure 5.5 (b), (f), and (j), and (c), (g), and (k) shows the residence times for the buffer, FBC, and Non-FBC regions, respectively. The residence times for the buffer, FBC, and Non-FBC regions, respectively. The residence times for the buffer, FBC, and Non-FBC regions denote the buffer residence time, FBC residence time, and Non-FBC residence time, respectively. The median, mean and standard deviation of the residence times and the buffer residence times are shown in Table 5.4. The median, mean and standard deviation of the FBC and Non-FBC residence times are shown in Table 5.5.

Table 5.4 Statistics of Residence Time for the Entire Model Space and the Buffer Region for 9 Cases

<table>
<thead>
<tr>
<th>Case</th>
<th>Residence time [yr]</th>
<th>Buffer residence time [yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Median</td>
<td>Mean</td>
</tr>
<tr>
<td>A</td>
<td>2.12E+02</td>
<td>5.07E+02</td>
</tr>
<tr>
<td>B</td>
<td>6.37E+01</td>
<td>9.33E+01</td>
</tr>
<tr>
<td>C</td>
<td>4.92E+01</td>
<td>6.45E+01</td>
</tr>
<tr>
<td>D</td>
<td>3.16E+02</td>
<td>8.77E+02</td>
</tr>
<tr>
<td>E</td>
<td>1.40E+02</td>
<td>2.34E+02</td>
</tr>
<tr>
<td>F</td>
<td>5.99E+01</td>
<td>8.52E+01</td>
</tr>
<tr>
<td>G</td>
<td>7.31E+01</td>
<td>1.18E+02</td>
</tr>
<tr>
<td>H</td>
<td>5.45E+01</td>
<td>7.84E+01</td>
</tr>
<tr>
<td>I</td>
<td>4.89E+01</td>
<td>6.42E+01</td>
</tr>
</tbody>
</table>

Table 5.5 Statistics of Residence Time for the FBC and Non-FBC Regions for 9 Cases

<table>
<thead>
<tr>
<th>Case</th>
<th>FBC residence time [yr]</th>
<th>Non-FBC residence time [yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Median</td>
<td>Mean</td>
</tr>
<tr>
<td>A</td>
<td>7.58E-04</td>
<td>1.56E-01</td>
</tr>
<tr>
<td>B</td>
<td>1.70E-04</td>
<td>2.20E-04</td>
</tr>
<tr>
<td>C</td>
<td>1.07E-04</td>
<td>1.17E-04</td>
</tr>
<tr>
<td>D</td>
<td>1.45E-03</td>
<td>1.24E+00</td>
</tr>
<tr>
<td>E</td>
<td>3.12E-04</td>
<td>2.74E-02</td>
</tr>
<tr>
<td>F</td>
<td>1.46E-04</td>
<td>1.84E-04</td>
</tr>
<tr>
<td>G</td>
<td>2.61E-04</td>
<td>1.05E-03</td>
</tr>
<tr>
<td>H</td>
<td>1.58E-04</td>
<td>1.81E-04</td>
</tr>
<tr>
<td>I</td>
<td>9.83E-05</td>
<td>1.04E-04</td>
</tr>
</tbody>
</table>

* Mass absorption rate at the outer boundary is used as a comparable quantity to mass release rate at the boundary. See Section 5.4.2 for more details.
Figure 5.5  Cumulative distribution functions of the residence times of $10^4$ particles.
The residence times of $10^4$ particles for 9 cases are calculated by observing the detailed tracks of each particle. Particles are initially located uniformly around the surface of the waste canister with a small distance (0.01m) away from the canister. Water flow rate in the buffer region is very small as shown in Table 3.6 for all 9 cases. The water-saturated bentonite-filled buffer region is assumed to be homogeneous isotropic with the effective molecular diffusivity of $3.2 \times 10^{-3} \text{ m}^2/\text{yr}$. Due to a very small Peclet number ($P_e \sim 10^6$) in the buffer region for all realizations for 9 cases, molecular diffusion is dominant for transport.

For cases G, H, and I in Figure 5.5 (j), the differences of the buffer residence times for these 3 cases are negligibly small. This is because the non-FBC regions for these cases occupy small areas in the NFR due to well-connected fracture network as shown in Figure 3.27, and thus, particles out of the buffer region move along the streamline without re-entering the buffer region. However, for other cases (A–F) as shown in Figures (b) and (l), particles getting out of the buffer region can re-enter the buffer region by molecular diffusion from the non-FBC and the FBC region due to slow advection. These particles, which re-entered the buffer region, make the difference of the buffer residence times for cases from A to F.

Particles released from the buffer region move either into FBC or to Non-FBC region by molecular diffusion. For cases B, C, F, G, H, and I, the networks are well connected (see Figure 3.27), so thus have a greater FBC region which covers most of the model space. For these cases, most particles out of the buffer move along the streamline around the buffer to the outer boundary without entering the non-FBC region. These particles have zero non-FBC residence time as shown in Table 5.6. The FBC residence times range narrowly from $10^5$ to $10^2$ yr for cases B, C, F, G, H, and I.

**Table 5.6  Number of Particles Which Has Zero Non-FBC Residence Times**

<table>
<thead>
<tr>
<th>Case</th>
<th>Number of particles which has zero Non-FBC residence times for $10^4$ particles for each case</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>861</td>
</tr>
<tr>
<td>B</td>
<td>6659</td>
</tr>
<tr>
<td>C</td>
<td>9676</td>
</tr>
<tr>
<td>D</td>
<td>433</td>
</tr>
<tr>
<td>E</td>
<td>1772</td>
</tr>
<tr>
<td>F</td>
<td>7553</td>
</tr>
<tr>
<td>G</td>
<td>5618</td>
</tr>
<tr>
<td>H</td>
<td>8281</td>
</tr>
<tr>
<td>I</td>
<td>9882</td>
</tr>
</tbody>
</table>

For cases A, D, and E, a greater non-FBC region exists due to not well-connected networks (see Figure 3.27). Particles in the non-FBC region can move into the FBC region by diffusion. If particles move into the FBC, where the water velocity is very small, they take a relatively long time to arrive at the outer boundary, resulting in the wide variation of the FBC residence times as shown in Figure 5.5 (c) and (g). The FBC residence times for these cases are ranged widely from $10^5$ to $10^{-2}$ yr.

If the particle does not move into the FBC region before it gets out of the model space, zero FBC residence time occurs. 2 out of $10^4$ particles have zero FBC residence time for case A, and 1 out of $10^4$ particles for case D. This is possible when the particle moves into the Non-FBC region directly from the buffer region and is absorbed at the outer boundary without going into the FBC region. Zero FBC residence time is not observed for cases B, C, E, F, G, H, and I.

If a particle moves into the FBC region directly from the buffer region and was absorbed at the outer boundary, zero non-FBC residence time occurs. The number of particles, which has zero non-FBC residence time, is shown in Table 5.6. Due to the occurrence of zero non-FBC residence time, the CDFs of the non-FBC residence times range not from the zero but from the ratio of the number of particles whose have zero non-FBC residence time to the $10^4$ particles as shown in Figure 5.5 (d), (h), and (l).

The residence time of a particle in the entire model space is obtained by summing the residence times in the buffer, FBC, and non-FBC regions. The residence times for $10^4$ particles are summarized in Table 5.4 and Table 5.5.

The FBC residence time shows that the median values range between $10^4$ yr and $10^3$ yr, whereas the residence time in the entire model space has the median values ranging between 50 yr and 300 yr. Thus, the contribution of

---

* The FBC region especially adjacent to the non-FBC region usually has an extremely low water velocity.
FBC region to the residence time in the entire model space is negligible. On the other hand, residence times in the buffer and in the non-FBC are comparable to the residence time.

For a medium with a greater FBC region due to well-connected fracture network such as cases B, C, F, G, H, and I, the residence time is mainly determined by the buffer residence time. For a medium with a smaller FBC region due to not well-connected fracture network such as cases A, D, and E, the residence time is mainly determined by the non-FBC residence time.

5.4.1.2 Effects of Aperture Correlation

Particle transport has been simulated based on the water velocity profiles obtained in Section 3.6.2.3 for a model with a heterogeneous NFR for cases A and B with the length-aperture correlation (2.7).

Figure 5.6 and Figure 5.7 show the CDFs of the residence times of $10^4$ particles both for the cases with and without the length-aperture correlation for cases A and B, respectively. In Figure 5.6 and Figure 5.7, the dashed lines labeled as “correlated” represent the CDF for the correlated aperture with the length of fracture by (2.7). The solid lines in the figures labeled as “uncorrelated” are the same as in Figure 5.5 (a)–(d). For uncorrelated case, aperture of a fracture segment is generated based on the given lognormal distribution as shown in Table 3.3. The median, mean and standard deviation of the residence times and the buffer residence times both for the cases with and without the length-aperture correlation for cases A and B are shown in Table 5.7. The median, mean and standard deviation of the FBC and Non-FBC residence times are shown in Table 5.8.

![Figure 5.6](image)

Cumulative distribution functions of the residence times for correlated aperture for case A
Table 5.7  Statistics of Residence Time for the Entire Model Space and the Buffer Region for Correlated Aperture for Cases A and B

<table>
<thead>
<tr>
<th>Case</th>
<th>Residence time [yr]</th>
<th>Buffer residence time [yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Median</td>
<td>Mean</td>
</tr>
<tr>
<td>A</td>
<td>2.63E+02</td>
<td>6.29E+02</td>
</tr>
<tr>
<td></td>
<td>(2.12E+02)</td>
<td>(5.07E+02)</td>
</tr>
<tr>
<td>B</td>
<td>6.04E+01</td>
<td>8.98E+01</td>
</tr>
<tr>
<td></td>
<td>(6.37E+01)</td>
<td>(9.33E+01)</td>
</tr>
</tbody>
</table>

The values in parentheses are for uncorrelated case, same as in Table 5.4

Table 5.8  Statistics of Residence Time for the FBC and non-FBC Regions for Correlated Aperture for Cases A and B

<table>
<thead>
<tr>
<th>Case</th>
<th>FBC residence time [yr]</th>
<th>Non-FBC residence time [yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Median</td>
<td>Mean</td>
</tr>
<tr>
<td>A</td>
<td>1.97E-05</td>
<td>1.57E-01</td>
</tr>
<tr>
<td></td>
<td>(7.58E-04)</td>
<td>(1.56E-01)</td>
</tr>
<tr>
<td>B</td>
<td>4.96E-06</td>
<td>1.26E-05</td>
</tr>
<tr>
<td></td>
<td>(1.70E-04)</td>
<td>(2.20E-04)</td>
</tr>
</tbody>
</table>

The values in parentheses are for uncorrelated case, same as in Table 5.5

Figure 5.7  Cumulative distribution functions of the residence times for correlated aperture for case B
As shown in Figure 5.6 (b) and Figure 5.7 (b), the difference of the buffer residence times between the case with the length-aperture correlation and the case without the correlation is negligible because the fracture networks are identical except for apertures both for the cases with and without the length-aperture correlation for each realization.

As shown in Figure 5.6 (c) and Figure 5.7 (c), the FBC residence time for the correlated case is smaller than that for the uncorrelated case due to the higher water velocity for the correlated case than that for the uncorrelated case. In Figure 5.6 (c), the FBC residence time for the correlated case ranges widely from $5.79 \times 10^{-8}$ to $3.43 \times 10^1$ yr than that for the uncorrelated case as from $3.6 \times 10^{-5}$ to $3.19 \times 10^1$ yr. This is because the flow becomes more heterogeneous for the correlated case, where the water flows through a few long fractures (see Section 3.6.2.3).

The difference of the residence times in the entire model space both for the cases with and without the length-aperture correlation is negligible for cases A and B because the contribution of the FBC residence time is negligible.

5.4.1.3 Effects of Modeling Approach for NFR

To observe effects of modeling approach for the NFR, particles transport has also been simulated for a homogenized NFR by the uniformization for 100 realizations for nine cases in Table 3.4. The median, mean, and standard deviation of the residence times for the entire model space, buffer region, and FBC regions are shown in Table 5.9 and Table 5.10. In the homogenized NFR by the uniformization, the entire NFR is considered as a FBC region, and is represented by single values of hydraulic properties. Thus, non-FBC region has been smeared with FBC region.

### Table 5.9 Statistics of Residence Times for the Entire Model Space and the Buffer Region for 9 Cases by the Uniformization

<table>
<thead>
<tr>
<th>Case</th>
<th>Residence time [yr]</th>
<th>Buffer residence time [yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Median</td>
<td>Mean</td>
</tr>
<tr>
<td>A</td>
<td>4.49E+01</td>
<td>5.79E+01</td>
</tr>
<tr>
<td>B</td>
<td>4.42E+01</td>
<td>5.78E+01</td>
</tr>
<tr>
<td>C</td>
<td>4.49E+01</td>
<td>5.86E+01</td>
</tr>
<tr>
<td>D</td>
<td>4.46E+01</td>
<td>5.83E+01</td>
</tr>
<tr>
<td>E</td>
<td>4.52E+01</td>
<td>5.83E+01</td>
</tr>
<tr>
<td>F</td>
<td>4.49E+01</td>
<td>5.81E+01</td>
</tr>
<tr>
<td>G</td>
<td>4.46E+01</td>
<td>5.75E+01</td>
</tr>
<tr>
<td>H</td>
<td>4.56E+01</td>
<td>5.87E+01</td>
</tr>
<tr>
<td>I</td>
<td>4.56E+01</td>
<td>5.87E+01</td>
</tr>
</tbody>
</table>

### Table 5.10 Statistics of FBC Residence Times for 9 Cases by the Uniformization

<table>
<thead>
<tr>
<th>Case</th>
<th>FBC residence time [yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Median</td>
</tr>
<tr>
<td>A</td>
<td>6.65E-05</td>
</tr>
<tr>
<td>B</td>
<td>6.24E-05</td>
</tr>
<tr>
<td>C</td>
<td>6.44E-05</td>
</tr>
<tr>
<td>D</td>
<td>6.40E-05</td>
</tr>
<tr>
<td>E</td>
<td>6.42E-05</td>
</tr>
<tr>
<td>F</td>
<td>6.24E-05</td>
</tr>
<tr>
<td>G</td>
<td>6.41E-05</td>
</tr>
<tr>
<td>H</td>
<td>6.41E-05</td>
</tr>
<tr>
<td>I</td>
<td>6.27E-05</td>
</tr>
</tbody>
</table>
For a model with a homogenized NFR, the residence time distributions are mainly determined by the buffer region because the non-FBC region does not exist and the contribution of the FBC residence time to the residence time is negligible due to the small magnitude of the FBC residence time with median and median of order of $10^{-2}$ yr. Thus, the residence time distributions for a model with a homogenized NFR are always smaller than those for the heterogeneous NFR as shown in Figure 5.8.

The difference in the residence time between the heterogeneous NFR and the homogenized NFR is negligible for cases C, F, H, and I. For cases A, D, and E, the difference of the residence time is significant because the Non-FBC covers a greater area of NFR.

Figure 5.9 shows the comparison of the 90% confidence intervals of residence times for the entire model space between a model with a homogenized NFR by the uniformization and a model with a heterogeneous NFR by the local homogenization for 100 realizations for 9 cases. Symbols ♦ and ▲ represent the median of the total discharges at the outer boundary for 100 realizations for each case for a heterogeneous NFR and for a homogenized NFR, respectively.

Observations from the comparison of the Figure 5.9 are as follows.
First, for the network with the same fracture geometry parameters, such as cases A, B, and C, a greater connectivity exhibits a shorter residence time of particles because of higher flow rate and smaller water-stagnant regions, which cause the delay of the particle movement by molecular diffusion.

Second, the residence times for the entire model space for a homogenized NFR are shorter and range narrowly than those for a heterogeneous NFR.

Third, the residence times for the homogenized NFR for all cases are almost identical, whereas those for the heterogeneous NFR are strongly dependent on the heterogeneity of the NFR. This result occurs due to following reasons. For the homogenized NFR, because the non-FBC region does not exist and the contribution of the FBC residence time to the residence time for the entire model space is negligible, the residence time in the entire model space is mainly determined by the buffer region, which is identical for all cases, and is independent on the heterogeneity of the NFR.

Fourth, a difference between the local homogenization and the uniformization decreases as the connectivity increases. For cases C, F, and I with connectivity of 6.0, the local homogenization and uniformization give similar results.

5.4.2 Effects of Heterogeneity of NFR and Modeling Approach for NFR on Mass Absorption Rate

In some previous performance assessment studies, the mass release rate of radionuclides was obtained as one of the outputs from the transport analysis in the near field, and used as input data for the far-field transport [Gylling, 1997; JNC, 2000 (Vol. 1, p.V-5)]. In this study, as a comparable quantity to the particle release rate at the outer boundary, particle absorption rate [particles/time] at the boundary is considered. Particle absorption rate is obtained by counting the number of particles being absorbed at the boundary per unit time. For the comparison, the fractional absorption rate [yr⁻¹] at the outer boundary is calculated by normalizing the particle absorption rate by the total number of particles.

Figure 5.10 shows the fractional absorption rate at the outer boundary for a model with a heterogeneous NFR by the local homogenization ((a)~(c)) and a model with a homogenized NFR by the uniformization ((d)~(f)) for 10⁴ particles of cases A, B, and C. Cases A, B, and C have the same statistics of the fracture geometry parameters as shown in Table 3.3 and Table 3.4 except for the connectivity. For case A, the network is sparse due to the small connectivity as 1.2, and has irregular shape of FBC due to the large standard deviation of the fracture length. By increasing the connectivity to 3.0 (case B) and to 6.0 (case C) for the same fracture geometry parameters, the network becomes better connected and covers a greater area of the NFR.
Because fractional absorption rate at the outer boundary is identical to the probability density function (PDF) of the particles being absorbed at the outer boundary per unit time, i.e., differential forms of CDFs of the residence times in Figure 5.8 with respect to the time, detailed explanations in previous sections are valid for Figure 5.10. Table 5.11 shows the maximum fractional absorption rate and time when the maximum fractional absorption occurs at the outer boundary both for heterogeneous NFR and homogenized NFR for cases A, B, and C.

Figure 5.10 (a), (b), and (c) show that the strong dependency of the mass absorption rate at the outer boundary on the connectivity. For the model with a heterogeneous NFR, the mass of radionuclide absorbed at the outer boundary increases as the connectivity increases for the same fracture geometry parameters.

For case A, about 4 times greater mass is absorbed at the outer boundary with shorter residence time with a homogenized NFR (Figure 5.10 (d)) than that with a heterogeneous NFR (Figure 5.10 (a)). For case C, however, the models with the homogenized NFR and the model with the heterogeneous NFR yield the similar mass absorption rate at the outer boundary.

Figure 5.10 (d), (e), and (f) show that the mass absorption rate at the outer boundary by the homogenized NFR is almost identical for 3 cases, whereas the strong dependency on connectivity is observed for the heterogeneous NFR as shown in Figure 5.10 (a), (b), and (c).

Table 5.11  Maximum Fractional Absorption Rate at the Outer Boundary

<table>
<thead>
<tr>
<th>Case</th>
<th>Model with a heterogeneous NFR</th>
<th>Model with a homogenized NFR</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Maximum fractional absorption rate [yr⁻¹]</td>
<td>Time for maximum fractional absorption rate [yr]</td>
</tr>
<tr>
<td>A</td>
<td>4.6E-3</td>
<td>54.4</td>
</tr>
<tr>
<td>B</td>
<td>1.2E-2</td>
<td>38.1</td>
</tr>
<tr>
<td>C</td>
<td>1.6E-2</td>
<td>19.5</td>
</tr>
</tbody>
</table>

Figure 5.10  Fractional absorption rates at the outer boundary for 10⁴ particles for cases A, B, and C with heterogeneous NFR ((a)–(c)) and homogenized NFR ((d)–(f))
5.5 Conclusions

A model for the particle transport analysis has been established for the one-waste canister configuration based on the flow model developed in Chapter 3. A mathematical basis of the random walk for constant water velocity and diffusivity has been developed. Particle transport is simulated by a random walk tracking method (RWTM) for the advection and molecular diffusion. Subroutines for particle transport have been implemented into FFDF code.

Effects of the heterogeneity of the NFR (i.e. connectivity) on the residence time and the mass absorption rate are investigated for a model with a heterogeneous NFR by local homogenization by performing the particle transport analysis for different sets of statistics of fracture geometry parameters.

Numerical results show that:
- The residence times of particles in the flow-bearing region (i.e. FBC), water-stagnant region (i.e. Non-FBC), and the entire model space distribute more widely, as the connectivity of the fracture network becomes smaller (see Figure 5.5).
- The residence time in the entire model space is determined mainly by that in the buffer region for a network with a large connectivity. If the connectivity is small, the residence in the water-stagnant region also becomes comparable to that in the buffer (see Figure 5.5).
- A network with a greater connectivity exhibits a shorter residence time of particles and a higher mass absorption rate at the outer boundary because of a higher flow rate and smaller water-stagnant regions (see Figure 5.9 and Figure 5.10).
- A difference in the residence times both for the cases with and without the length-aperture correlation is negligible because the contribution of the residence time in the flow-bearing region is negligibly small (see Figure 5.6 and Figure 5.7).

Effects of modeling approaches for the NFR have been investigated by comparing the residence time of particles and the mass absorption rate at the outer boundary between the heterogeneous NFR by local homogenization and the homogenized NFR by uniformization.

Numerical results show that:
- The residence time obtained for a model with a homogenized NFR is smaller, and ranges more narrowly than that obtained for a model with a heterogeneous NFR (see Figure 5.9).
- The fractional mass absorption rate for the homogenized NFR is larger, and distributes more narrowly than that for the heterogeneous NFR (see Figure 5.10).
- Difference in the residence time and the fractional mass absorption rate between the homogenized NFR and the heterogeneous NFR becomes greater as the connectivity becomes smaller (see Figure 5.9 and Figure 5.10).
- The homogenized NFR yields almost same residence time and the absorption rate of particles for different characteristics of the NFR (i.e. fracture geometry parameters, connectivity), whereas those obtained for a heterogeneous NFR are sensitive to the characteristics of the NFR (see Figure 5.9 and Figure 5.10).
- For the homogenized NFR, the residence time of particles is mainly determined by the bentonite-filled buffer region (see Table 5.9).

The homogenized NFR cannot reproduce the long tail of distribution for residence time on the large value side, especially for low connectivity cases. However, the homogenized NFR gives conservative results, i.e., underestimation of the residence time and overestimation of the mass absorption rate. For a conservative safety assessment, using a homogenized NFR assumption may be justified by this fact.

While the near-field model treating the heterogeneous NFR as a homogeneous continuum yields conservative results for particle transport, it might not be used for site selection because it can not differentiate candidate rocks.

5.6 Limitations & Future Studies

In this dissertation, waste dissolution, sorption, and radioactive decay are neglected for the transport analysis. Cases in this study can be considered as radionuclide with long half-life and low sorption distribution coefficient, such as I-129.

After failure of the canister (1000 years), nuclides in the waste have been assumed to be released instantaneously by contacting with groundwater, and to be distributed homogeneously around the canister with a small distance (0.01m) away from it. An instantaneous pulse input has been used as the initial source condition. The instantaneous pulse input condition is used in this analysis because the residence time for a more generalized release
model can be obtained by convolution. For HLW repository performance assessment, realistic conditions, such as congruent release and solubility-limit release, should be incorporated.

This study shows that the analytical formulae \( < x(t) > = v_f \) and \( < x(t)^2 > = (v_f)^2 + 2Dt \) derived in Section 5.2.2 are both necessary and sufficient conditions for the step equation only for constant velocity and diffusivity. Further study is required for the space and time dependent water velocity and diffusivity.

In this chapter, for the simulation of the particle transport, the step equation obtained for an infinite domain with constant \( v \) and \( D \) has been applied without any justification to the current one-waste canister model, which consists of a large number of finite triangular elements. A proper step equation is required for more rigorous treatment in the future.

The mesh size affects the determination of the water-flowing region (\( i.e. \) FBC) and water-stagnant region (\( i.e. \) Non-FBC) for a model with a heterogeneous NFR. For the same fracture network, the flow-flowing region or water-stagnant region is changed if the different mesh size applies. Thus, we need further studies to investigate the effect of the finite element mesh on the particle transport in the future.
6. Evaluation of Coefficient C in Kozeny-Carman Equation

6.1 Introduction

The coefficient C in Kozeny-Carman equation (3.3) for the local homogenization in Section 3.4.1, and (3.9) for the uniformization in Section 3.4.2 is assumed to be unity in the numerical analysis for the water flow (Chapter 3). In this chapter, the coefficient C is evaluated.

If C is uniform over the model space and identical for both x and y directions, then C is factored out in (3.17). In such a case, the potential distribution, \( \phi(x, y) \), obtained in Chapter 3 applies for any constant value of C. However, because the value of the water discharge is evaluated by (3.15) and (3.16), the water discharge is proportional to the value of C. According to Carman [1956], the coefficient C is dependent on the shape of cross-sectional area normal to flow \( (c_0) \) and the tortuosity \( (\tau) \). One of the ways to express the coefficient C is given by Carman [1956] as

\[
C = \tau / c_0,
\]

where \( \tau \) is a tortuosity factor and is given by

\[
\tau = \left( \frac{L}{L'} \right)^2,
\]

where \( L \) and \( L' \) are defined by Carman [1956] as the length of the test-piece, and the average length of the path of a streamline through the pore space, respectively.

The values of C are always less than unity because \( \tau \leq 1 \) since \( L \leq L' \) and \( c_0 > 1 \) [Carman, 1956]. For a medium with a rectangular cross-sectional area (i.e. a parallel slit), the value of \( c_0 \) is 3 [Carman, 1956].

Tortuosity is related to the geometrical shape of the path for water flow. In this chapter, the tortuosity is quantitatively estimated by using detailed information about the water flow paths through the fracture network. In this study, using a single value of tortuosity \( \tau \) obtained for the entire FBC, a single value of coefficient C is calculated by (6.1).

6.2 Tortuosity

Tortuosity has been defined as a ratio between the average length of the path of a streamline, \( L' \), and the length of test piece. L. Bear [1972] defined the tortuosity as \( (L/L')^2 \) while Kozeny [1927] defined the tortuosity as \( (L/L') \). Carman [1937; 1956] defined the tortuosity as \( (L'/L)^2 \).

Kozeny [1927] obtained the velocity \( v_k \) through the granular bed based on apparent path \( L \) along the streamline by solving the Navier-Stokes equations for all channels through a cross section normal to flow. The velocity \( v_k \,[m/s] \) is defined as the quotient of the amount of water discharges to the total cross sectional area. Kozeny assumed that the granular bed is equivalent to a stream tube with total cross sectional area consisting of a group of parallel channels with an equivalent open cross section. In order to take into account the actual complicated path of length \( L' \), Kozeny introduced the reduced pressure gradient term corrected with \( (L/L') \).

Carman [1937] modified the velocity \( v_k \) derived by Kozeny [1927] as \( v_k(L/L') \) because the actual path pursued by an element of the fluid is tortuous. This newly introduced term \( (L/L') \) by Carman and the reduced pressure gradient term \( (L/L') \) by Kozeny yield the definition (6.2) \( (L/L')^2 \). The term \( (L'/L)^2 \) is called the tortuosity factor by Carman [1956].

Bear [1972] explained the tortuosity factor by Carman [1937] by introducing the effects of tortuosity in two ways. The term \( (L/L') \) introduced by Kozeny [1927] is due to the influence of tortuosity on the driving force. Another term \( (L/L') \) introduced by Carman [1937] is due to the effect of tortuosity on the velocity.

Carman [1937] found that the average angle between the streamline and the x-axis is \( \theta_{av} = 45^\circ \) from the motion of a colored streamline through a bed of large glass spheres. Carman [1937] adopted the average angle \( \theta_{av} \) of 45° to the direction of flow and hence used \( L/L' = \cos \theta_{av} = 1/\sqrt{2} \). However, because the angle \( \theta \) between the streamline and x-axis could not have a constant value but varied from position to position in the porous medium [Fowler, et al., 1940], Carman [1956] claimed that the correct average for \( (L/L')^2 \) should not be \( \cos^2 \theta_{av} \) but \( < \cos^2 \theta > \) as

\[
\left( \frac{L}{L'} \right)^2 = \cos^2 \theta > .
\]
where \( \langle \cos^2 \theta \rangle \) denotes the average value of \( \cos^2 \theta \) taken over all values of local angle \( \theta \) in the porous medium.

It should be noted that (6.3) was obtained for the incompressible fluid and viscous flow through a block of porous medium of constant cross-sectional area. In this study, (6.3) is used to estimate the value of tortuosity in a fracture network (see Section 6.3.2).

6.3 Evaluation of Tortuosity

Tortuosity for a fracture network is estimated in two different ways. First, tortuosity is calculated by the definition of the tortuosity given in (6.2), which is based on the path length for water flow (Section 6.3.1). Second, tortuosity is calculated by (6.3), which is based on the orientation angle of the flow paths (Section 6.3.2). In the following sections, a single value of tortuosity over the entire fracture network is considered.

6.3.1 Evaluation of Tortuosity by Path Length

Tortuosity by path length, i.e. \( \tau_L \), is defined based on (6.2) as

\[
\tau_L \equiv \left( \frac{L}{L_e} \right)^2,
\]

where \( L_e \) denotes the average length of the paths through a fracture network*, and \( L \) denotes the medium length in pressure (or potential) applied direction (e.g. \( x \)-axis).

To simply the calculation, a square model space is considered. A two-dimensional square (L×L) model space (Figure 6.1) is used for the evaluation of the tortuosity. A fracture segment is defined as a line element with length \( l \) and aperture \( b \), which is the same as in Chapter 3 (see Figure 3.1). The left side of the square (\( x=-L/2 \)) and right side of the square (\( x=L/2 \)) are called the left and right boundaries, respectively, in this chapter. \( L \) is set to be \( L=1 \) for simplicity without losing generality.

![Figure 6.1 Model space for tortuosity estimation.](image)

6.3.1.1 Average Length of Paths

Fractures are generated based on given statistics of the fracture geometry parameters by random sampling. For the purpose of discussion in this section, the uniform distribution is assumed for the statistical distributions of the fracture parameters, i.e. location, orientation (0–2\( \pi \)), and aperture \( (10^{-4}-10^{-2}) \). Length of a fracture segment is set to be \( l=1 \). For a discrete fracture network generation in the model space, each fracture is generated independently and then superimposed in the model space. Whenever a fracture is added in the model space, the interconnectivity of the fractures and the connection of the interconnected fractures with the two boundaries (left and right boundaries) are

* It should be noted that \( L_e \) in (6.4), which is defined in a fracture network, is different from \( L'_e \) in (6.2), which is defined in a porous medium.

91
checked. If the first connection occurs between the two boundaries through the interconnected fractures, no more fracture is added.

![Fracture network generation in unit square domain.](image)

(a) Fracture network generation in unit square domain. (b) Interconnected fractures connecting the left and right boundaries. (c) Interconnected fractures with assigned labels at the intersections.

Table 6.1 List of Connected Points for Figure 6.2 (c)

<table>
<thead>
<tr>
<th>Points</th>
<th>Connected points</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
</tr>
<tr>
<td>6</td>
<td>1,7,8</td>
</tr>
<tr>
<td>7</td>
<td>6,9</td>
</tr>
<tr>
<td>8</td>
<td>6,10</td>
</tr>
<tr>
<td>9</td>
<td>2,7,11</td>
</tr>
<tr>
<td>10</td>
<td>3,8,11</td>
</tr>
<tr>
<td>11</td>
<td>4,5,9,10</td>
</tr>
</tbody>
</table>

Figure 6.2 (a) shows a fracture network generation in the unit square model. In Figure 6.2 (a), the first connection occurs at the 7th fracture. The interconnected fractures (thick lines) will be considered for the tortuosity evaluation. Figure 6.2 (b) shows the interconnected fractures connecting the left and right boundaries. Figure 6.2 (b) is utilized to measure an average length $L_e$ of the paths in the model space. A path will be defined below.

The procedures of measuring the average length of the paths are as follows.

1. Each intersection of fractures including the intersection of the fracture with the left and right boundaries is labeled (Figure 6.2(c)). Intersection point is simply called “point” in this chapter.

2. All paths connecting the left and right boundaries through the interconnected fractures are identified (see Appendix G). A path is defined as sets of interconnected fractures between two points on the left and right boundaries requiring that each point included in the set should be visited at most once. 8 paths are identified based on the list of connected points shown in Table 6.1 (see Appendix G for detail). The identified 8 paths are as follows.

- $(1-6-7-9-2)$, $(1-6-7-9-11-4)$, $(1-6-7-9-11-5)$, $(1-6-7-9-11-10-3)$, $(1-6-8-10-3)$, $(1-6-8-10-11-4)$, $(1-6-8-10-11-5)$, and $(1-6-8-10-11-9-2)$.

3. A length of a path is calculated by summing the distances between neighboring points consisting of a path.

For example, a length of a path, $(1-6-7-9-2)$, is obtained by summing the distances between 1 and 6, 6 and 7, 7 and 9, and 9 and 2. Similarly, lengths of the 8 paths mentioned in (2) are obtained as 1.091, 1.137, 1.192, 1.425, 1.256, 1.378, 1.432, and 1.608, respectively.

4. An average length of paths, $L_a$, is calculated by the arithmetic mean of the lengths of the all identified paths. For the case in Figure 6.2 (c), $L_a$ is 1.315.

5. A value of tortuosity, $(L/L_a)^2$, for the fracture network in Figure 6.2 is calculated as 0.578 using $L_a=1.315$ and $L=1$.

Procedures (1) to (5) should be repeated to establish the statistics of tortuosity.

### 6.3.1.2 Average Length of Flow Paths

The paths in the previous sections are identified by geometrical consideration. The geometrical paths are not necessarily actual flow paths. Actual flow would occur in the direction from a “high-potential” point to a “low-
potential” point. In this section, the flow paths will be identified for the fracture network by solving the potential distribution at the intersections of fractures (see Appendix H).

![Fracture network with assigned labels](image)

**Figure 6.3** Fracture network with assigned the label at the intersections and boundary conditions for water flow.

As boundary conditions, constant pressures are prescribed as \( P_L=1 \) at the left \((x=0.5)\) boundary and as \( P_R=0 \) at the right \((x=0.5)\) boundary. No flow boundary conditions are prescribed at the top \((y=0.5)\) and the bottom \((y=-0.5)\) of the unit square domain. Potential distribution of the fracture network in Figure 6.3 is obtained by solving the mass balance equations of the flow rate at each intersection. The potentials at the points on the left and right boundaries are given as \( P_1=1 \), \( P_2=P_9=P_6=P_5=0 \). Potentials at the intersections are numerically obtained as \( P_6=2.97E-1 \), \( P_7=2.43E-1 \), \( P_8=2.01E-1 \), \( P_9=7.57E-2 \), \( P_{10}=6.20E-2 \), \( P_{11}=3.03E-2 \) [kg/ms²].

For the procedures to identify the flow paths through the interconnected fractures given in the previous section, one more rule is added. Because the water can flow from a higher potential to a lower potential, connected points in the 2nd column in Table 6.1 should have lower values of potential than those of the points in the 1st column in Table 6.1. By this potential consideration as an additional rule to identify a flow path, a list of connected points is simplified as shown in Table 6.2. As a result of considering the potential, 6 flow paths for Figure 6.3 are identified based on Table 6.2 as \((1-6-7-9-11-2)\), \((1-6-7-9-11-4)\), \((1-6-7-9-11-5)\), \((1-6-8-10-3)\), \((1-6-8-10-11-4)\), and \((1-6-8-10-11-5)\). Two paths, \((1-6-7-9-11-10-3)\) and \((1-6-8-10-11-9-2)\), which are identified in previous section by geometrical consideration, are eliminated from the flow paths.

The average length of paths, \( L_c \), is calculated for these 6 flow paths as 1.248. The value of tortuosity, \((L/L_c)^2\), is calculated as 0.642 using \( L_c=1.248 \) and \( L=1 \).

<table>
<thead>
<tr>
<th>Points</th>
<th>Connected points</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
</tr>
<tr>
<td>6</td>
<td>7, 8</td>
</tr>
<tr>
<td>7</td>
<td>9</td>
</tr>
<tr>
<td>8</td>
<td>10</td>
</tr>
<tr>
<td>9</td>
<td>2, 11</td>
</tr>
<tr>
<td>10</td>
<td>3, 11</td>
</tr>
<tr>
<td>11</td>
<td>4, 5</td>
</tr>
</tbody>
</table>

**Table 6.2** List of Connected Points based on Potential Distribution in Figure 6.3

### 6.3.2 Evaluation of Tortuosity by Orientation Angle

In this section, tortuosity is evaluated by orientation angle of fractures. Two formulae are considered. First, tortuosity \( \tau_0 \) is evaluated by orientation angle \( \theta \) of all fractures included in the interconnected fractures which connect the left and right boundaries. Second, the tortuosity \( \tau_{\theta^*} \) is evaluated by orientation angle \( \theta^* \) of fractures which form the actual flow paths through the fracture network.
\( \tau_0 \) is defined [Fowler, et al., 1940; Carman, 1956] as
\[
\tau_0 = \cos^2 \theta ,
\]
where \( \langle \cos^2 \theta \rangle \) denotes the average value of \( \cos^2 \theta \) taken over values of local orientation angle \( \theta \) of all fractures included in the interconnected fractures which connect the left and right boundaries.
\( \tau_{st} \), is defined as
\[
\tau_{st} = \cos^2 \theta^s > ,
\]
where \( \langle \cos^2 \theta^s \rangle \) denotes the average value of \( \cos^2 \theta^s \) taken over values of local orientation angle \( \theta^s \) of all fractures which form the actual flow paths through the fracture network.

In this study, fractures which form the actual flow paths are identified from the interconnected fractures as follows. First, the fractures whose have only one intersection point are identified. Second, the fractures whose have the same values of potential for all intersection points on those fractures are identified. Because water cannot flow through the fractures identified in the first and second procedures, fractures forming the actual flow paths are determined by excluding those fractures identified in the first and second procedures.

The \( \tau_0 \) is calculated for the same fracture network as used for obtaining \( L_e \), where \( \theta \) is the orientation of the fractures included in the interconnected fractures (thick lines in Figure 6.2(b) and (c)). A value of \( \tau_0 \) is 0.604 for the network in Figure 6.2(c). In Figure 6.2(c), \( \tau_0 \) equals to \( \tau_{0t} \) since all interconnected fractures form the actual flow paths.

### 6.4 Numerical Results and Observations

For the same fracture network, the value of tortuosity over the fracture network is calculated by three different formulae given in this section, i.e. \( \tau_L \) in (6.4), \( \tau_0 \) in (6.5) and \( \tau_{st} \) in (6.6).

#### 6.4.1 Effect of the Size of Fracture Length on Tortuosity

Three cases are selected to calculate the tortuosity through a fracture network in the unit square domain as shown in Table 6.3.

For case 1, the first connection between the left (\( x=-0.5 \)) and right (\( x=0.5 \)) boundary through the interconnected fractures can occur with few long fractures. For case 3, due to the given short length of fracture (\( l=0.5m \)), more fractures are required to occur the first connection than that for case 1. Case 2 is selected as \( l=0.75 \) to see the effect in between \( l=1.0 \) and \( l=0.5 \). To see the effect of the size of fracture length on the tortuosity, other fracture geometry parameters are kept the same for these 3 cases.

Figure 6.4 shows the cumulative distribution functions (CDFs) of tortuosities \( \tau_L, \tau_0 \) and \( \tau_{st} \) for 100 realizations for the 3 cases. The means and standard deviation (S.D.) of \( \tau_L, \tau_0 \) and \( \tau_{st} \) for 100 realizations are shown in Table 6.4. The median values of \( \tau_L, \tau_0 \) and \( \tau_{st} \) for 100 realizations are shown in Table 6.5. Figure 6.5 shows the fracture networks, interconnected fractures (thick lines) connecting the left and right boundaries, and interconnected fractures form actual flow paths for a selected realization at the most probable tortuosity of \( \tau_L \) (indicated by dot in Figure 6.4) from 100 realizations for each case.

A smaller value of \( \tau_L \) means that the flow path is more tortuous (see (6.4)). For tortuosity greater than 0.6 in Figure 6.4, differences among the 3 curves are not significant. For tortuosity smaller than 0.4, the differences among 3 curves are more significant as the length \( l \) of fracture segments decrease.

The median values of \( \tau_0 \) for the 3 cases in Figure 6.4 are approximately 0.5, i.e. 0.507, 0.496, and 0.495 for cases 1, 2, and 3, respectively. This is because the continuous uniform distribution is assumed for \( \theta \) (see Table 6.3). The \( \tau_0 \) for the entire square domain can be calculated for a given continuous uniform distribution of orientation as
\[
\tau_0 = \cos^2 \theta > \int_0^{2\pi} \frac{1}{2\pi} \cos^2 \theta \, d\theta = 0.5 .
\]

The median values of \( \tau_{st} \) in Figure 6.4 are 0.560, 0.515, and 0.523 for cases 1, 2, and 3, respectively. The values of \( \tau_0 \) and \( \tau_{st} \) are identical if all interconnected fractures form the actual flow paths through the fracture network.

A difference between \( \tau_0 \) and \( \tau_{st} \) (i.e. \( \tau_0=0.422 \) and \( \tau_{st}=0.561 \) for a realization of case 1 in Figure 6.5(a)) comes from the fact that some of fractures included in the interconnected fractures are not included in the fractures forming...
Among the three formulae for tortuosity, $\tau_{0*}$ gives the largest median values for three different fracture lengths. The difference between $\tau_0$ and $\tau_{0*}$ is not significant. $\tau_L$ gives the smallest value among the three, which makes the water flow rate smallest.

Because $\tau_L$ is considered to be the most rigorous definition among three, $\tau_L$ should be used. However, in more realistic situations, where thousands to hundreds of thousands of fractures are included, calculating the average path length is time consuming. For a practical application, where conservative estimation of water flow rates need to be obtained, $\tau_0$ or $\tau_{0*}$ may be used.

Table 6.3 Statistics of the Fracture Geometry Parameters for Tortuosity

<table>
<thead>
<tr>
<th>Case</th>
<th>Length, $l$ [m]</th>
<th>Aperture, $b$ [m]</th>
<th>Orientation, $\theta$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Range</td>
<td>Distribution</td>
<td>Range</td>
</tr>
<tr>
<td>1</td>
<td>$10^{-4}$ to $10^{-2}$</td>
<td>Uniform</td>
<td>$0$ to $2\pi$</td>
</tr>
<tr>
<td>2</td>
<td>$10^{-4}$ to $10^{-2}$</td>
<td>Uniform</td>
<td>$0$ to $2\pi$</td>
</tr>
<tr>
<td>3</td>
<td>$10^{-4}$ to $10^{-2}$</td>
<td>Uniform</td>
<td>$0$ to $2\pi$</td>
</tr>
</tbody>
</table>

Table 6.4 Statistics of $\tau_L$, $\tau_0$, and $\tau_{0*}$

<table>
<thead>
<tr>
<th>Case</th>
<th>$\tau_L$</th>
<th>Standard deviation</th>
<th>$\tau_0$</th>
<th>Standard deviation</th>
<th>$\tau_{0*}$</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.69E-01</td>
<td>1.79E-01</td>
<td>5.27E-01</td>
<td>1.18E-01</td>
<td>5.64E-01</td>
<td>1.30E-01</td>
</tr>
<tr>
<td>2</td>
<td>4.18E-01</td>
<td>1.87E-01</td>
<td>5.12E-01</td>
<td>1.09E-01</td>
<td>5.31E-01</td>
<td>1.16E-01</td>
</tr>
<tr>
<td>3</td>
<td>3.48E-01</td>
<td>1.52E-01</td>
<td>5.09E-01</td>
<td>8.59E-02</td>
<td>5.24E-01</td>
<td>9.43E-02</td>
</tr>
</tbody>
</table>

Table 6.5 Median Values of $\tau_L$, $\tau_0$, and $\tau_{0*}$

<table>
<thead>
<tr>
<th>Case</th>
<th>Median</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\tau_L$</td>
</tr>
<tr>
<td>1</td>
<td>4.26E-01</td>
</tr>
<tr>
<td>2</td>
<td>3.72E-01</td>
</tr>
<tr>
<td>3</td>
<td>3.14E-01</td>
</tr>
</tbody>
</table>

**Figure 6.4** Cumulative distribution functions (CDFs) of $\tau_L$, $\tau_0$, and $\tau_{0*}$ for $l=1.0$ (a), and $l=0.75$ (b), and $l=0.5$ (c) for 100 realizations.
Fracture network generation

Interconnected fractures connecting the left and right boundaries

Interconnected fractures forming actual flow paths

Figure 6.5 Fracture network, interconnected fractures (thick lines) connecting the left and right boundaries, and interconnected fractures forming the actual flow paths for a selected realization for each case.
6.5 Conclusions & Discussions

The values of the coefficient $C$ in Kozeny-Carman equation for the entire FBC in the square model space have been calculated by three different formulae, i.e. $\tau_L/c_0$, $\tau_0/c_0$, and $\tau_0^*/c_0$. The value of $c_0$ is assumed to be 3 in this study. The values of the tortuosity are calculated by the three formulae as $\tau_L=(L/L_0)^2$, $\tau_0=<\cos^2 \theta>$, and $\tau_0^*=<\cos^2 \theta^*>$. Among three, $\tau_L$ is the most direct formula.

A numerical scheme to calculate the average of the path length of the discrete fracture network has been developed. $\tau_0$ and $\tau_0^*$ have also been calculated by using orientation angles of fractures included in the FBC extracted from the DFN. The theoretical value of $\tau_0$ for a uniform angle distribution between 0 and $2\pi$ has been obtained to be 0.5. Numerical results also show that the $\tau_0$ value is close to 0.5. Comparing the three formulae, $\tau_L$ gives the smallest value, whereas difference between $\tau_0$ and $\tau_0^*$ is not significant. Because $\tau_0$ gives conservative (over)estimate for tortuosity, with which the water flow rate in the fractured rock is overestimated, $\tau_0$ may be used for a performance assessment modeling.

Among three different methods for calculation of tortuosity, $\tau_0$ is most practical in terms of numerical efforts because $\tau_0$ can be calculated immediately after identifying the interconnected fractures (i.e. FBC). For $\tau_0^*$, additional numerical work (e.g. potential values at the intersections of fractures in this study) is required to identifying the fractures forming actual flow paths from the discrete fracture network. For $\tau_L$, the potential values at the intersections of the fractures included in the FBC must be calculated to identify the flow paths. Also, identification of all flow paths through the FBC requires the computational efforts. For a system contains large number of interconnected fractures, the methods for $\tau_L$ and $\tau_0^*$ require considerable amount of computation.

The average value of the coefficient $C$ is calculated by $\tau_0/c_0=0.5/3=0.167$. In Chapter 3, it has been assumed that $C=1$. Thus, with tortuosity correction, the water flow rate through FBC in the NFR becomes about 1/6 of the value obtained in Chapter 3.

Although $\tau_L$ and $\tau_0^*$ are not used to evaluate the coefficient $C$ in this study, it should be noted (i) that $\tau_L$ is the most direct method to evaluate the tortuosity for the fracture network, and (ii) that $\tau_0^*$ is more realistic than $\tau_0$ because the only orientation angles $\theta^*$ of fractures forming the actual flow paths are considered.

---

* For $\tau_L$, the calculation time is over a day with Pentium III-500 personal computer if the number of intersection points is larger than 200. For the calculation of $\tau_0^*$ in this study, fractures which form the actual flow paths should be identified. For the identification, potential values at intersections of fractures are used in this study. To calculate potential values at the intersections, $N$ (number of intersection points) linear equations should be solved.
7. Flow Evaluation with Tortuosity Correction

7.1 Introduction

In the flow model developed in Chapter 3, a flow-bearing cluster (FBC) extracted from a discrete-fracture network (DFN) has been transformed into a heterogeneous continuum by the local homogenization (Section 3.4.1) and a homogeneous continuum by the uniformization (Section 3.4.2). In Chapter 6, tortuosity correction to the permeability for the entire FBC has been discussed, and a single value of $C$ was obtained for the FBC. It has been concluded that for a conservative overestimate of water flow rates, $\tau_0$ may be used.

In this chapter, the water flow analysis through a fracture network is made in two different ways, i.e. a DFN model, and a homogeneous continuum model. In the DFN model, water flow rate through the fracture network is calculated by solving mass conservation equations at intersection points of fractures [Long, et al., 1982; Schwartz, et al., 1983; Robinson, 1984; Long, 1985; Andersson, et al., 1987; Dverstorp, et al., 1992]. In the homogeneous continuum model developed in Section 3.4.2, tortuosity by the orientation angle $\tau_0$ is incorporated in the coefficient $C=\tau_0/c_0$. Results from these approaches are compared.

7.2 Flow Rate through a Fracture Network

7.2.1 Model Space and Boundary Conditions

A two dimensional unit square domain is defined as shown in Figure 7.1. A line element represents a fracture with length $l$ and aperture $b$. A fracture is generated based on given statistics of the fracture geometry parameters. For a fracture network generation, total number of fractures $N_f$ is prescribed in this chapter. Figure 7.2 shows a fracture network with $N_f=7$ for constant length ($l=1.0$ m), constant aperture ($b=10^{-4}$ m), and uniform orientation ($0\sim2\pi$) of fractures.

To calculate the flow rate in the model space, boundary conditions are prescribed as shown in Figure 7.1. Constant head boundary conditions are prescribed at the left boundary ($x=-0.5$) as $\phi=0.1$ [m] and at the right boundary ($x=0.5$) as $\phi=0$ [m]. No flow boundary conditions are prescribed at the top ($y=0.5$) and the bottom ($y=-0.5$) boundaries.

![Figure 7.1](image)

Figure 7.1  Model space for flow rate calculation

* In this chapter, a heterogeneous continuum by local homogenization is not considered because the coefficient $C$ has been obtained not for the local triangular elements but for the entire NFR in Chapter 6.

** Tortuosity is not required to calculate the flow through a network of parallel fractures. In this study (see Chapters 3 and 5), however, because the flow rate is obtained by transformation of the FBC into a continuum using Kozeny-Carman equation for the permeability, tortuosity is needed.
7.2.2 Discrete Fracture Network (DFN) Approach

Water flow through the fracture network has been modeled by the DFN approaches [Long, et al., 1982; Schwartz, et al., 1983; Robinson, 1984; Long, 1985; Elsworth, 1986; Andersson, et al.,1986; Andersson, et al., 1987; Long, et al.,1987; Dershowitz, et al., 1994]. In the DFN approaches, individual fractures are considered to determine the flow rate of water. A fracture is modeled as parallel-plate water conducting channel. Water velocity through a cross-section normal to flow is obtained by solving the Navier-Stokes equations for a time-independent, laminar flow in a viscous, incompressible fluid.

The flow rate through individual fracture for \( w=1 \text{[m]} \) is written as:

\[
Q_f = \frac{\rho gb}{12\mu_w} \frac{\left[ \Delta \phi \right]}{L},
\]

where \( \mu_w (0.799 \times 10^{-3} \text{ N.s/m}^2 \text{ for } 30^\circ \text{C}) \) is the viscosity of water, \( \rho(996 \text{ kg/m}^3 \text{ for } 30^\circ \text{C}) \) is the density of water, \( g(9.8 \text{ m/s}^2) \) is the constant for gravity, \( b \) is the aperture of a fracture, and \( \phi \text{[m]} \) is the hydraulic head. Hydraulic head is the sum of the elevation head \( (z) \) and the pressure head \( (P/\rho g) \),

\[
\phi = z + \frac{P}{\rho g},
\]

where \( P \text{[kg/m}^2\text{]} \) is the pressure.

In Figure 7.3, the hydraulic heads at points 1, 2 and 3 are prescribed as \( \phi_1=\phi_2=0.1, \) and \( \phi_3=0 \text{[m]} \). The hydraulic heads at 8 internal points from 4 to 11 are unknown. The distribution of the hydraulic head \( \phi \) at all intersections is calculated by solving the \( N \) (the number of intersections of fractures, \( i.e., N=8 \text{ in Figure 7.3} \)) linear equations with assumption of mass balance at intersections of fractures (see Appendix H). The values of unknown hydraulic heads in Figure 7.3 are calculated numerically as \( \phi_{9}=5.530\text{E-2}, \phi_{10}=7.272\text{E-2}, \phi_{11}=6.824\text{E-2}, \phi_{12}=8.897\text{E-2}, \phi_{13}=4.124\text{E-2}, \phi_{14}=3.849\text{E-2}, \phi_{15}=5.134\text{E-2}, \) and \( \phi_{16}=4.126\text{E-2} \text{[m]} \). Then, a flow rate through each fracture is calculated by (7.1) with these obtained values of \( \phi \). For example, a flow rate from points 9 to 3, \( Q_{9,3} \), is calculated as

\[
Q_{9,3} = \frac{\rho gb}{12\mu_w} \frac{\left[ \phi_9 - \phi_3 \right]}{L_{9,3}} = 1.024\times 10^{-5} \text{[m}^3/\text{s}],
\]

* To calculate the water flow rate through the fracture network, the hydraulic (or potential) head at the intersections of fractures is not necessarily needed. In Appendix I, the water flow rate is calculated for a simple fracture network without calculating the values of potential head at the intersections of fractures [Chambré, 2001].
where $L_{3,9}$ is the distance between points 3 and 9, and obtained numerically as 3.826E-1 [m]. The positive quantity means that water flow from intersection 9 to intersection 3.

Figure 7.3  Distribution of hydraulic head at the intersections of fractures

Flow rates between 1 and 7, and 2 and 7 are calculated by (7.1) as $Q_{f,1-7}=8.481E^{-8}$ [m$^3$/s] with $L_{1-7}=1.324E^{-1}$ [m] and $Q_{f,2-7}=1.758E^{-8}$ [m$^3$/s] with $L_{2-7}=6.387E^{-1}$ [m]. The sum of the flow rates through individual fractures, which intersect the boundary, yields the total flow rate of water at that boundary ($Q_{DFN}$). $Q_{DFN}=Q_{f,9-3}=1.024E^{-7}$ [m$^3$/s] is the total outflow rate at the right boundary. $Q_{DFN}=Q_{f,1-7}+Q_{f,2-7}=1.024E^{-7}$ [m$^3$/s] is the total inflow rate at the left boundary. The numerical results, which show the equal amount of inflow and outflow rate, confirm that the mass conservation of the model space.

It should be noted that the tortuosity is not required to calculate the flow through a network of parallel fractures as shown in Figure 7.3.

7.2.3  Homogeneous Continuum Approach

Water flow through the fracture network has been analyzed by transformation of the DFN into a continuum in Chapter 3. For a homogeneous continuum by the uniformization in Section 3.4.2, single values of the porosity ($\bar{\varepsilon}$), the specific surface area ($\bar{M}$), the permeability ($\bar{k}$), and the hydraulic conductivity ($\bar{K}$) are obtained for the entire FBC in Figure 7.2 by (3.7), (3.8), (3.9), and (3.10), respectively. Area $A$ in (3.7) and (3.8) denotes the area of the entire NFR region. Since the entire square model space in Figure 7.1 represents the NFR, $A=1$ [m$^2$] is used in this section. In order to take into account the effect of tortuous flow paths (see Chapter 6) through the fracture network, the coefficient $C$ in (3.9) is calculated with the tortuosity by orientation angle of fractures as

$$C = \tau_{\gamma} = \frac{<\cos^2 \theta>}{c_{0}},$$  \hspace{1cm} (7.4)

where $<\cos^2 \theta>$ denotes the average value of $\cos^2 \theta$ taken over all values of local orientation angle $\theta$ of fractures included in the interconnected fractures which connect the left and right boundaries. $c_{0}$ is 3 [Carman, 1956].

Table 7.1  Uniformized Hydraulic Properties for the Fracture Network in Figure 7.2.

<table>
<thead>
<tr>
<th>$\bar{\varepsilon}$</th>
<th>$\bar{M}$ [1/m]</th>
<th>$&lt;\cos^2 \theta&gt;$</th>
<th>$\bar{C}$</th>
<th>$\bar{k}$[m$^3$/s]</th>
<th>$\bar{K}$[m/s]</th>
<th>$Q_{DFN}$[m$^3$/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.555E-4</td>
<td>1.111E+1</td>
<td>3.068E-1</td>
<td>1.023E-1</td>
<td>1.422E-13</td>
<td>1.737E-6</td>
<td>1.737E-7</td>
</tr>
</tbody>
</table>

$\mu_w=0.799\times10^{-3}$ [N-s/m$^2$], $\rho=996$ [kg/m$^3$], $g=9.8$ [m/s$^2$]

For the calculation of the hydraulic conductivity for the entire FBC by (3.10), the system temperature of 30$^\circ$C is assumed. Numerically obtained hydraulic properties for the entire fracture network in Figure 7.2 are shown in Table 7.1. In this table, $<\cos^2 \theta>$ in the third column is obtained by averaging $\cos^2 \theta$ taken over all values of local
orientation angle $\theta$ of seven fractures in Figure 7.2. A flow rate through a homogeneous domain $Q_{\text{HOMO}}$ [m$^3$/s] (i.e. 1x1 homogeneous continuum) is calculated approximately by Darcy’s law as:

$$Q_{\text{HOMO}} = \frac{\Delta \phi}{\mu L} \cdot \frac{0.737 \times 10^{-3}}{1} \cdot A = 1.737 \times 10^{-7} [m^3/s],$$

(7.5)

where

$$\bar{K} = 1.737 \times 10^{-3} [m/s], \quad \Delta \phi = \frac{0.737}{1}, \quad A = 1[m^2].$$

(7.6)

### 7.3 Numerical Results

Table 7.2 shows the flow rates through the fracture network in Figure 7.2 by DFN ($Q_{\text{DFN}}$) and homogeneous continuum ($Q_{\text{HOMO}}$). In Table 7.2, $Q_{\text{HOMO}}$ is observed to be larger than $Q_{\text{DFN}}$.

Water flow rates through the fracture networks are calculated for four cases in Table 7.3 for 100 realizations. For each realization of DFN, water flow rates are calculated by the DFN approach in Section 7.2.2 and by the homogeneous continuum approach in Section 7.2.3.

#### Table 7.2 Flow Rates through the Fracture Network in Figure 7.2

<table>
<thead>
<tr>
<th>Flow rate [m$^3$/s]</th>
<th>$Q_{\text{DFN}}$</th>
<th>$Q_{\text{HOMO}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.024E-7</td>
<td>1.737E-7</td>
</tr>
</tbody>
</table>

For case 1 in Table 7.3, 30 fractures with a constant length $l=1$ [m] and aperture $b=10^{-4}$ [m] are generated in the model space. The orientation angles of fractures are distributed uniformly between 0 and $2\pi$. For case 2, to investigate the effects of the number of fractures, the same fracture geometry parameters are used as case 1 except for the number of fractures. For case 3, to investigate the effects of the length of fractures, the same fracture geometry parameters are used as case 2 except for the length of fractures. A half times shorter length of fractures for case 3 than that for case 2 is prescribed. For case 4, to investigate the effects of distribution of length, a lognormal distribution with mean and standard deviation of 0.5 (i.e. $\alpha_1=0.833$ and $\beta_1=0.354$ by (2.6)) is considered.

#### Table 7.3 Parameters for Water Flow Rate

<table>
<thead>
<tr>
<th>Cases</th>
<th>Number of Fractures, $N_f$</th>
<th>Length $l$ [m]</th>
<th>Aperture $b$ [m]</th>
<th>Orientation, $\theta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>30</td>
<td>1.0</td>
<td>$10^{-4}$</td>
<td>0~2$\pi$ Uniform</td>
</tr>
<tr>
<td>2</td>
<td>60</td>
<td>1.0</td>
<td>$10^{-4}$</td>
<td>0~2$\pi$ Uniform</td>
</tr>
<tr>
<td>3</td>
<td>60</td>
<td>0.5</td>
<td>$10^{-4}$</td>
<td>0~2$\pi$ Uniform</td>
</tr>
<tr>
<td>4</td>
<td>60</td>
<td>Lognormal distribution with $\alpha_l=8.33E-1$ and $\beta_l=3.54E-1$</td>
<td>$10^{-4}$</td>
<td>0~2$\pi$ Uniform</td>
</tr>
</tbody>
</table>

#### Table 7.4 Flow Rates by DFN ($Q_{\text{DFN}}$) and Homogeneous Continuum ($Q_{\text{HOMO}}$) Approaches for 100 Realizations for 4 Cases in Table 7.3.

<table>
<thead>
<tr>
<th>Case</th>
<th>Median $Q_{\text{DFN}}$ [m$^3$/s]</th>
<th>Mean $Q_{\text{DFN}}$ [m$^3$/s]</th>
<th>Standard deviation $Q_{\text{DFN}}$</th>
<th>Median $Q_{\text{HOMO}}$ [m$^3$/s]</th>
<th>Mean $Q_{\text{HOMO}}$ [m$^3$/s]</th>
<th>Standard deviation $Q_{\text{HOMO}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7.52E-7</td>
<td>7.62E-7</td>
<td>1.38E-7</td>
<td>1.10E-6</td>
<td>1.09E-6</td>
<td>1.44E-7</td>
</tr>
<tr>
<td>2</td>
<td>1.77E-6</td>
<td>1.78E-6</td>
<td>1.78E-6</td>
<td>2.18E-6</td>
<td>2.19E-6</td>
<td>1.97E-7</td>
</tr>
<tr>
<td>3</td>
<td>6.82E-7</td>
<td>6.73E-7</td>
<td>1.44E-7</td>
<td>1.31E-6</td>
<td>1.30E-6</td>
<td>1.14E-7</td>
</tr>
<tr>
<td>4</td>
<td>5.61E-7</td>
<td>5.55E-7</td>
<td>1.85E-7</td>
<td>1.09E-6</td>
<td>1.10E-6</td>
<td>1.61E-7</td>
</tr>
</tbody>
</table>
Table 7.4 shows the median, mean, and standard deviation of the flow rate by DFN \(Q_{DFN}\) and homogeneous continuum \(Q_{HOMO}\) approaches for 100 realizations for 4 cases in Table 7.3. Figure 7.4 shows the cumulative distribution functions of the flow rate by DFN (solid) and homogeneous continuum (dashed) approaches for 100 realizations for four cases in Table 7.3.

For case 2, a difference in median values between the flow rate by DFN \(Q_{DFN}\) and the flow rate by homogeneous continuum \(Q_{HOMO}\) is 23.2%. Cases 1 and 2 represent the networks with the same geometry of fractures but different number of fractures. By increasing the number of fractures from \(N_f=30\) to \(N_f=60\), the flow rate increases as the number of fractures is increased, and a discrepancy between the median values of \(Q_{DFN}\) and \(Q_{HOMO}\) are decreased from 46.3% to 23.2%.

For case 3, a difference in median values between the flow rate by DFN \(Q_{DFN}\) and the flow rate by homogeneous continuum \(Q_{HOMO}\) is 92.1%. Cases 2 and 3 represent the networks with the same number of fractures but different size of fracture length. By decreasing the size of fracture length \(l=1\) to \(l=0.5\), a discrepancy between the median values of \(Q_{DFN}\) and \(Q_{HOMO}\) are increased from 23.2% to 92.1%.

For case 4, a difference in median values between the flow rate by DFN \(Q_{DFN}\) and the flow rate by homogeneous continuum \(Q_{HOMO}\) is 94.3%. Cases 3 and 4 represent the networks with the same geometry of fractures but different distribution of length. By generating the larger and smaller fracture lengths than its mean value in lognormal distribution, flow rates range more widely than those for the network with a constant length of fractures.

Figure 7.4  CDFs of the flow rate by DFN (solid) and homogeneous continuum (dashed) approaches for 100 realizations for four cases in Table 7.3.
7.4 Conclusions & Discussions

In this chapter, the water flow analysis through a fracture network has been made by a discrete-fracture network (DFN) model and by a homogeneous continuum model. For the homogeneous continuum model, the tortuosity correction has been incorporated in the coefficient $C = \tau_0 / C_0$ in the permeability as shown in (3.3). For the same fracture network, the flow rates obtained by two models are compared.

Numerical observations are summarized for the same fracture geometry parameters as follows:

- As the number of fractures increases, the water flow rate increases, and a difference between the median values of $Q_{DFN}$ and $Q_{HOMO}$ decreases.
- As the size of fracture length decreases, the water flow rate decreases, and a difference between the median values of $Q_{DFN}$ and $Q_{HOMO}$ increases.
- As the length of fractures varies from its mean value, water flow rates range more widely.

For all cases considered in this study, the homogeneous continuum approach yields the overestimated water flow rates compared with those by the DFN approach. The current study could justify the conservatism of the model treating the discrete fracture network as a homogeneous continuum.

In this chapter, particle transport has not been simulated because the fractional mass absorption rate for the homogeneous continuum (i.e., uniformized NFR) is less dependent on the degree of the heterogeneity of the NFR (i.e., connectivity) (see Figure 5.10). However, the residence time of particles in the uniformized NFR could be different because the residence time in the NFR decreases (or water flow rate increases) as the connectivity increases.

For the transformation of the FBC into a continuum, only homogeneous continuum by the uniformization is considered in this chapter because the coefficient $C$ with tortuosity correction is assumed to be uniform for the entire FBC (see Chapter 6).
8. Conclusions

In the near-field rock (NFR), interconnected fractures are major conduits for groundwater flow and radionuclide transport. Heterogeneity of the transport path in the NFR can significantly affect results for HLW repository performance assessment. However, in the previous near-field models for water-saturated HLW repository performance assessments, the heterogeneity of the NFR was not included in the radionuclide transport analysis.

The objectives of this dissertation are to develop a near-field model incorporating the heterogeneity of the NFR in the groundwater flow and particle transport analyses, and to investigate effects of the heterogeneity of the NFR and effects of the modeling approaches for the NFR on the groundwater flow rate and particle transport in the near field. A hypothetical, simplified region including one canister, the buffer, and the near-field rock is considered.

A two-dimensional model for the groundwater flow simulation has been developed for the time-independent, incompressible Darcy’s flow. To incorporate the heterogeneity of the NFR explicitly, a discrete fracture network is generated in the NFR. A flow-bearing cluster (FBC) of fractures is extracted from the fracture network by checking the interconnectivity of fractures. The FBC is transformed into a heterogeneous continuum and a homogeneous continuum to compare the modeling approaches for the NFR. The Kozeny-Carman equation is used for permeability. A finite element solution has been derived for the spatial distribution of the hydraulic potential in the FBC.

The numerical model developed for flow analysis has been bench-marked against a mathematical model by comparing the results by the numerical solution with those by the analytical solution for the given special cases. A model for the particle transport simulation has been established based on the flow model by applying the random walk tracking method.

A computer code, FFDF, has been developed for the water flow and the particle transport.

Effects of the heterogeneity of the NFR and effects of the modeling approach for the NFR have been investigated for different sets of statistics of fracture geometry parameters by comparing the groundwater flow rates, the particle residence times, and mass absorption rates between the model with a heterogeneous NFR by locally homogenizing the DFN in the NFR and the model with a homogenized NFR by uniformizing the DFN over the entire NFR.

The coefficient $C$ in Kozeny-Carman equation for the permeability has been evaluated by calculating tortuosity for the fracture network using three formulae $\tau_1$, $\tau_0$, and $\tau_0^*$.

The homogeneous continuum model, transformed from the discrete fractures by uniformization, incorporating the coefficient $C = \tau_0/d_{eq}$ with tortuosity correction has been compared with the conventional DFN model for the same fracture network.

For the performance assessment of the water-saturated HLW repository, the current study shows that:

- For water flow analysis in fractured rock, the NFR as a homogeneous continuum is not an appropriate approach because it does not necessarily yield a conservative water flow rate.
- The simplification (i.e. the NFR was treated as the homogeneous continuum) introduced in previous near-field models for radionuclide transport is justified by the fact that a homogeneous continuum yields conservative results, i.e., underestimates the residence time and overestimates the mass absorption rate, compared to the models incorporating the heterogeneity of the NFR (i.e. DFN, heterogeneous continuum).
- If the NFR is treated as a homogeneous continuum for radionuclide transport, (1) the bentonite-filled buffer plays an important role as a barrier for the release of radionuclides, and (2) the effects of the heterogeneity of the NFR on the radionuclide transport are negligible.
- To incorporate the tortuosity correction to the permeability, $\tau_0$ could be used for a performance assessment modeling because (1) $\tau_0$ conservatively overestimates the tortuosity, and thus the water flow rate in the NFR is overestimated, and (2) $\tau_0$ requires the least computational efforts among three methods.
- The length-aperture correlation, which is considered to exist, but which is very difficult to obtain by field measurements, could be neglected for the performance assessment because the effect of the length-aperture correlation on the transport in the near-field is negligible.

For the purpose of the site selection, in which performance of various kinds of host rocks needs to be differentiated, the current study shows that:

- For a sparsely fractured rock, a homogeneous continuum by uniformizing the rock is not an appropriate approach to model the water flow and particle transport because (1) it cannot properly reproduce high and low tails of the flow rates, the residence time of particles, and the mass absorption rates, whereas the heterogeneous continuum by locally homogenizing the rock can generate those tails properly, and
(2) it wipes out the differences in the residence time and the absorption rate (or release rate) of solute among different rocks.
REFERENCES


Japan Nuclear Cycle Development Institute (JNC), Second progress report on research and development for the geologic disposal of HLW in Japan, H12: Project to establish scientific and technical basis for HLW disposal in Japan, JNC TN1400 2000-001-005, 2000.


Appendix A: Random Sampling for Lognormal Distribution

There is no exact method to generate a single normal (or lognormal) variate from a single uniform variate [Bratley, et al., 1983]. The Box-Muller method [Box, et al., 1958] is used in a computer code (FFDF)* to generate a pair of lognormally distributed random numbers from a pair of uniformly distributed random number between 0 and 1.

The lognormal distribution (2.1) of variable $x$ can be written as a normal distribution $f(z)$ of variable $z$ for zero mean and unit standard deviation

$$
f(z) = \frac{1}{\sqrt{2\pi}} \exp \left[ -\frac{z^2}{2} \right], \ -\infty < z < \infty,
$$

(A.1)

where $\alpha_L$ is the shape parameter and $\beta_L$ is the scale parameter of the lognormal distribution.

The joint probability density functions (PDF) of two independent variables, $z_1$ and $z_2$, is the product of the individual PDFs [Box, et al., 1958].

$$
f(z_1, z_2) = f(z_1) \cdot f(z_2) = \frac{1}{\sqrt{2\pi}} e^{-z_1^2/2} \cdot \frac{1}{\sqrt{2\pi}} e^{-z_2^2/2} = \frac{1}{2\pi} e^{-z_1^2/2} e^{-z_2^2/2}.
$$

(A.3)

By conversion from the Cartesian coordinates with $z_1$ and $z_2$ axes to the polar coordinates $r_\gamma$ and $\theta_\gamma$ (see Figure A.1), the joint PDF in (A.3) is written as [Bratley, et al., 1983]

$$
f(r_\gamma, \theta_\gamma) = \frac{r_\gamma}{2\pi} e^{-r_\gamma^2/2}.
$$

(A.4)

* Features of FFDF are given in Appendix D
Using direct inversion of the CDF [Press, et al., 1992], the desired deviate $f(r_j)$ can be obtained from a uniform deviate $U_2$ between 0 and 1 as

$$r_j = \sqrt{-2 \ln(1-U_2)} = \sqrt{-2 \ln(U_2)}. \quad (A.7)$$

Now, $z_1$ and $z_2$ can be obtained by uniformly distributed angle $\theta_j$ as $2\pi U_1$, and the relationship between two coordinates shown in Figure A.1,

$$z_1 = r_j \cos \theta_j = \sqrt{-2 \ln(U_2)} \cdot \cos(2\pi U_1), \quad (A.8)$$

$$z_2 = r_j \sin \theta_j = \sqrt{-2 \ln(U_2)} \cdot \sin(2\pi U_1). \quad (A.9)$$

Using (A.8) and (A.9), two independent random numbers $z_1$ and $z_2$, which are distributed normally, are generated from the two uniform random numbers $U_1$ and $U_2$ between 0 and 1. By the definition of (A.2), two lognormally distributed, independent random numbers, $x_1$ and $x_2$, also can be obtained from the two uniform random numbers between 0 and 1,

$$x_1 = \beta_z \cdot e^{\alpha_z z} = \beta_z \cdot \exp[\alpha_z \cdot \sqrt{-2 \ln(U_2)} \cdot \cos(2\pi U_1)], \quad \text{where } \beta_z, \alpha_z > 0 \text{ and } 0 < U_1, U_2 < 1 \quad (A.10)$$

$$x_2 = \beta_z \cdot e^{\alpha_z z} = \beta_z \cdot \exp[\alpha_z \cdot \sqrt{-2 \ln(U_2)} \cdot \sin(2\pi U_1)], \quad \text{where } \beta_z, \alpha_z > 0 \text{ and } 0 < U_1, U_2 < 1 \quad (A.11)$$

Equations (A.10) and (A.11) are utilized to generate lognormally distributed random numbers in FFDF code. Figure A.2 shows lognormal distributions for $\beta_z=0.3m$ and $\alpha_z=1.0$ obtained by analytical expression (2.1) and by numerical solution by (A.10) and (A.11). $10^3$ samples have been made in Figure A.2.

**Figure A.2** Lognormal distribution by Analytical solution using (2.1) and by numerical solution using equations (A.10, A.11)
Appendix B: Parameters for Occurrence of FBC

In this study, the percolation of the system (i.e., whether a FBC occurs in the system or not) is crucial because water can flow into the buffer region only through the FBC due to the assumption of impermeable rock matrix. The amount of water supplied to the buffer region depends on fracture geometry parameters. In this section, important parameters for percolation are investigated. By simple numerical simulations, orientation is found to be the most important parameter for percolation.

B.1 Orientation

Figure B.1 shows a particular realization for a fracture network generation for sets of statistics of fracture geometry parameters in Table 3.1. To see the effect of orientation on percolation, a constant value of the orientation (θ=π/4) is assumed instead of isotropy (uniform distribution from 0 to 2π). Distributions for other parameters and their values are the same as given in Table 3.1.

Figure B.1 Fracture network generation

Figure B.2 shows a fracture network generation with the constant orientation (θ=π/4). No intersection occurs in this case, whereas the fracture network with uniform orientation in Figure B.1 yields 907 intersections. This result indicates that orientation primarily determines percolation.

Figure B.2 Fracture network generation with constant orientation.

B.2 Length

To see the effect of fracture length on percolation, a constant length both for the primary and secondary fractures are assumed. Other parameters are the same as given in Table 3.1. Figure B.3 shows a fracture network with the constant length of 0.3m (short fractures), and Figure B.4 shows a fracture network with the constant length of 3.0 m (long fractures). 83 intersections occur for the case with short fractures in Figure B.3, whereas 4986 intersections occur for the case with long fractures in Figure B.4. Percolation occurs only for the long-fracture case.
Notice that both cases are for isotropic orientation. If the constant orientation (0.25π) is assumed for the case with the long fractures, no intersection occurs as shown in Figure B.5. This result implies that the orientation is more important than the length.

Figure B. 3 Fracture network with the constant length of 0.3m (short fractures).

Figure B. 4 Fracture network with the constant length of 3.0m (long fractures).

Figure B. 5 Fracture network with constant length (3.0m) and orientation (0.25π).

B.3 Aperture

Generally, intersection can occur more likely with a greater aperture than with a smaller aperture. To see the effect of fracture aperture on percolation, a constant aperture of 10^{-4} m is assumed, while other parameters are the same given in Table 3.1. Figure B.6 shows the fracture network generated with the constant aperture of 10^{-4} m.
Figure B.6 appears to be identical to Figure B.1. Thus, aperture effect on percolation is negligibly small because the aperture is sufficiently smaller than the length.

In a computer code (FFDF), a line is treated as a point if a certain parameter (i.e. length or aperture) is smaller than the system dimension dividing by a factor of 1000. The factor of 1000 has been determined empirically by running the FFDF code. For example, if a system diameter is 10m, a fracture with length smaller than or equal to 0.01m can be treated as a point rather than a line. Similarly, a fracture with aperture as small as 100μm can be represented as a line rather than a rectangle since 100μm < 0.01m.

![Fracture network with the constant aperture](image)

**Figure B. 6 Fracture network with the constant aperture**

In summary, orientation, which is assumed to be uniform for simplicity, is the most important parameter to occur the FBC (i.e. percolation).
Appendix C: Example for Assembling Global Matrix

In (3.43), all three matrices, $[\zeta]$, $[\phi]$, and $[\Omega]$ are called global matrices. By summing all elemental matrices, with subscript $e$, global matrices can be obtained. To show how to assemble the global matrix equation from the element matrix and solve the global matrix equation, a simple example (Figure C.1) is given. The domain has 5 nodes and 4 elements. At nodes 1 and 2, by the $C_1$ boundary condition, the potential head is prescribed. At nodes 4 and 5, by the $C_2$ boundary condition, zero flux is prescribed. By mass balance, the flux $Q_3$ is zero at node 3.

![Figure C.1 Simple example for water flow analysis.](image)

The global matrix equation is written as

$$[\zeta][\phi] = [\Omega]. \quad (C.1)$$

The global matrix $[\zeta]$ can be obtained by superimposing all of the elemental matrices as

$$[\zeta] = \sum_{e=1}^{5} [\zeta_e]. \quad (C.2)$$

because the domain consists of four elements.

Element (1) has three nodes, 1, 2, and 3. Because there are five nodes in the domain, the global matrix has $5 \times 5$ matrix. By (3.46),

$$[\zeta_1] = \frac{K_1}{4\Delta_1} \begin{bmatrix}
\beta_1 \beta_{1,1} + \gamma_{1,1} \gamma_{1,1} & \beta_1 \beta_{1,2} + \gamma_{1,2} \gamma_{1,2} & \beta_1 \beta_{1,3} + \gamma_{1,3} \gamma_{1,3} & 0 & 0 \\
\beta_1 \beta_{1,1} + \gamma_{1,1} \gamma_{1,1} & \beta_1 \beta_{1,2} + \gamma_{1,2} \gamma_{1,2} & \beta_1 \beta_{1,3} + \gamma_{1,3} \gamma_{1,3} & 0 & 0 \\
\beta_1 \beta_{1,1} + \gamma_{1,1} \gamma_{1,1} & \beta_1 \beta_{1,2} + \gamma_{1,2} \gamma_{1,2} & \beta_1 \beta_{1,3} + \gamma_{1,3} \gamma_{1,3} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix} \quad (C.3)$$

$$[\zeta_2] = \frac{K_2}{4\Delta_2} \begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & \beta_2 \beta_{2,2} + \gamma_{2,2} \gamma_{2,2} & \beta_2 \beta_{2,3} + \gamma_{2,3} \gamma_{2,3} & \beta_2 \beta_{2,4} + \gamma_{2,4} \gamma_{2,4} & 0 \\
0 & \beta_2 \beta_{2,2} + \gamma_{2,2} \gamma_{2,2} & \beta_2 \beta_{2,3} + \gamma_{2,3} \gamma_{2,3} & \beta_2 \beta_{2,4} + \gamma_{2,4} \gamma_{2,4} & 0 \\
0 & \beta_2 \beta_{2,2} + \gamma_{2,2} \gamma_{2,2} & \beta_2 \beta_{2,3} + \gamma_{2,3} \gamma_{2,3} & \beta_2 \beta_{2,4} + \gamma_{2,4} \gamma_{2,4} & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix} \quad (C.4)$$

$$[\zeta_3] = \frac{K_3}{4\Delta_3} \begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix} \quad (C.5)$$

116
\[
\begin{bmatrix}
\beta_i \beta_{i1} + \gamma_i \gamma_{i1} & 0 & \beta_i \beta_{i3} + \gamma_i \gamma_{i3} & 0 & \beta_i \beta_{i5} + \gamma_i \gamma_{i5} \\
0 & 0 & 0 & 0 & 0 \\
\beta_i \beta_{i1} + \gamma_i \gamma_{i1} & 0 & \beta_i \beta_{i3} + \gamma_i \gamma_{i3} & 0 & \beta_i \beta_{i5} + \gamma_i \gamma_{i5} \\
0 & 0 & 0 & 0 & 0 \\
\beta_i \beta_{i1} + \gamma_i \gamma_{i1} & 0 & \beta_i \beta_{i3} + \gamma_i \gamma_{i3} & 0 & \beta_i \beta_{i5} + \gamma_i \gamma_{i5}
\end{bmatrix}
\]

By the assumed boundary conditions, the values of \(\phi_1, \phi_2\) are prescribed. The homogenized hydraulic conductivity, \(K_n\), is assumed for each element. The values of \(Q_i\) and \(Q_5\) are prescribed zero. The value of \(Q_3\) is zero by the mass balance. Then, the global matrix can be divided into the known and unknown matrices as

\[
\begin{bmatrix}
\zeta_{11} & \zeta_{12} & \zeta_{13} & \zeta_{14} & \zeta_{15} \\
\zeta_{21} & \zeta_{22} & \zeta_{23} & \zeta_{24} & \zeta_{25} \\
\zeta_{31} & \zeta_{32} & \zeta_{33} & \zeta_{34} & \zeta_{35} \\
\zeta_{41} & \zeta_{42} & \zeta_{43} & \zeta_{44} & \zeta_{45} \\
\zeta_{51} & \zeta_{52} & \zeta_{53} & \zeta_{54} & \zeta_{55}
\end{bmatrix}
\begin{bmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\phi_4 \\
\phi_5
\end{bmatrix}
= \begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
0
\end{bmatrix},
\]

where \(*\) represents unknown parts

and

\[
[\zeta_7]_{11} = \begin{bmatrix}
\zeta_{11} & \zeta_{12} \\
\zeta_{21} & \zeta_{22}
\end{bmatrix}, \text{ and so on.}
\]

Equation (C.8) can be explicitly written by two matrix equations:

\[
[\zeta_7]_{11}[\phi_1]_h + [\zeta_7]_{12}[\phi_2]_h = [Q_7]_h^T,
\]

\[
[\zeta_7]_{21}[\phi_1]_h + [\zeta_7]_{22}[\phi_2]_h = [0].
\]

The unknown matrix \([\phi_1]_h\) is obtained by solving (C.11), and \([Q_7]_h\) is obtained by solving (C.10) after substituting the obtained \([\phi_2]_h\) into (C.10).
Appendix D: Features of FFDF Code

FFDF (Finite-element Flow and transport code for Discrete-Fracture networks) is a two-dimensional numerical code for simulating water flow and particle transport in the near field of geologic repository for the one-waste canister configuration. FFDF is developed by the author at Nuclear Waste Research Laboratory in University of California at Berkeley. For analyses of water flow and particle transport through a fractured rock, DFN in the near-field rock (NFR) is transformed into a heterogeneous continuum by the local homogenization (Section 3.4.1) or a homogeneous continuum by the uniformization (Section 3.4.2). With the FFDF code, a steady-state spatial potential distribution in the water-flowing regions is obtained based on the assumptions of time-independent, incompressible Darcy’s flow. The finite element method (Galerkin’s method) is applied for solving the potential equation in the two-dimensional domain with the heterogeneous distributions of the porosity (Section 3.4.1.1) and the hydraulic conductivity (Section 3.4.1.2). The governing equation and the boundary conditions for the flow analysis used in FFDF code are (3.17), (3.18), and (3.19), respectively. Equations from (3.43) to (3.50) are the numerical solutions implemented in the FFDF code. Particle transport is simulated considering the advection and molecular diffusion by random walk tracking method (RWTM) on the top of the flow model. The governing equation for transport analysis used in FFDF code is (5.68). As boundary conditions, reflecting boundary condition is prescribed at the surface of the canister, and absorbing boundary condition is prescribed at the outer boundary.

FFDF for a near-field model with a heterogeneous NFR by the local homogenization, performs

1. the generation of DFN, which includes:
   - determination of proper statistics for fracture geometry parameters by the user.
   - generation of a fracture segment based on determined statistics for fracture geometry parameters.
   - 2 random numbers for the determination of location.
   - 1 random number for the determination of length.
   - 1 random number for the determination of orientation.
   - 1 random number for the determination of aperture.
   - superposition of individual fractures in the model space until the required number of fractures is achieved.

2. identification of the FBC by inspecting the interconnection of fractures,
3. generation of triangular finite elements over the FBC and the bentonite-filled buffer region,
4. calculation of the equivalent permeability and porosity for each element,
5. calculation of the spatial potential distribution in the FBC and the bentonite-filled buffer region, and the total discharge of water at the interface between the buffer region and the NFR region, and the total discharge at the outer boundary,
6. calculation of the residence time of the particles by random walk tracking method.

To obtain a statistical distribution, procedures (1) to (5) are repeated for water flow analysis only. The procedure (1) to (6) should be repeated for the particle transport analysis.

FFDF for a near-field model with the homogenized NFR by the uniformization performs the same procedures as those for the model with the heterogeneous NFR except for (4), where the permeability and porosity for the entire NFR are calculated by procedures shown in Section 3.4.2.
Appendix E: Analogy to Transport Equation

In this appendix, it is checked if the step equation (5.35) satisfies the transport equation by showing if the probability density function, \( w(x,t) \), satisfies the transient transport equation for one and two-dimensional cases.

First, for one-dimensional x-coordinate, the probability, \( w(x,t) \), that the particle has been displaced by advection and diffusion in the time \( t \) to a region between \( x \) and \( x+\Delta x \) is given in (5.25) as

\[
w(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right), \quad t \geq 0, -\infty < x < \infty.
\] (5.25)

A differential equation for \( w(x,t) \) in one-dimensional x-coordinate for advection and diffusion with constant \( v \) and \( D \) is

\[
\frac{\partial w(x,t)}{\partial t} + v \frac{\partial w(x,t)}{\partial x} - D \frac{\partial^2 w(x,t)}{\partial x^2} = 0.
\] (E.1)

If (5.25) satisfies (E.1), (5.25) is a solution of the differential equation (E.1).

Substituting (5.25) into the first term of left-hand side in (E.1) yields

\[
\frac{\partial w(x,t)}{\partial t} = \frac{ND[x^2 - v^2t^2 - 2Dt]}{8(Dt)^{3/2} \sqrt{\pi}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right)
\] (E.2)

Substituting (5.25) into the second term of left-hand side in (E.1) yields

\[
v \frac{\partial w(x,t)}{\partial x} = v \frac{N(v(t-x))}{4Dt\sqrt{\pi Dt}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right)
\] (E.3)

Substituting (5.25) and \( \frac{\partial w(x,t)}{\partial x} \) obtained in (E.3) into the third term of left-hand side in (E.1) yields

\[
D \frac{\partial^2 w(x,t)}{\partial x^2} = D \frac{N}{4Dt\sqrt{\pi Dt}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right) \left(\frac{(x-vt)^2 - 2Dt}{2Dt}\right)
\] (E.4)

Substituting (E.2), (E.3), and (E.4) into the left-hand side of (E.1) gives the zero, which is the same as that of right-hand side of (E.1).

\[
\frac{ND[x^2 - v^2t^2 - 2Dt]}{8(Dt)^{3/2} \sqrt{\pi}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right) + v \frac{N(v(t-x))}{4Dt\sqrt{\pi Dt}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right) - D \frac{N}{4Dt\sqrt{\pi Dt}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right) \left(\frac{(x-vt)^2 - 2Dt}{2Dt}\right)
\] (E.5)

Since (5.25) satisfies (E.1), (5.25) is a solution of (E.1). Thus, resulting mass distribution of a large number of particles by the step equation for this case is equivalent to that given by the one-dimensional transport equation (E.1)

Second, for a two-dimensional \( x, y \) coordinates, similar to \( w(x,t) \) as shown in (5.25), the probability, \( w(y,t) \), that a particle has been displaced in the time \( t \) to a region between \( y \) and \( y+dy \), can be written as

\[
w(y,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{(y-y_0)^2}{4Dt}\right), \quad t \geq 0, -\infty < y < \infty.
\] (E.6)

Since movements of particles in x-coordinate are independent of those in y-coordinates, the probability, \( w(x,y,t) \), that the particle has been displaced in the time \( t \) to a region between \( x \) and \( x+dx \), and between \( y \) and \( y+dy \), can be expressed as a product of solutions as

\[
w(x,y,t) = w(x,t)w(y,t) = \frac{1}{4\pi Dt} \exp\left(-\frac{(x-x_0)^2 + (y-y_0)^2}{4Dt}\right), \quad t \geq 0, -\infty < x < \infty, -\infty < y < \infty.
\] (E.7)
A differential equation in two-dimensional \((x,y)\) coordinates for advection and diffusion with constant \(v_x\), \(v_y\), and \(D\) is

\[
\frac{\partial w(x,y,t)}{\partial t} + v_x \frac{\partial w}{\partial x} + v_y \frac{\partial w}{\partial y} - D \frac{\partial^2 w}{\partial x^2} - D \frac{\partial^2 w}{\partial y^2} = 0
\]  
(E.8)

If (E.7) satisfies (E.8), (E.7) is a solution of the differential equation (E.8). Substituting (E.7) into the first term of left-hand side in (E.8) yields

\[
\frac{\partial w(x,y,t)}{\partial t} = -\left[4Dt + (v_x^2 + v_y^2 - x^2 - y^2)\right] e^{-\frac{(x-v_xt)^2+(y-v_yt)^2}{4Dt}}
\]  
(E.9)

Substituting (E.7) into the second term of left-hand side in (E.8) yields

\[
v_x \frac{\partial w}{\partial x} = -\frac{[xv_y - v_y^2]}{8D^2\pi^2} e^{-\frac{(x-v_xt)^2+(y-v_yt)^2}{4Dt}}
\]  
(E.10)

Substituting (E.7) into the third term of left-hand side in (E.8) yields

\[
v_y \frac{\partial w}{\partial y} = -\frac{[yv_x - v_x^2]}{8D^2\pi^2} e^{-\frac{(x-v_xt)^2+(y-v_yt)^2}{4Dt}}
\]  
(E.11)

Substituting (E.7) into the fourth term of left-hand side in (E.8) yields

\[
D \frac{\partial^2 w}{\partial x^2} = De^{-\frac{(x-v_xt)^2+(y-v_yt)^2}{4Dt}} \left[-\frac{1}{8D^2\pi^2} + \frac{(x-v_xt)^2}{16D^2\pi^2}\right]
\]  
(E.12)

Substituting (E.7) into the fifth term of left-hand side in (E.8) yields

\[
D \frac{\partial^2 w}{\partial y^2} = De^{-\frac{(x-v_xt)^2+(y-v_yt)^2}{4Dt}} \left[-\frac{1}{8D^2\pi^2} + \frac{(y-v_yt)^2}{16D^2\pi^2}\right]
\]  
(E.13)

Substituting (E.9), (E.10), (E.11), (E.12), and (E.13) into the left-hand side of (E.8) gives the zero, which is the same as that of right-hand side of (E.8).

\[
e^{-\frac{(x-v_xt)^2+(y-v_yt)^2}{4Dt}} \left[-\frac{4Dt + (v_x^2 + v_y^2 - x^2 - y^2)}{16D^2\pi^2} - \frac{[xv_y - v_y^2]}{8D^2\pi^2} - \frac{[yv_x - v_x^2]}{8D^2\pi^2}\right]
\]

\[
- \frac{D(x-v_xt)^2}{8D^2\pi^2} + \frac{D(y-v_yt)^2}{16D^2\pi^2}
\]  
(E.14)

\[
= 0
\]

Thus, (E.7) satisfies (E.8). Since (E.7) is a solution of (E.8), distribution of particles in \(x, y\) coordinates, \(w(x,y,t)\), in (E.7) is equivalent to the resulting distribution by the two-dimensional transient advection-diffusion transport equation with constant \(v_x\), \(v_y\), and \(D\) in (E.8)
Appendix F: Imaginary Absorbing Boundary for Transport

Increasing the size of triangular elements leads to increase the gap between the outer (circular) boundary \((r=R_2)\) and the elements. The gap regions are shown in Figure F.1 as shaded regions. The gap regions are created by circular domain discretization with triangular elements, and are neither FBC region nor Non-FBC region. To avoid a numerical error due to the gap regions for the particle transport, imaginary absorbing boundary with radius of \(R_2'\) as shown in Figure F.1 (b) is set as \(R_2'=R_2-h_{\text{gap}}\), where \(h_{\text{gap}}\) is the maximum thickness of the gap region.

Maximum thickness of the gap, \(h_{\text{gap}}\), is evaluated using an example in Figure F.2. Parameter \(R_2\) and \(\theta\) in Figure F.2 should be prescribed for numerical calculation. In this study, \(R_2=5\) m is used for all numerical simulations. The values of \(\theta\), depended on the size of elements, are \(2\pi/10\), \(2\pi/20\), \(2\pi/40\), and \(2\pi/80\) for cases 1, 2, 3, and 4 in Figure 3.22, respectively.

The value of \(R_2'\) for the triangle with \((x_1, y_1)\), \((x_2, y_2)\), and \((x_3, y_3)\) in Figure F.2 can be obtained using the area of the triangle \(\Delta\) and the distance between \((x_2, y_2)\), and \((x_3, y_3)\), \(L_{\text{gap}}\), by cosine rule as:

\[
R_2' = \frac{2\Delta}{L_{\text{gap}}},
\]

where

\[
2\Delta = \begin{vmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \end{vmatrix}, \quad L_{\text{gap}} = \sqrt{2R_2^2(1-\cos \theta)}.
\]

The values of \(R_2'\) and \(h_{\text{gap}}\) \((h_{\text{gap}} = R_{2'}-R_2)\) for case 3 in Figure 3.22 (c) are calculated as 4.98 m and 0.02 m, respectively, by (F.1) with \((x_1=0, y_1=0)\), \((x_2=0.782, y_2=4.938)\), \((x_3=0, y_3=5.0)\), \(R_2=5\), and \(\theta=2\pi/40\).

Numerical results in Chapter 3 and Chapter 5 are based on the domain discretization with the same size of elements as case 3 in Figure 3.22 (c). Thus, a radius of the imaginary absorbing boundary for transport analysis in Chapter 5 is \(R_2'=4.98\) m.
Figure F. 2 Calculation of the maximum thickness of the gap region $h_{gap}$. 
Appendix G: Example for Identification of Paths

The procedures of identifying paths through the interconnected fractures connecting the left and right boundaries are given as follows. The fracture network in Figure G.1, which is the same as Figure 6.2 (c), is used for the purpose of explanation of the procedures.

First, the list of connected points is made for all points as shown in Table G.1. In the first column in Table G.1, points located on the right boundary (“2”, “3”, “4”, and “5”) are not considered. The connected points in the second column in Table G.1 are the nearest points along the interconnected fractures from the given point in the first column in the table. For example, points “2” and “8” in Figure G.1 are not the connected points with point “7” because the points “6” and “9” are the nearest points along the connected fractures from “7”.

Second, points consisting of a path are identified based on the list in Table G.1. Points on the left boundary is “1”, and points on the right boundary is “2”, “3”, “4”, and “5”. In Figure G.2, the points on the right boundary, which are the last points for possible paths, are shown as boxed numbers. To identify a path, let’s start from the point “1” which is located on the left boundary. Point “6” is the next point for a possible path because “1” is connected with only “6”, denoted as (1-6). Point “6” is connected “1”, “7” and “8”. By definition of a path (see Section 6.3.1.1), point “1” is not considered any more for this particular path because point “1” is already visited. Thus, next point for a path is either “7” or “8”. Let’s take “7” first as (1-6-7). “8” will be taken later, and becomes the remaining point for “6”. The next possible point for “7” is “9” because “6” is already visited (1-6-7-9). As a next point for “9”, “2” and “11” are possible. Let’s take “2” first, and “11” becomes the remaining point for “9”. Since “2” is on the right boundary, the first path is identified as (1-6-7-9-2) as shown in Figure G.2.

For the second path, identified previous path (1-6-7-9-2) is used. During the identification of the first path, there are two remaining points as “8” for “6” and “11” for “9”. For the identification of a next path, the remaining points are checked from the reverse direction of the previous path (1-6-7-9-2). In this case, identification of a next path is started from the point “8” by keeping all upper level points of “9” as (1-6-7-9). Because “11” is the only remaining point for “9”, a next point for a path is “11” (1-6-7-9-11). For (1-6-7-9-11), next possible points are “4”, “5”, and “10”. Let’s take “4” first, and “5” and “10” become remaining points for “11”. The second path is identified as (1-6-7-9-11-4) since “4” is located on the right boundary.

Similarly, by checking the remaining point from the reverse direction of the previous path, the third and fourth paths are identified as (1-6-7-9-11-5), (1-6-7-9-11-10-3). A point, which has no more connected point, is called dead-end point in this study. For a point “8” in (1-6-7-9-11-10-8), a next point cannot be determined because “6” and “10” are already visited in this particular possible path. Thus, “8” is dead-end point for (1-6-7-9-11-10-8) as shown in Figure G.2. Therefore, (1-6-7-9-11-10-8) is not a path. By checking the remaining point of the upper levels of “8”, identification processes are performed until there is no more remaining point up to the starting point (i.e. “1” in this case). By these processes, fifth, sixth, seventh, and eighth paths are identified as (1-6-8-10-3), (1-6-8-10-11-4), (1-6-8-10-11-5), and (1-6-8-10-11-9-2), respectively. If there is no more remaining point up to the starting point (i.e. “1” in this case), identification processes can start from another point on the left boundary if it is available (“1” is the only point on the left boundary in Figure G.1). If another point exists, identification processes are repeated as above. In this new processes starting from another point on the left boundary, information of the remaining points for all points are initiated as given in the list of connected points.

In summary, total 8 paths are identified for the fracture network in Figure G.1. 8 paths are (1-6-7-9-2), (1-6-7-9-11-4), (1-6-7-9-11-5), (1-6-7-9-11-10-3), (1-6-8-10-3), (1-6-8-10-11-4), (1-6-8-10-11-5), and (1-6-8-10-11-9-2).

![Figure G.1](image-url) Interconnected fracture network same as Figure 6.2 (c)
Table G.1  List of Connected Points for Figure G.1

<table>
<thead>
<tr>
<th>Points</th>
<th>Connected points</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
</tr>
<tr>
<td>6</td>
<td>1,7,8</td>
</tr>
<tr>
<td>7</td>
<td>6,9</td>
</tr>
<tr>
<td>8</td>
<td>6,10</td>
</tr>
<tr>
<td>9</td>
<td>2,7,11</td>
</tr>
<tr>
<td>10</td>
<td>3,8,11</td>
</tr>
<tr>
<td>11</td>
<td>4,5,9,10</td>
</tr>
</tbody>
</table>

Figure G.2  Identification of paths from the list in Table G.1
Appendix H: Potential Distribution in the Fracture Network

To calculate the potential distribution at intersections, a simple fracture network in the unit square domain is considered as shown in Figure H.1. Boundary conditions are prescribed as shown in Figure H.2 (a). Constant pressures are prescribed as $P_1=1$ kg/ms$^2$ at the left ($x=-0.5$) boundary and as $P_2=0$ kg/ms$^2$ at the right ($x=0.5$) boundary. No flow boundary condition is prescribed at the top ($y=0.5$) and the bottom ($y=-0.5$) of the unit square domain.

Flow rate of water normal to flow through a fracture (parallel plate) of a length $\Delta L$ with a difference of potential head $\Delta P$ is calculated approximately as the product of the average velocity of water through the fracture with aperture ($b$) and the cross-sectional area ($b \cdot w$) normal to flow, where $w$ is the width of a fracture normal to $x$-$y$ plane. The flow rate for $w=1$[m] is written as:

$$Q = -\frac{b}{12\mu_w} \frac{\Delta P}{\Delta L}.$$  \hspace{1cm} (H.1)

where $\mu_w$ (0.799×10$^{-3}$ N·s/m² for 30°C) is the viscosity of water, $b$ is the aperture of a fracture, and $P$ [kg/ms$^2$] is the pressure.

Equation (H.1) can be written in terms of hydraulic head by substituting $\Delta \phi=\Delta P/\rho g$ (see (7.2)) as

$$Q = -\frac{\rho g b}{12\mu_w} \frac{\Delta \phi}{\Delta L}.$$  \hspace{1cm} (H.2)

where $\rho$ (996 kg/m$^3$ for 30°C) is the density of water, $g$(9.8 m/s$^2$) is the constant for gravity, and $\phi$ [m] is the hydraulic head.

---

Figure H.1  Simple example of fracture network

Figure H.2  A fracture network with boundary conditions
Figure H.2 (b) shows the fracture network with labeled points at the intersections. Parameters $L_{1,3}$ and $b_{1,3}$ denote the distance between points 1 and 3, and aperture of a fracture including both points 1 and 3, respectively.

In Figure H.2 (b), potentials at points 1 and 2 are known by given boundary conditions as $P_1=1$ kg/ms$^2$ and $P_2=0$ kg/ms$^2$ while those at points 3 and 4 are unknown. Unknown potentials $P_3$ and $P_4$ at points 3 and 4, respectively, can be calculated by assuming the mass balance of water at each point similar to the Kirchoff’s current law (the sum of current at each point is zero) in electrical circuit. Mass balance equations (sum of the volumetric flow rate at each point is zero) of water at points 3 and 4 by (H.1) are:

$$\begin{align*}
K_{1,3}' \frac{P_3 - P_2}{L_{1,3}} + K_{3,4}' \frac{P_3 - P_4}{L_{3,4}} &= 0, \\
K_{3,4}' \frac{P_3 - P_4}{L_{3,4}} + K_{4,2}' \frac{P_3 - P_4}{L_{4,2}} &= 0,
\end{align*}$$

(H.3)

where $K_{i,j}' [m^3/s/kg] = -\frac{b_{i,j}}{12\mu_w}$

Equation (H.3) can be written as a matrix form.

$$\begin{bmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
-K_{1,3}' / L_{1,3} & 0 & K_{1,3}' / L_{1,3} + K_{3,4}' / L_{3,4} & -K_{3,4}' / L_{3,4} & 0 \\
0 & -K_{4,2}' / L_{4,2} & -K_{4,2}' / L_{4,2} & K_{4,2}' / L_{4,2} + K_{4,2}' / L_{4,2} & 0
\end{bmatrix} \begin{bmatrix}
P_1 \\
P_2 \\
P_3 \\
P_4
\end{bmatrix} = \begin{bmatrix}
1 \\
0 \\
0 \\
0
\end{bmatrix}$$

(H.4)

Potentials at points 3 (i.e. $P_3$) and 4 (i.e. $P_4$) are calculated by solving the matrix in (H.4) with respect to $P_3$ and $P_4$ as

$$P_3 = \frac{K_{1,3}' (K_{1,3}' L_{1,3} + K_{3,4}' L_{3,4})}{K_{1,3}' K_{4,2}' L_{4,2} + K_{1,3}' K_{4,2}' L_{4,2} + K_{3,4}' K_{4,2}' L_{4,2}},$$

H.5

$$P_4 = \frac{K_{1,3}' K_{4,2}' L_{4,2}}{K_{1,3}' K_{4,2}' L_{4,2} + K_{1,3}' K_{4,2}' L_{4,2} + K_{3,4}' K_{4,2}' L_{4,2}}.$$

Numerical scheme incorporated into the code is verified by the analytical solution (H.5) for the case where $K_{1,3}'=8.12E-7$ m$^3$/kg, $K_{3,4}'=2.66E-8$ m$^3$/kg, $K_{4,2}'=2.66E-8$ m$^3$/kg, and $b_{1,3}=1.98E-3$ m, $b_{1,3}=b_{2,4}=6.34E-4$ m, and $L_{1,3}=7.39E-1$ m, $L_{3,4}=1.52E-1$ m, and $L_{4,2}=2.30E-1$ m. Numerically obtained values of $P_3=0.940$ kg/ms$^2$ and $P_4=0.566$ kg/ms$^2$ are verified by analytical solution as $P_3=0.940$ kg/ms$^2$ and $P_4=0.566$ kg/ms$^2$. 

126
Appendix I: Analytical Fracture Flow Model

In this appendix, an analytical fracture-flow model is developed [Chambré, 2001]. A mathematical problem in this appendix is to solve a water flow rate through a fracture network in Figure I.1 (see Appendix H for more details of the model space).

\[ Q_{i,j} = \alpha \left( \frac{b_{i,j}}{L_{i,j}} \right) \Delta P_{i,j}, \]  

(I.1)

where

\[ \alpha = \frac{1}{12\mu_w}, \]  

(I.2)

where \( b_{i,j} [\text{m}] \) and \( L_{i,j} [\text{m}] \) denote the aperture and length of a fracture with points \( i \) and \( j \), respectively. \( \mu_w (0.799\times10^{-3} \text{ Ns/m}^2 \text{ for } 30^\circ\text{C}) \) is the viscosity of water, and \( \Delta P_{i,j} [\text{kg/ms}^2] = P_i - P_j \).

By the condition (1), the same volumetric flow rate \( Q \) passes through each fracture, i.e. 1-3, 3-4, and 4-2, where 1-3 denotes a flow path from point 1 to point 3.

\[ Q = Q_{1,3} = Q_{3,4} = Q_{4,2}. \]  

(I.3)

(I.1) can be written using (I.3) as

\[ \Delta P_{i,j} = \frac{Q}{\alpha} \left( \frac{L_{i,j}}{b_{i,j}} \right), \]  

(I.4)

where \( \Delta P_{i,j} > 0 \) for each path since the right hand side of (I.4) is larger than zero.

(I.4) can be written for 3 paths in Figure I.1 as

\[ P_1 - P_3 = Q \frac{1}{\alpha} \left( \frac{L_{1,3}}{b_{1,3}} \right), \]  

(I.5)

\[ P_3 - P_4 = Q \frac{1}{\alpha} \left( \frac{L_{3,4}}{b_{3,4}} \right), \]  

(I.6)

\[ P_4 - P_2 = Q \frac{1}{\alpha} \left( \frac{L_{4,2}}{b_{4,2}} \right), \]  

(I.7)
\[ P_1 - P_2 = Q \frac{1}{\alpha \left( \frac{L_{1,3}}{b_{1,3}^3} \right)} . \]  

(I.7)

Summation from (I.5) to (I.7) yields

\[ P_1 - P_2 = Q \frac{1}{\alpha} \left( \frac{L_{1,3}}{b_{1,3}^3} + \frac{L_{3,4}}{b_{3,4}^4} + \frac{L_{4,2}}{b_{4,2}^4} \right). \]  

(I.8)

From (I.8), \( Q \) is obtained as

\[ Q = \alpha \frac{(P_1 - P_2)}{\left( \frac{L_{1,3}}{b_{1,3}^3} + \frac{L_{3,4}}{b_{3,4}^4} + \frac{L_{4,2}}{b_{4,2}^4} \right)}. \]  

(I.9)

As shown in (I.9), volumetric flow rate \( Q \) through a fracture network can be calculated without knowing the values of pressure head at points 3 and 4.

For an example, \( Q \) is calculated as 6.54E-8 m\(^3\)/s by (I.9) using same input data used in Appendix H such as \( \alpha=104.3 \text{ m}^3/\text{N}\cdot\text{s} \), \( P_1=1 \text{ kg}/\text{ms}^2 \), \( P_2=0 \text{ kg}/\text{ms}^2 \), \( b_{1,3}=1.98\text{E}-3 \text{ m} \), \( b_{3,4}=b_{4,2}=6.34\text{E}-4 \text{ m} \), and \( L_{1,3}=7.39\text{E}-1 \text{ m} \), \( L_{3,4}=1.52\text{E}-1 \text{ m} \), and \( L_{4,2}=2.30\text{E}-1 \text{ m} \).

The value of \( Q=6.54\text{E}-8 \text{ m}^3/\text{s} \) obtained by (I.9) for the data used in Appendix H is the same as that calculated by (H.1) for \( Q_{1,2} \), where \( Q=Q_{1,2}=Q_{3,4} \).

The method for calculation \( Q \) described in this appendix can be applied to more complicated fracture network than that in Figure I.1, which has only one flow path. For example, a fracture network which has the two flow paths, i.e. 1-3-4-2 and 5-3-4-2, is given in Figure I.2.

![Figure I.2 A fracture network which has two inlets.](image)

The flow of water through the fracture network can be simulated by the flow of an electric current in an analog [Bear, 1972].

Equivalent arrays of resistors to the fracture networks in Figure I.1 and Figure I.2 are shown in Figure I.3 (a) and (b), respectively. An electric circuit in Figure I.3 (b) can be simplified by using Ohm’s law for resistor in parallel (see Figure I.4) as

\[ \frac{1}{R'} = \frac{1}{R_{1,3}} + \frac{1}{R_{3,5}}, \]  

(I.10)

where \( R' \) [ohm] denotes a resistance for a simplified flow path from the two paths.
Figure I. 3  Equivalent array of resistors to the fracture network in Figure I.1 (a) and the fracture network in Figure I.2 (b). $R_{ij}$ [ohm] denotes the resistance between points $i$ and $j$ in electrical circuit.

Figure I. 4  Simplified array of resistors from Figure I.3 (b) by Ohm’s law for resistors in parallel.

Since a circuit in Figure I.3 (a), which is equivalent to Figure I.1, is the same as a circuit in Figure I.4, which is equivalent to Figure I.2, the volumetric flow rate $Q$ for a fracture network in Figure I.2 can be calculated by the method used for Figure I.1, i.e. (I.4)–(I.9), using the Ohm’s law for resistor in parallel as follows.

Bear [1972] showed that the resistance $R$ [ohm] in electric circuit corresponds to the hydraulic properties as

$$R_{ij} = \frac{1}{\alpha b_i^j},$$  \hspace{1cm} (I.11)

where subscripts $i$ and $j$ denote the starting and end points of flow paths.

By substituting (I.11) into (I.10), a simplified resistance $R'$ in Figure I.4 is obtained from $R_{1,3}$ and $R_{3,5}$ as

$$R' = \frac{1}{\alpha} \left( \frac{L_{i,j} L_{j,k}}{L_i^b b_j^k + L_j^b b_k^i} \right).$$  \hspace{1cm} (I.12)

By (I.1) and (I.11), a following relationship is obtained as

$$\Delta P_{ij} = Q_{ij} R_{ij}.$$  \hspace{1cm} (I.13)

Substituting (I.12) into (I.13) with $Q_{ij} = Q$ yields

$$\Delta P_{i,j} = Q \frac{1}{\alpha} \left( \frac{L_{i,j} L_{j,k}}{L_i^b b_j^k + L_j^b b_k^i} \right).$$  \hspace{1cm} (I.14)

Since $\Delta P_{3,4}$ and $\Delta P_{4,2}$ in Figure I.4 are the same as those in (I.6) and (I.7), respectively, the volumetric flow rate $Q$ for a fracture network in Figure I.2 is calculated by summing (I.14), (I.6) and (I.7) as
\[ Q = \alpha \left( P_1 - P_2 \right) \left( \frac{L_{3,3}}{L_{5,5} b_{1,1} \left( L_{5,5} b_{1,1} + L_{1,1} b_{3,3} \right) + L_{5,5} b_{1,1}} + \frac{L_{4,4}}{b_{1,1}^{b_{3,3}}} + \frac{L_{4,4}}{b_{1,1}^{b_{3,3}}} \right) \]  

(I.15)

It should be noted that with an analytical model described in this appendix, water flow rate through the fracture network can be calculated without calculating the potential head at the intersections of fractures, whereas the method used in Chapter 7 requires the values of the potential head at the intersections of fractures.