Workflow for the integration of 3D geometrical and numerical models applied to contaminant transport in fractured porous media

Research Proposal

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1. Introduction

1.1 General Background

Geosciences, or the Earth Sciences, are all the sciences related to the planet Earth. Hydrogeology, like most geosciences, is an interdisciplinary subject which deals with water flowing through geological formations. Groundwater resources are precious assets as a source for drinking water and for human industrial and agricultural activities. They are subject of increased interest from the science community, together with an ever-increasing realization of their primary importance for human life. In the actual world context, water is going to become a limiting factor for human development and problems will arise to maintain a good balance between water resources availability and their exploitation. With the world’s population explosion, combined with increasing pollution and wide-scale irrational management (excessive withdrawal), a critical water shortage may occur in the future. Because remediation of contaminated aquifer is prohibitively costly and in some cases impossible, it is extremely important to take care of these precious resources.

A possible and very dangerous contamination source is the release of man-made radionuclides in the environment. A radionuclide is a radioactive chemical that is found in water and its contamination is a developing issue. Radioactivity in ground water is usually, but not always, naturally occurring (natural sources are element such as radon, radium, or uranium). Discharges from nuclear power plants and medical facilities have caused man-made radioactivity to find its way into drinking water sources. Speaking about nuclear power plants, one of their biggest problems is the management of the wastes produced. There are different kinds of waste, depending on their radioactivity level. The Nuclear Regulatory Commission separates wastes into two broad classifications: high-level or low-level waste. The former comes primarily from the fuel used by reactors to produce electricity. The latter comes from reactor operations and from medical, academic, industrial, and other commercial uses. Others waste types are sometimes cited, such as mine tailings, intermediate-level or transuranic waste. Since the only way radioactive wastes become harmless is through decay -which for some isotopes contained in high-level wastes can take
hundreds of thousands of years- they must be stored in a way that provides adequate protection for very long times.

After years of study, most countries have concluded that permanent geologic burial is the most acceptable solution for the final disposition of high-level nuclear waste. Nuclear waste has sometimes been called the Achilles’ heel of the nuclear power industry. Much of the controversy over nuclear power plant is on the lack of a dumping system for the highly radioactive spent fuel removed from operating reactors. As a result, progress on nuclear waste disposal is widely considered a prerequisite for any future growth of nuclear power IB [3]. Repositories for disposal of radioactive waste generally rely on a multi-barrier system to isolate the waste from the biosphere. It is defined as a multi-barrier system because it includes the natural (geological) barrier provided by the host rock and an engineered barrier system (EBS). An EBS must be tailored to the specific environment in which it is to function. Consideration must be given to factors such as the heat that will be produced by the waste, the pH and redox conditions that are expected, the expected groundwater flux, the local groundwater chemistry, the possible interactions among different materials in the waste and in the EBS, the mechanical behavior of the host rock after repository closure and the evolution of all these conditions over time. Ensuring that an EBS will perform its desired functions requires an integration of site characterization data, data on waste and engineering barrier materials properties, “in situ and laboratory testing” and modeling (OECD - NEA O [1]).

Scientists have studied a broad range of options for managing spent nuclear fuel and high-level radioactive waste. The U.S. Department of Energy (Office of Civilian Radioactive Waste Management) lists several options to manage waste: leaving it where it is, burying it in various ways (sub-sea beds, very deep-holes, polar ice sheets), sending it into space, injecting the waste in liquid form very deep underground, making it safer through advanced technologies (transmutation). The international scientific consensus holds that these materials should eventually be disposed of deep underground in what is called a geologic repository. In a recent special report, the National Academy of Sciences summarized the various studies and emphasized that geologic disposal is ultimately necessary (Board on

1.2 Problem Definition

This Ph.D. work is part of the GEOIDE project, whose title is GeoTopo3D - “Development of a 3D predictive modeling platform for exploration, assessment and management of mineral, petroleum and groundwater resources” - (D.Kirkwood, J.Pouliot, R.Therrien, K.MacQuarrie, S.Li, M.Mostafavi). Since 1998, GEOIDE has been a federal-funded Network of Centers of Excellence administrated by the business centre GEOIDE inc. based at Laval University. This ‘network of networks’ brings together skills, technology and people from different communities of practice, in order to develop and consolidate the Canadian competences in geomatics. GEOIDE wants to change the ways geomatics research and development are carried out, to ensure dramatically enhanced circulation of knowledge across disciplines, regions, and between researchers, industry and government users to establish a permanent legacy of cooperation IB [1]. There are 19 projects in the third GEOIDE phase (2005-2009) and they are classified in three application sectors called “Thrusts” and three science and technology domains called “Themes”. GeoTopo3D is placed in the thrust named “Sustainable marine and land resources” (SLM) and in the theme “Data fusion and management” (DFM). It is organized into three principal scientific areas: Geomodels, 3D GIS and 3D Numerical Modeling. A Geomodel is built in specific software platforms (such as Gocad) and it constitutes a 3D representation of geological structures (see Chapter 2). Numerical Modeling deals with mathematical models that give a description of a physical phenomenon. In the hydrogeological context, numerical models should provide a solution to the equations governing groundwater flow and mass transport. Eventually, the term “model”, identify at the same time the software built to solve these equations and the mathematical scheme used to solve them. The goal of the GeoTopo3D project is to facilitate users’ access to Geomodels and to help modelers to build Geomodels, in order to enable a more efficient use of and integration of geoscientific data. Moreover, the objective is to allow a better and larger exploitation of Geomodels, especially taking advantage of the link with 3D GIS and Numerical Models.
My own research is placed in the integration between Geomodels and Numerical Models. In particular, it relies on the development of a workflow for numerical modeling of groundwater flow and solute transport in fractured media adapted to the Gocad platform. The research direction that has been chosen is to use the code Hydrogeosphere (Therrien et al., 2005) to model a fractured aquifer, whose geometry will be built in the Gocad platform. Furthermore, we would like to apply this integration between the two kinds of models (Geomodel and Numerical) to an existing site. For this application, the area chosen surrounds the Finnish nuclear power plant at Olkiluoto site, an island on the South Finnish coast, where a final deep geological disposal facility for nuclear waste is being excavated.

Gocad is a visualization software whose acronym stands for Geological Object Computer Aided Design and it is a product of the Gocad international consortium. This software is based on an interpolation method for modeling natural objects and representing a wide variety of complex data. As opposed to traditional CAD systems, that simply create nice geometrical entities without any constraint, Gocad has been conceived to generate more complex structures and take into account the physical properties attached to each object.

Numerical modeling in hydrogeology has become increasingly important in fields like contaminant transport, waste disposal, geothermal energy and groundwater supply management. Modeling requires a large quantity of input data to describe the configuration of the hydrogeological system, such as geometry and topography data, geology and hydrogeology issues, water and porous medium chemical properties, boundary and initial conditions. The domain geometry, where the simulations will be carried out, has to be first defined and then discretized.

A large amount of data is usually available for a site chosen to be a nuclear waste disposal, like the one selected for this work. Such data are continuously updated and they constitute a large database for modeling purposes. Dumping of nuclear waste is really a crucial matter and countries with nuclear power plants are more and more involved in it, facing all related problems. Surveys and all kind of studies (e.g. geological, mechanical, structural, hydrogeological and chemical) are essential to assess properties of the natural system and imperative to ensure a safe disposal of wastes for human beings.
1.3 Objectives

In the context of nuclear waste disposal it is important to have a detailed knowledge of the groundwater flow, in order to be able to foresee how it might lead to the transport of radionuclides eventually released from the canisters. Therefore, this work focuses on a hydrogeological study to analyze the groundwater pathways through the host geological formation.

The central idea is to create a geometrical model of the geological environment where a repository for nuclear waste is going to be built. The geometry created has to be transferred to the numerical code which allows analyzing groundwater flow and mass transport through the system. A grid, merely a discretization of the geometrical domain in smaller elements, is necessary to solve the partial differential equations governing physical phenomena like, in this case, groundwater flow and mass transport. In other words, one of the challenges in this research project is to find a good compromise between a high-resolution model that represents geological structure with a high degree of fidelity and a lower resolution model more suited for a large number of calculations. Thus, the focus is on creating flow and transport model grids that capture the geometric detail of a particular geological model as it is mentioned in Bower B [4]. Nevertheless, a seamless incorporation of that data into numerical models for fluid flow and transport still does not exist. Development is thus needed to create an efficient link between Geomodels and numerical models, such that the latter benefits from the knowledge gained in constructing Geomodels (Kirkwood et al. K [5]).

A mesh must satisfy some conditions, such as being conformed to the shape of the domain studied and grading from small to large elements, even if across a short distance. Moreover, its elements cannot have any configuration, but they should have a right size and shape, to avoid numerical instabilities or oscillations. It is a key challenge to generate gridded reservoir descriptions that incorporate the structural complexity of the geology while maintaining model sizes that are practical for flow simulations (Prevost et al. P [4]).

The idea in this work is to develop an interface between the Gocad platform and the code Hydrogeosphere, to allow a simple and quick data transfer between them. Through numerical simulations, we would like to analyze the hydrogeological system – fractured
aquifer- existing at Olkiluoto. Groundwater flow modeling really constitutes an important part of the ongoing site investigation program for the repository design and safety assessment and in the last few years modeling has been carried out at Olkiluoto. The only way the radioactive material may be released from the repository into the biosphere is as a result of dissolution in the groundwater and subsequent migration and propagation through the discontinuities or the porous matrix, until reaching surface water systems. That is why hydrogeological modeling is fundamental in this context.

1.4 Current knowledge and bibliography

Previous works on linking Geomodels and Numerical models include Mancini M [2], Andenmatten and Kohl A [5], Kalbacher at al. K [1], but the connection made between the two kinds of models was quite weak and difficult to be implemented. Moreover, in the first work cited, the geometry of the geological site was very simple, consisting in homogeneous crystalline rock not taking into account discontinuities.

In Andenmatten and Kohl (2003), the discretization of a geological site in Switzerland was made by means of the TGridlab Gocad plug-in and the numerical analysis of geothermal resources was carried out with FRACture (Kohl and Hopkirk, 1995). TGridlab is dedicated to the generation of 3D unstructured meshes from geological surface models (tetrahedral meshes, modular hybrid flow grids). It is based on the Frame Model, a gridding framework developed by Lepage, 2003 (Prevost et al. P [4]). Its utilization seemed to be quite tricky and some tests were necessary to verify its capabilities, characterizing a time-consuming phase of the project.

The other two comparable studies are applications of the numerical code Rockflow (University of Hannover, ISEB and Tübingen, ZAG), which allows doing simulation of flow, mass and heat transfer and deformation in fractured porous rock. In the first work (Mancini M [2]), the mesh was simply generated in the Gocad platform through Tsolid elements. Tetrahedra generation was realized from closed surfaces, which were created from polylines imported in a dxf file. Some attempts were made in order to find an optimal densification rate, as the triangulate mesh characterizing the surface comes from the nodes
distance in the border polyline. Nevertheless, in this case a homogeneous crystalline rock was considered, not taking into account fractures or discontinuities.

The last, but maybe more interesting work (Kalbacher et al K [1]) is again about a coupling with the finite element program Rockflow, but in this case the geological medium is a fractured rock. The geometrical model has been generated in the Gocad platform and a CAD interface was developed to ensure the model transfer to the numerical code. The mesh generation was provided with the GMSH tool. In this work, fractures are introduced as plane surfaces and intersections were produced. During mesh generation, the intersection lines are applied to ensure an exact fit of the finite elements of one surface with the next. Moreover, Kalbacher et al. (2005) affirm that mesh generation within Gocad has some disadvantages: particularly some complex challenges can cause numerical errors during the mesh generation. These effect are hard to locate, analyze, comprehend and difficult to remove afterwards.

Dealing with the simulation of flow and mass transport at the ONKALO site, we can say that some studies have been carried out on a domain distinguished by a big number of fracture planes -33 fracture planar zones- based on revised bedrock version, as reported in Lofman and Mészáros L [4]. The numerical code used was FEFTRA™ program package, developed by VTT Processes (Technical Research Centre of Finland) and based upon a quadtree/octree family of algorithm. In this study the sparsely fractured rock was meshed with hexahedral elements and the fractures and the repository with triangular and quadrilateral elements. Another mesh process is cited in Vieno et al. V [2], where tetrahedral elements represent the rock matrix and then triangular elements are added to the faces of tetrahedral elements to represent fractures. Modeling was carried out in order to assess disturbances caused by construction and operation of ONKALO and to study baseline conditions at Olkiluoto. Some results of these simulations are published and they can be used as comparison with the results that would be obtained at the end of the modeling part of this work.
1.5 Methodology

The first phase in a modeling work is to create a conceptual model. It is a scheme to represent all important elements that characterize the system. It requires an understanding of hydrogeology and dynamics of groundwater flow, in order to define the most important features (e.g. hydrogeological units involved in transmission of water, impermeable layers and presence of fractures). It is important to regard the medium as an entity in relation to groundwater flow: its behavior towards water establishes its hydrogeological definition, regardless of its lithology. For this reason, different rock types may have the same hydraulic properties (e.g. hydraulic conductivity, specific storage) and can be incorporated in the same aquifer unit. Once the hydrogeological components of the system are identified, it is possible to build the correspondent 3D geological model with modeling software (definition of shape and size of the system to be modeled).

In brief, the steps and phases planned for this research program are:

- Link the Geomodel and existing ONKALO data:
  - Visualization and data interpretation
  - Establishment of a link between geology and hydrogeology: describing site-specific relationships between fluid flow and geological structure
  - Creation of the 3D sub-surface model: fracture zones and repository area

- Generate the mesh: the geological model should constitute the input geometry of the numerical code.
  - Mesh fitting s to the geometry of the 3D Model
  - Refinement and smoothing where necessary (where solution is expected to have steep changes)
  - Connectivity control
  - Right topological relation between 2D elements (fractures) and 3D tetrahedra (rock matrix)

- Assure compatibility between file describing the mesh generated and the Hydrogeosphere software:
- Creation of an interface to create a readable input file according to the numerical code format file
- Modification of some part of the Hydrogeosphere code to make it possible to read tetrahedral mesh and fractures zones constituted by triangulated surfaces
- Improvement of wells representation (linear regular elements representing the axis of the well)

• Make required intermediate steps before simulations:
  - Assessment thematic information to the model (e.g. permeability, dispersivity, porosity, trasmissivity, specific storage, solute characteristics).
  - Definition of boundary and initial conditions

• Run numerical simulations to analyze flow paths and mass transport (radionuclides) in the fractured aquifer in the bedrock at the Onkalo site, in the Olkiluoto municipality (Finland). Objectives are to evaluate influence of fractures in groundwater flow and to analyze contaminant transport (its space and time evolution) and eventually salinity evolution.
2. Geomodeling

At the basis of Geomodels there is the 3D representation of the subsurface objects and structures, such as stratigraphic units and their depositional style, fractures, fault and folds. Thus, 3D Geomodels are a collection of data that describe the geometry, the topology and other information linked to geological structures, such as thematic properties of the objects (e.g. porosity, saturation, hydraulic conductivity). A definition of Geomodeling explains the general background of this topic: Geomodeling consists of the set of all mathematical methods allowing to model in an unified way the topology, the geometry and the physical properties of geological objects while taking into account any type of data related to these objects (Mallet M [1]). Thus a Geomodel is a 3D representation of subsurface geological structures, which are neither directly accessible nor wholly known. Actually, they are underground objects. Therefore we don’t have much available data to describe them and, when available, the data are scattered and not evenly distributed. Thus, a Geomodel should help to create and increase knowledge of geological systems, which are mostly unknown. Moreover, in Geoscience the primary concern is to be able to reproduce constraints, which are a kind of restrictions to orient geometry and properties interpolation (such as control nodes or fixed borders that cannot move during interpolation process) and complicated shapes that can be found in nature.

Application of 3D modeling to geosciences objects led to the development of new tools that could replace traditional C.A.D. (Computer Aided Design) software. In the context of the Gocad research project started in 1989 at Nancy (ENSG), a new approach for discrete modeling of natural objects was applied. It is based on the following criteria IB [2]:

- the geometry of any object is defined by a finite set of nodes (points) in the 3D space;
- its topology is modeled by links bridging these nodes;
- its physical properties are modeled as values attached to these nodes.

This approach calls for a powerful mathematical tool able to interpolate the physical properties and the location of nodes defining the objects in the 3D space. This tool is called “Discrete Smooth Interpolation", whose development mainly contributed Jean-Laurent Mallet (1989). Discrete models allow representation of complex natural objects. This tool
consists in interpolating a function on a set of points, while respecting some constraints that can be applied to the discrete model.

As mentioned above, geological objects are mostly unknown and only incomplete and indirect information is accessible. Therefore, it is necessary to build a representation of something that is hidden underground by means of scattered punctual information. Data comes, for example, from core samples observations, optical borehole images, geophysical surveys or hydraulic tests. Geological properties arising from data available rarely can be represented as continuous and simple mathematical functions and sometimes it is even impossible to find this function. Additionally, continuous representations are poorly adaptable to model geological discontinuities as faults, fractures or erosion surfaces. Thus, discrete representations are more suitable for geological properties modeling.
3. Site description

3.1 Olkiluoto island geology

The Olkiluoto Island (12 km²) is situated on the Finnish coast of the Bothnian Sea (Figures 3.1 and 3.2). The coast is characterized by shallow bays surrounded by small archipelagos. It is a low-lying island that emerged from the sea about 3000-2500 years BP. Land uplift is still active, at a rate of about 6 mm/y. The whole local hydrogeochemical and biological system is affected by this postglacial land uplift. The average island topographic height is about 5 m a.s.l. The soil, mainly stony moraine originated, is no more than 1.5 m thick and usually less than 0.8 m. Between organic soil and the bedrock an overburden layer is found: it is made of till and fine sand, sand and silt. Its average thickness is 3 m and nowhere exceeds 10 m. The crystalline bedrock lays deeper. It is a part of the Precambrian Fennoscandian Shield. The Olkiluoto area is located in an area mainly composed of metasedimentary migmatic mica gneisses. Other lithologies intersect the gneiss, as grey gneiss, granite pegmatite, diabase dykes and amphibolite, but they constitute only a little fraction of the geology structure.

Figure 3.1 – Geographic location.

Figure 3.2 – Olkiluoto Island location.
(From Posiva Report 2005-03 P [2])
### 3.2 Finland nuclear energy

Most of the data presently used to create the geological model comes from the Posiva Oy, a Finnish waste-disposal company. Posiva, established in 1995, is an expert organization responsible for the final disposal of spent nuclear fuel, research into final disposal and for other expert nuclear waste management tasks and it has some international partners.

Finland has two nuclear power plants, each with two reactor units. The power plants are at Olkiluoto in Eurajoki, on the Finnish west coast, and at Hästholmen in Loviisa, on the Finnish south coast. The combined output of the two reactors at Teollisuuden Voima Oy’s power plant at Olkiluoto is 1,680 MW and that of the two reactors at Fortum Power and Heat Oy’s power plant in Loviisa (Figure 3.1) is 976 MW. Finland made a decision in principle in 2002 to build a fifth reactor unit. The new reactor unit (OL3) being built at Olkiluoto will have an output of 1600 MW. Legislation passed in Finland requires nuclear waste generated in Finland to be processed, stored and finally disposed of in Finland.

### 3.3 Geological repository general information

The deep geological disposal of nuclear waste is based on the idea of a multi barrier concept, where natural and engineered barriers system –EBS- act together to isolate the waste from humans and environment. The natural barriers include the host rock and the groundwater and geochemical systems, so it is important to take them into account for the choice of a site where the repository has to be built. An EBS may itself comprise a variety of components of the waste package, such as the waste form, waste canisters, buffer, backfill, seals, and plugs (Figure 3.3). The disposal concept proposed by the SKB (Swedish Nuclear Fuel and Waste Management Company) is based on copper canisters with a cast iron insert, where the spent fuel assemblies will be placed. The insert provides mechanical strength and radiation shielding, and keeps the fuel assemblies in a fixed configuration (Figure 3.4). This canister design, called KBS-3, is also taken in consideration by Posiva Oy for the Onkalo repository. According to the SKB, canisters may be placed in vertical deposition holes (KBS-3V) or in horizontal deposition drifts (KBS-3H).
Typical plans call for disposal of long lived and high level wastes in stable geological formations, at a depth up to several hundred meters (IAEA I [3]). Four host geological formations are being widely considered for disposal: crystalline rocks, salt formations, argillaceous formations and tuff.

This study concerns about repository constructed in crystalline bedrock. Thus, its characteristics are briefly listed (IAEA I [2]):

- Crystalline rocks have high mechanical strength. Stable shaft, tunnel and gallery openings can be excavated at depths appropriate for geological disposal.
- In general, they are poorly transmissive and flow predominantly takes place through interconnected networks of fractures.
- They usually contain minerals both in the matrix and as fillings along fractures that sorb radionuclides (retarded solute transport by sorption).
- They frequently have both low matrix permeability and low matrix porosity: transport through the rock matrix is primarily by diffusion.
- Crystalline rocks have very low solubility. Creation of new pathways for groundwater flow or transport by dissolution is not a concern. However, soluble minerals may have been precipitated along fractures in the rock and these could be redissolved.
They normally have good thermal conductivity. Consequently, any heat generated by the waste can be dissipated so that thermal effects on both the engineered barriers and the surrounding rock will be minimized.

In the third point of the previous list, radionuclides are mentioned. A radionuclide is an atom that emits radiations spontaneously, as its nucleus has not a stable level of energy. Thus, it releases its extra energy through ionizing radiation in the form of alpha and beta particles or the more penetrating gamma rays. Each radionuclide contained in the waste has a half-life, that is the time taken for half of its atoms to decay and thus for it to lose half of its radioactivity. Sooner or later all radioactive wastes decay into non-radioactive elements. The main objective in disposing of radioactive waste is to protect people and the environment, avoiding any dangerous radionuclide release to the biosphere. High level nuclear waste (mainly spent fuel coming from reactors), requires the most important protecting measures. It is usually immobilized in an insoluble matrix such as borosilicate glass or synthetic rock, sealed inside a corrosion-resistant container, such as a canister made of stainless steel and copper. Then it is located deep underground in a stable rock structure and finally surrounded with an impermeable backfill such as bentonite clay. Bentonite has low permeability, high swelling capability, and high adsorption capacity and has been examined as the preferred material for the EBS considering required functions such as buffering chemical conditions, dissipating decay heat, supporting overpack, and buffering external stress over a long period of time (Kurosawa and Ueta, K [7]). Once final disposal is complete, the encapsulation plant will be decommissioned and dismantled, the tunnels filled with a mixture of bentonite and crushed stone and the shafts and tunnels leading to the repository sealed. After this there will be no need to supervise the site.

There is wide international agreement that at present, geological final disposal is currently the best-known long-term solution to nuclear waste management (allowing future generations to retrieve wastes). In Canada, the NWMO (Nuclear Waste Management Organization) has the purpose to develop collaboratively with Canadians a management approach for the long-term care of Canada's used nuclear fuel that is socially acceptable, technically sound, environmentally responsible and economically feasible (NWMO Annual
Report, 2005 N [3]). Ongoing research is on the construction of a deep geological repository in a suitable rock formation, such as the crystalline rock of the Canadian Shield or Ordovician sedimentary rock. Moreover, Ken Nash, Chairman at NWMO, in February 23, 2006, (N [1]) spoke about the Canada’s Strategy for Long-Term Waste Management. He said “Looking internationally, over $10 B has been spent world-wide on repository research and numerous safety reviews have concluded that geologic repositories can be built to provide a high level of long-term safety”. In fact, natural and technical release barriers characterizing a geological repository should prevent the radionuclides emitted by spent nuclear fuel from coming into contact with organic nature, for a very long period of time, at least 100000 years.

3.3.1 Geological waste disposal around the world

Countries that use nuclear energy include Canada, China, Finland, France, Germany, India, Japan, Pakistan, Russia, Sweden, Switzerland, United Kingdom, United States of America. In 2005, there were 441 commercial nuclear generating units throughout the world, with a total capacity of about 368 gigawatts, providing about 16-18% of the world’s electrical energy IB [7].

The first countries to consider disposal of nuclear waste in deep geological repository were Germany in the years 1960, then Sweden in 1970. An underground laboratory in crystalline rock has been built in 1994 at Aspo (Sweden) with participation of seven countries (Germany, Canada, Finland, France, Japan, United Kingdom and Switzerland). Germans are studying a dome salt formation at Gorleben. In the USA, in 1978, the Department of Energy (DOE) promoted searches and investigation to find out a site for a deep nuclear waste repository. Yucca Mountain (Nevada) area has been chosen. In addition, a shallow repository for transuranic wastes is currently active in New Mexico (WIPP, waste isolation pilot plant). In Canada, Ontario Power Generation is now proceeding with the approvals and licensing process associated with implementing a long-term management of low and intermediate level radioactive waste received from the Pickering, Bruce and Darlington stations. In Switzerland, there is an underground research laboratory for high-level waste repository sited in the Opalinus Clay of the Zürcher Weinland. Scandinavians countries have highly developed techniques for nuclear waste management, such as at
Onkalo, an underground rock characterization system located in Finland, in the Olkiluoto Island, which this work is about.

### 3.4 Onkalo underground facility

ONKALO is an acronym based on the Finnish language expression for Olkiluoto Rock Characterization for Final Disposal. The word ONKALO also means a cave in Finnish. Onkalo is located in the East part of the Olkiluoto Island. Its precise location can be seen is shown in Figure 3.5, where the boreholes identification codes (KR followed by the well number) are also shown. Boreholes are the main direct way to analyze the bedrock characteristics, such as geological structures, rock mechanics, hydrogeology and hydrochemistry. All these aspects are indispensable for bedrock excavations phases and repository design conception.

Figure 3.5 – Olkiluoto island: boreholes –KR- and Onkalo area -tick oval-.

(From Ahokas and Koskinen, A [2])
3.4.1 Site general information

ONKALO is an underground research laboratory (URL), whose development has been partly based on the experience from other URLs. However, all currently existing underground laboratories in crystalline rock are of the generic type, i.e. they are not located on the actual disposal sites and have been designed for generic studies only. Compared to these facilities (such as Åspö Hard Rock Laboratory in Sweden and the URL in Canada, Manitoba) ONKALO is to a greater extent focused on the characterization of the site-specific properties of the rock mass, and specific underground experiments are mainly related to tests and experiments in which the site-specific conditions at Olkiluoto have to be taken into account (Posiva Oy P [3]).

ONKALO is an underground rock facility constructed to allow the assessment of the geological conditions and the acquisition of information needed for detailed design of repository. Then these investigations allow testing the designed solutions and constitute the support to make possible to obtain construction license for disposal facility. It will later serve the deep repository. Construction work started in July 2004 and is expected to complete in 2010. The application of the construction license is to be submitted to the authorities by the end of 2012. The underground parts of ONKALO consist of a system of exploratory tunnels accessed by an access spiraling tunnel and a ventilation shaft. The final disposal facility will be excavated at about 500 meters deep in the Olkiluoto bedrock. The total underground volume of ONKALO is approximately 330 000 m$^3$ and the combined length of tunnels and the shaft is 8500 m. After a very large number of studies, tests and analyses, the bedrock has been judged mechanically and chemically stable. Moreover, at this depth groundwater is almost oxygen free and flow rates are minor. These two last aspects reduce the corrosive action of water on the canisters that will be containing the nuclear wastes.
3.4.2 Site description and conceptual model

Many data are accessible and several reports are constantly written up with earlier information which comes from current working. The principal documents used as reference to build the geological model are the “Bedrock Model, version 2003/01” written by Vaittinen et al. V [1] and the information related to a simplified model built by Ahokas and Koskinen A [2]. In the former, the modeled volume covers an area of 35 km² (5 km x 7 km) and its limiting coordinates are 6790000–6795000 Northing and 1522000–1529000 Easting, corresponding to the whole Olkiluoto Island (Figure 3.5). In the latter, the model domain is of approximate 1 cubic kilometer, 6791492–6792492 Northing and 1525424–1526424 Easting. This area is shown as a red rectangle in Figure 3.7 and its 3D model in Figure 3.9.

The bases for the fracture structure definition have been to identify the borehole core intersections belonging to each structure. A structure is defined as being any deterministic feature of structural significance within the model, including both fracture and crushed zone, and hydraulic feature (Vaittinen et al. V [1]). A borehole intersection is a fixed point to be modeled, as it represents a core borehole interval having properties that are important from a rock engineering and/or hydrogeological point of view and differ from the average borehole properties, such as in the core sample image shown in Figure 3.6, coming from the borehole KR09. As in this work the focus is on hydrogeology, only the structures distinguished by special hydrogeological feature have been considered. Identification of similar intersections in different boreholes brings to the definition of correlated structures. In fact, each borehole intersection should be included in the correlation process that brings to the definition of quasi-planar structures in 3D, as said in Vaittinen et al. V [1]. Each one of these structures will be then considered as a fracture zone in the context of this project.

As already pointed out in Section 1.2, a large amount of data is available. It could be helpful for a complete and precise description of the site, but at the same time it becomes tricky to find the definitive structural elements of the model because each report is updated with new interpretations, changes in the structures names and code identifications. Also criteria used to define structural intersections in boreholes have changed during early modeling phases.
I based my analysis mainly upon the classification showed in the Bedrock Model Version 2003/1, where 23 boreholes core samples covering an area of about 1.1 km x 1.5 km are available (Figure 3.7) and where three main types of structures are described:

1) H: a descriptive attribute to identify an hydraulic feature ($K > 5 \cdot 10^7$ m/s)
2) R: a descriptive attribute to identify a fracture feature ($IF > 10$ fractures/m)
3) RH: a descriptive attribute to identify both the fracture and hydraulic features
Correlation is made between structure intersections belonging to different boreholes, assuming that fractures represent parts of quasi-planar structures in 3D. Structures with a single borehole intersection have been modeled as discs with a diameter of 100 m, but they are not taken in consideration to create the 3D model for the groundwater flow simulations, as they don’t form network for significant flow. Only structures having at least two direct observed intersections have been considered, as we are interested in groundwater preferential pathways across a large distance in a network of fractures. Thus, from a hydrogeological point of view, 11 structures have been chosen: RH9, RH19A, RH19B, RH20A, RH20B, RH20C, RH21, RH24, RH26, RH80 and H79. The H79 is the only simple hydraulic structure, while the other ones belong to the two models (structural and hydrogeological). Nevertheless, after first construction phases of the Geomodel, it has been found that H79 has a small areal extent, if compared to other structures, and probably it will not be considered. Structures just mentioned above are shown in Figure 3.8.
Figure 3.8 - Structures having at least two correlated direct observations, view towards the west.

(From Vaittinen et al, V [1])

Some studies have been carried out on a domain distinguished by a bigger number of fracture planes, like 33 fracture planar zones, based on a revised bedrock model by Saksa et al. (1998). The numerical code used was FEFTRA™ program package, developed by VTT Processes (Technical Research Centre of Finland).

A more recent simplified geological model has been developed in order to study the effect of hydraulic connection under a long-term pumping test made in June 2004 (Ahokas and Koskinen A [2], JP-Fintact J [1]). Accessible data from this study show that the number of deep boreholes in March 2005 was 33 and the accumulated quantity of the site data is very extensive. This model is composed of 9 fracture structures (Figure 3.9). Two of them are added for flow modeling purpose (transport of cement along vertical structures). Moreover, three other fractures (RH20A, RH20B and RH20B_alt) were simplified to only one. The most significant difference between the Task 7A model version and the 2003/1 is that in the former some new structures are introduced at the location of RH19A and RH19B. The new formations have been individuated by the geophysical interpretation called “mise-à-la-masse anomalies”, at shallow depth around structures RH19A and RH19B. They are structures
SGP1, SGP2, SHGP1, SHGP2 (S=structure, H=hydrogeological, GP=geophysical). Nevertheless, for the flow model the SHGP2 is neglected.

Figure 3.9 - Model box (1 km$^3$) and structures used in Task 7.
(From Ahokas and Koskinen A [2])
4. Mesh Generation

There are a wide variety of geological applications where accurate representation of complex engineering systems and geologic structure and stratigraphy are critical to producing accurate numerical models of fluid flow and mass transport. Oil and gas reservoir production, structural geology, groundwater resource development and waste disposal in a geologic repository are examples of the areas where modeling is used to predict the long term behavior of the system. Most tools available for representing complex geologic surfaces and volumes are not designed for producing optimal grids for flow and transport computation (Gable et al. G [1]). This is the central problem of this study, where a tool able to generate a finite element mesh of a geological model created in Gocad must be found. Actually, grid generation is a key link between the geoscientific information systems and numerical models. Grids must capture complex geometry and insure the computational resources are optimized to produce accurate and stable solutions (Gable et al. G [2]).

4.1 Mesh types

Meshes can be classified according to their geometrical or topological characteristics into regular and irregular or structured and unstructured, respectively. Topology defines how nodes are interconnected. Geometry identify where nodes are placed in the 3D space. Geometrical criterion describes nodes distribution, how their position is defined by a mathematical function so that all point locations could be found and the whole grid could be recreated. If the mesh is irregular, nodal coordinates don’t follow a specified geometry (square or triangles of same dimensions repeated in the whole mesh) and they have to be stored independently. According to a topological standard, meshes are either structured or unstructured, depending on their connectivity. In a structured mesh, the indices of the neighbors of any node can be calculated using simple calculations, e.g. the node of indices (i,j) has as neighbors nodes (i+1, j), (i-1,j), (i,j-1), (i,j+1). Hence, structured meshes are characterized by a foreseeable rule which describes node connectivity with neighboring nodes. On the contrary, unstructured meshes necessitate the storage of a list of each node’s neighbors, as it has no regular topology. In fact, there is not a repeatable pattern describing
nodes connectivity, as relations between nodes change all over the domain. Unstructured and irregular meshes are the most general ones and they are broadly employed in geological models, especially in finite elements problems. The division between structured and unstructured meshes usually extends to the shape of the elements: two-dimensional structured meshes typically use quadrilaterals, while unstructured meshes use triangles (Bern and Plassmann B [3]).

Well-studied geometric constructions such as Delaunay triangulation are central to unstructured mesh generation (Bern and Plassman B [3]). It is an often suitable way to tessellate a domain in 2D into triangles. They become tetrahedra in the 3D space. Some different approaches and mesh generation algorithms exist. All of them require that circumsphere (circumcircle in 2D) defined by each tetrahedron (triangle in 2D) encloses no mesh nodes in its interior (Figures 4.1 and 4.2). The Delaunay triangulation is related to the Voronoi diagram (its dual): the circle circumscribed about a Delaunay triangle has its center at the vertex of a Voronoi polygon (Figure 4.3).

Figure 4.1 - 2D Delaunay triangulation: each circumcircles is empty i.e. no nodes in its interior. (From Shewchuk S [1])

Figure 4.2 – 3D Delaunay tetrahedron and its circumsphere. (From Shewchuk S [1])

Figure 4.3 – 2D Delaunay triangulation (green) and Voronoi diagram (blue). (From Eppstein, E [1])
In 3D, tetrahedral meshes offer some important advantages over hexahedral ones: unique interpolation vertices to interior, greater flexibility in fitting complicated domains and greater convenience for refinement and derefinement. In order to meet these advantages, tetrahedral meshes are almost always unstructured (Bern and Plassman B [3]).

4.2 Meshing characteristics

Before diving into more detailed matters, it is important to clarify and to answer some fundamental questions, like what is meshing? Given an input domain, mesh process divide it into simple cells. This is an indispensable preprocessing step for the finite element method used to solve partial differential equations. A mesh is characterized by its elements type, shape and size. The number of elements is also a key feature, as higher element number implies slower solution time (more CPU time required). Mesh generation is carried out through some steps, like generate initial point placement, determine mesh connectivity and then mesh smoothing and refinement. Connectivity is generated by different kind of algorithms such as Delaunay and constrained Delaunay triangulation or octree and quadtree.

4.2.1 How to generate the mesh

The central problem of this project is grid generation of a 3D geological model. It is a challenging goal to achieve and many solutions have been evaluated. Grid generation is a very large research domain. It is essential to look for the better tool that can generate the required mesh in a straightforward way, in order to be able to plan all steps required for this project in a timeframe of three years. Several mesh generators exist and each one has specific characteristics useful for special tasks. Gocad was not conceived for generation of mesh required as input in Numerical Models. Some plug-ins were developed in order to accomplish mesh generation, such as the TGridlab I mentioned in Section 1.4. Unfortunately, this tool is not compatible with the Gocad version available at Laval University (Gocad release 2.1.4), but only with the older edition 2.0.

One of the most important targets of this study is to apply numerical modeling to complex 3D geometries. Thus the grid must reflect the geological structure. But the task of exporting data from a 3D geological model to a numerical model is quite difficult and time
consuming. After a long search for a mesh generator, a useful and convenient tool has been found. It is called LaGrit and it has been developed at Los Alamos Laboratory (see Section 4.2.2.2). Another option might be to try to generate the grid within Gocad, as explained in the next paragraph.

4.2.1.1 How to generate the mesh: Gocad

Modeling in Gocad has its foundation on working with basic geometric objects such as PointsSets, Curves, Surfaces, Solids, Voxets, SGrid, Well, Group, Channel, 2D-Grid, Model3d. They are the basis to edit all the other geometrical representation the user wants. In the context of this work, the most important are:

- **PointSet**: it is a set of discrete data points where each vertex is described by its number in the set and its coordinates.
- **Curve**: it is represented by a polygonal line composed of a set of points connected by segments.
- **Surface (TSurf)**: it is represented as a set of points connected by triangles.
- **Solid (TSolid)**: it is represented by a tetrahedron, which is composed of 4 vertices.

In Gocad, it is possible to apply constraints on a geometric structure, so that it will be respected when the DSI (Discrete Smooth Interpolation) is used to interpolate the geometry. Through constraint it is possible to limit the movement of some part of the object or to keep it in a certain way (e.g. a Control Node (CN) is a point that the DSI cannot move).

In the context of this work, the Solid object would be the most interesting elements. They can be created from a PointSet or a closed Surface. The former possibility is applied by digitizing points anywhere in the domain, with more points where a detailed solution is necessary (near fractures, near the repository site). Then, points are connected to form tetrahedra. The second approach, based on TSolids generated from a closed Surface, doesn’t allow an easy incorporation of intersecting fracture surfaces.

An application of TSolids built by closed surfaces, it is found in Mancini M [2], where the geological environment is a homogenous crystalline rock, but where fractures are not taken into account (see Section 1.4).
Create a TSolid from a closed surface is quite easy, but there are very few available tools to control the construction of the tetrahedra. Moreover, as in Gocad geometric elements don’t have a topological structure, there is no way to control the right topological relation between triangles on fracture zones (triangulated surfaces) and surrounding tetrahedra. Finally, there is little information available about TSolid and once they are generated there are few accessible tools to work with them.

4.2.1.2 How to generate the mesh: LaGriT

The LaGriT Code Development Team at Los Alamos National Laboratory is constituted by C.W. Gable et al. It is a software tool for generating, editing and optimizing multi-material unstructured finite element grids (triangles and tetrahedra). LaGriT maintains the geometric integrity of complex input volumes, surfaces, and geologic data and produces an optimal grid made of Delaunay-Voronoi elements. The LaGriT grid generation system has many special features tailored to geological applications.

The first step in LaGriT is to define a mesh object and create within it geometric regions as combinations of bounding surfaces. Then, nodes are added in the volume inside the surfaces. Finally, in the last step connection between nodes is realized, by means of a Delaunay tetrahedralization algorithm, as mentioned previously. After generated, the mesh may be manipulated by means of some tools that provide refinement and smoothing, useful to create a mesh adapted to numerical simulations.

The idea is to import in the mesh generator the surface created in Gocad. With the module written by C. W. Gable (Los Alamos National Laboratory, G [3]), it is possible to read the Gocad ASCII TSURF format. Once the file has been read, it might be defined as a sheet surface. A sheet surface is used for user provided surfaces described by a collection of connected triangles or quadrilaterals. Thus, surfaces generated in Gocad, constituted by connected triangles, can be imported in LaGriT environment. Moreover, nodes on these surfaces have to be included into the grid that should be generated. By then, other nodes will be added in order to represent the rock matrix surrounding the fracture zones.
5. Numerical Hydrogeological Modeling

5.1 Generalities

Numerical Modeling is based upon algorithms implemented by means of programming codes on computers. These algorithms allow solving mathematical equations which represent physical phenomena. There are different numerical techniques by which computer algorithms are derived from equations that govern the physical or chemical system modeled. In order to obtain a numerical model, the mathematical formulation for continuous variables has to be transformed into discrete form (Holzbecher and Sorek H [3]).

The purpose of modeling in hydrogeology is to represent reality and physical phenomena in such a way that the modeler can do one of several things:

- Understand physical and/or chemical phenomena and interpret data: improve knowledge of the hydrogeological system by reproducing it.
- Determine the causes of an observed condition (flow direction, contamination, subsidence, solute migration time and pathways).
- Predict the effects of changes to a system or its evolution (pumping, remediation, development, waste disposal).

A numerical solution always has an error associated to it, as it gives an approximation of the exact and real value. Nevertheless this is the only possible solution in many kinds of problems related to physical phenomena described by partial differential equation. This kind of equations describe mathematically a physical phenomenon when the unknown function (the hydraulic head, the pressure charge or the concentration for solute transport) depends on two or more independent variables, usually on time \( t \) and on one or several spatial variables \( (x, y, z) \) for a 3D problem. In most cases of practical interest, it is too difficult or even impossible to find an analytical solution to the equations and numerical techniques are employed, computing approximate values of the unknown function at the “mesh points”. Thus, this kind of solution requires some type of mesh generation, as numerical models find a solution of the governing equations of flow and transport over a grid system. The domain
analyzed is discretized in many elements, according to which the solution is carried out. All the methods that can be implemented (Finite Difference Methods FDM, Finite Element Methods FEM, Control Volume Finite Element Methods CVFEM) result in a linear system of similar structures, but the grid requirements may be quite different. The FDM usually relies on structured mesh, as the approximation is more accurate when the edges meeting at vertices are nearly orthogonal (Bern and Plassman  B [3]). The FDM approach gives a solution limited to each node of the grid. The refinement is however not very efficient. The mesh has to be regular because the FDM technique comes from the Taylor’s series, based on the discretization along the axes $x$ and $y$. All these aspects imply that a code based on FDM is easier to program than a FEM code. The FEM can overcome limitation of FDM techniques, even if the code is more difficult to write. With the FEM method there is the possibility to find the solution all over the domain, as the solution is continuous.

As a numerical method approximates the real value unknown, a criterion is needed to establish when the approximation is good enough to be considered acceptable. A technique usually employed to stop the calculations is based on convergence criteria. It means that when the change in the solution at each point is less than a specified target, called the convergence criterion, or sometimes epsilon ($\epsilon$), calculations are halted. Another important aspect of a numerical method is its stability. Algorithms are the basis of numerical methods and they have to be stable. This means that small changes in the input data should give only small changes in the final results, without producing unrealistic solutions or oscillations. Depending on the scheme adopted (explicit, implicit, type of weighting technique applied in spatial and temporal discretization) a numerical method can be conditionally stable, unconditionally stable or unstable. Methods conditionally stable should respect some stability constraints (e.g. Courant, Neumann).

Partial differential equations require that boundary and/or initial conditions be defined, to calculate a particular solution. Boundary conditions come from the fact that the modeled domain is only a portion of the surrounding natural system. Thus they describe how the analyzed system is coupled with the exterior, what is the link between them. These conditions are essential in the solution of the partial differential equations and they have a
great influence on the results. Initial conditions, on the other end, are mandatory in transient regime, as the initial state of the system from which the simulation starts must be known.

In hydrogeology there are physical and hydraulic boundaries. The former are fixed and may be characterized by lithological or structural changes or large body surface water. The latter results from special hydraulic conditions such as groundwater divide, streamlines or known piezometric maps (Figures 5.1 and 5.2). Furthermore, hydrogeologic boundaries can be defined through the three following types of mathematical conditions:

1. Specified head boundary, also called Dirichlet condition: the hydraulic head $h$ is imposed as a constant value.

2. Specified flow condition, also called Neumann condition: the derivative of the head (flux $q$) is given across a boundary, e.g. no-flow boundary for impermeable elements or streamlines. This condition would be mathematically written as $q = -K \nabla h = 0$.

3. Head-dependent flow boundary, also called Cauchy condition. It may be applied to take into account rivers or drains effects. Its mathematically expression would be $Q = -KA/L(h - h_{ext})$, where $h_{ext}$ is the hydraulic head in the river or drain having an influence on the groundwater flow field modeled.

![Image](image.png)

Figure 5.1 – Regional scale with physical boundaries on the left. Local domain with hydraulic boundaries. (From Anderson and Woessner A [6])
Although hydrogeologically defensible, exclusive use of flux boundaries generally should be avoided for a mathematical reason: the governing equation is written in terms of derivatives, or difference in head, so that the solution will be non unique if the boundary condition also are exclusively specified as derivatives (Anderson and Woessner A [6]). In order to represent correctly the hydrogeology of a system, many other parameters have to be included in the numerical model as, for example, the areal extent, the thickness and the hydraulic properties of the different hydrogeological units (hydraulic conductivity, specific storage, porosity, solute properties) and the surface water bodies nearby.

5.2 Fractured media

5.2.1 Generalities

Intact rock has pores and cracks related to mineral grains, thus linked to the rock origin and that constitute the rock. This kind of void space is called primary porosity. After it is formed, a rock may undergo mechanical stresses resulting from pressure and temperature variations. Consequently, the stresses can produce all kind of discontinuities such as joints, faults, fractures, which constitute the secondary porosity. The main difficulty in modeling fluid flow in fractured rock is to describe this heterogeneity that comes from the presence of fractures. Flow paths are controlled by the geometry of fractures and their open void spaces. Studies on fracture network have been encouraged for the last two decades by important
industrial applications such as fractured oil fields, exploitation of hot dry rock geothermal energy and underground waste repository projects (Adler et al. A [1]).

5.2.2 Conceptual model for fractured media

Research on this topic spans more than four decades. Two broad classes of models have appeared to describe hydrogeological systems: those that deal with porous media and those with fractured media (Fetter F [1]). Researchers have developed several conceptual models describing fluid flow in fractured porous media. Fundamentally, each method can be distinguished on the basis of the storage and flow capabilities of the porous medium and the fracture. The storage characteristics are associated with porosity, and the flow characteristics are associated with permeability. Accordingly to the kind of medium, the conceptual model is different and numerical solution needs some adjustments. The hydraulic response of a reservoir is further complicated by the hydraulic interaction between fractures and the surrounding porous matrix. Water flows unevenly through a complex network of different paths resulting from discontinuity intersections. If the surrounding rock matrix has a low fracture density and low permeability, as is the case in crystalline rocks, hydraulic characteristics mainly depend on fractures. The presence of fractures can greatly influence mass transport because they might represent preferential pathways for rapid contaminant migration. Because of the disparity between the rate of advective contaminant migration along the fractures and the slow, but persistent, advance in the adjacent porous matrix, vastly different time scales for transport can exist in fractured porous media (Therrien and Sudicky T [2]).

In order to model this kind of scenario, a conceptual approach has to be chosen, depending on the relative importance of the fracture network and matrix hydraulic nature. The choice of the conceptual representation depends on the results we are looking for, the input data available and the scale of the area modeled. There are two extreme applicable methods dealing with modeling of a fractured medium:

1) Systems with a few relatively major fractures in a relatively impermeable matrix.

2) Systems with a network of persistent highly interconnected fractures in a permeable matrix.
Three main approaches originate from these two views of geological medium:

1. **Equivalent continuum models**: the entire fractured porous medium is regarded as a single continuum. This approach can be applied when the number of fractures is extremely large in relation to the scale considered. This approach is based on the representative elementary volume (REV) definition (Bear, 1972; Marsily, 1986).

2. **Dual porosity models**: this concept is based on the modeling of fractures and matrix as two continua occupying the same control volume in space. Important interactions take place between these two media, as both of them contribute to groundwater flow and transport.

3. **Discrete fracture models**: they are applied when large-scale heterogeneities govern the flow and mass transport. In this case, each fracture is characterized by its own geometrical and hydraulic properties.

### 5.3 Hydrogeosphere

HydroGeosphere is the numerical code chosen to be applied in the hydrogeological modeling part of this work. Without going in detailed description of this software, its principal characteristics and equations governing the algorithm will be exposed. The numerical code, earlier called FRAC3DVS, is a three-dimensional numerical model describing fully-integrated subsurface and surface flow and solute transport and developed by René Therrien in collaboration with the University of Waterloo (Therrien R., McLaren R.G., Sudicky E.A). It can be applied to variably-saturated conditions and to porous and discretely-fractured media. Transport solution takes into account advection, diffusion, dispersion of non reactive and reactive solutes. The control volume finite-element method, sometimes also called finite volume approach, is employed. The CVFEM is based on the principle of mass conservation and on the idea that a continuum can be modeled as a configuration of discrete elements. A volume of influence is assigned to each node. Equations describing the interaction of the element with its neighbors are written for each element. This interaction is expressed by mean of a mass balance, which is a key concept implying that the difference between inflow and outflow in each control volume must be equal to the variation in fluid stored in the same volume. In steady state condition, there is
no storage variation and consequently inflow has exactly the same value of outflow, but opposite signs. Furthermore, this procedure is accomplished at the full domain scale and it ensures fluid conservation both locally (for each element) and globally (for the whole area discretized).

### 5.3.1 Groundwater flow equations

The general three-dimensional equation at the basis of the numerical modeling of groundwater flow used in Hydrogeosphere comes from a modified form Richards` equation. The following expression is applicable in transient conditions and for a variably-saturated porous medium. The exchange term \( \Gamma_{\text{ex}} \) allows coupling the model to a dual continuum (e.g. a fracture) linked to the porous medium:

\[
-\nabla (w_m q) + \sum \Gamma_{\text{ex}} \pm Q = w_m \frac{\partial}{\partial t} (\theta, S_w)
\]

(1)

Where:

- Volumetric fraction \( w_m \) [-]
- Volumetric fluid exchange rate \( \Gamma_{\text{ex}} \) \([L^3/L^3T]\]
- Source or sink terms \( Q \) \([L/T]\)

(\( \neq 1 \) Only if there is a second continuum)

- Darcy flux: \( q = -K \cdot k_r \nabla (\psi + z) \) \([LT^{-1}]\]
- Relative permeability: \( k_r = k_r (S_w) \) \([L/T]\]
- Pressure head: \( \psi \) \([L]\]
- Elevation head: \( z \) \([L]\]
- Saturation: \( S_w = \theta / \theta_s \) [-]
- Porosity: \( \theta_s \) [-]

- \( w_m \) Volumetric fraction
- \( q \) Darcy flux
- \( \Gamma_{\text{ex}} \) Volumetric fluid exchange rate
- \( Q \) Source or sink terms
- \( \psi \) Pressure head
- \( z \) Elevation head
- \( \theta \) Porosity
- \( \theta_s \) Saturation
- \( S_w \) Relative permeability
- \( k_r \) Darcy flux
In equation (1), the relative permeability is introduced for variably-saturated conditions. In the case of fully saturated conditions, $k_{rw} = 1$ and the equation simplify to (we will neglect the volumetric exchange rate, for sake of simplicity):

$$S_s \frac{\partial h}{\partial t} + \nabla q = Q = S_s \frac{\partial h}{\partial t} + \nabla \left( K \nabla h \right)$$

(2)

In (2), $S_s$ is the specific storage [L$^{-1}$], that is the volume of water released per unit volume of aquifer ($V_f$) for a unit decrease in hydraulic head. Equation (2) is the result of the combination of the continuity equation with the Darcy equation.

The fractures in Hydrogeospher are modeled as two-dimensional parallel plates. For a fracture of aperture $w_f$ and using the same analogy of Richards’ equation applied for the porous medium (equation 1) the governing equation becomes (if is an index meaning fracture):

$$-\nabla \cdot \left( w_f \cdot q_f \right) - w_f \cdot \Gamma_f = w_f \frac{\partial S_{sf}}{\partial t}$$

(3)

Where:

Darcy Flux:

$$q_f = -K_f \cdot k_{sf} \nabla \left( \psi_f + z_f \right)$$

The saturated hydraulic conductivity of a fracture is (Bear 1972):

$$K_f = \frac{\rho g w_f^2}{12 \mu}$$

The symbol $\nabla$ is the two dimensional gradient operator defined in the fracture plane (as fracture are represented by planar elements). All other parameters and their dimensions are the same as in the equation (1), but in this case are referred to a fracture.

### 5.3.2 Groundwater mass transport equations

After having solved the flow equation, the transport equation can be solved. Principal mechanisms governing mass transport are advection, dispersion and diffusion. In addition, also chemical and biochemical reactions can be simulated if the solutes considered undergo degradation or retardation. A general form of the transport equation appropriate for
variably-saturated conditions in a porous medium, as presented in the Hydrogeosphere Manual is:

\[-\nabla \cdot w_m(qc - \theta_s S_w D\nabla c) + [R\lambda c]_{\text{par}} + \sum \Omega_{ex} \pm Q_c = w_m\left[\frac{\partial}{\partial t}(\theta_s S_w Rc) + \theta_s S_w R\lambda c\right]\]  \hspace{1cm} (4)

A simpler expression can be written for a non-reactive solute (i.e. when neither degradation nor retardation take place), in saturated conditions and considering only one continuum:

\[-\nabla (qc) + \nabla \cdot (Dn\nabla c) \pm Q_c = \frac{\partial}{\partial t}(n \cdot c)\]  \hspace{1cm} (5)

In saturated conditions \(\theta_s\) is replaced by the porosity \(n\). In addition, if the fluid is incompressible \((\partial q_i / \partial x_i = 0)\) and porosity \(n\) is constant in time, a more simplified equation can be written:

\[-v_i \nabla c + \nabla D\nabla c \pm \frac{Q_c}{n} = \frac{\partial c}{\partial t}\]  \hspace{1cm} (6a)

\(q_i = v_i \cdot n\) \hspace{1cm} (6b)

The first term on the left part of equation (5) is the advective term, which represents the difference with the flow equation. In fact, without it, if \(c\) is replaced par \(b\) in (5), its form is similar to that of equation (2). To be more accurate, in equation (6b) the total porosity should be replaced by the effective porosity, that is the interconnected porosity which contributes to groundwater flow.

For example, for a one-dimensional transport mechanism of a reactive and degradable solute, equation (6a) becomes:

\[-\frac{v}{R} \frac{\partial c}{\partial x} + \frac{D}{R} \frac{\partial^2 c}{\partial x^2} - \lambda \cdot c \pm \frac{Q_c}{n} = \frac{\partial c}{\partial t}\]  \hspace{1cm} (7)

It is important to remind that the transport equation is a type of PDE (partial differential equation) that can change its behavior from parabolic to hyperbolic when advection dominates. This situation requires special attention when grid methods are used, because numerical dispersion can appear. Smaller grid sizes reduce numerical dispersion (Rausch et al. R [2]). Peclet number \((\text{Pe}=\Delta x/\alpha_i\Delta x\) is the grid element dimension, \(\alpha_i\) is the dispersivity) is a parameter that can be controlled to reduce problems: if it is smaller than 2,
the parabolic nature of the PDE will dominate and numerical dispersion won’t occur. As a general rule, numerical dispersion and oscillations can be avoided if the grid Peclet number is kept smaller than 2.

### 5.3.3 Radionuclides release from canisters

Hydrogeology must be considered in the characterization of a suitable location for a geological disposal system for nuclear wastes. In fact, groundwater plays a major role in this perspective, since the flow might be the most likely mechanism for radionuclides release to the biosphere. Migration of these contaminants is related to all the components of the engineered barrier system, EBS. The possible leakage of canisters containing radioactive materials is a very crucial issue that may motivate a study of contaminant migration in fractured systems. One of the principal barriers to the transport of radionuclides is that they may be sorbed onto mineral surfaces. However, one of the more recent concerns is that sorption onto colloids may actually enhance the transport of radionuclides, particularly those that have a low solubility (e.g., Pu, Am, and Np). There is considerable evidence that the presence of naturally occurring colloids (1 to 1000 nm in size) may enhance contaminant transport (Long and Ewing L [6]).

Mobile colloids in groundwater enhance the transport of chemicals sorbed to particle surfaces. Colloids are particles suspended in a fluid, with diameters ranging from 1 nm to 1 µm, with high surface area and electrostatic. Colloids in groundwater are mainly mineral particles in the form of metal oxides, humic macromolecules, bacteria and virus. In fractured media they are formed by microerosion of minerals present in the matrix as a result of formation crushing due to tectonic activity (Chrysikopoulos C [3]).

Actually, for the Onkalo repository there are some references to colloids content. In Report 2003-03 P [3] it is said that there is a need to plan and construct special equipment for colloid sampling. In Rickkola et al. R [3], colloids can be produced by the post closure effect of grouting material, as it may produce harmful mineralogical alteration in the bentonite buffer and creating a source of colloids in the geosphere. In addition, bentonite, used in the deposition hole where its function between the canister and the rock, should
have the ability to filter colloids, as mentioned in Tanskanen et al. T [1]. In general, all processes that contribute to eliminate colloids from the aqueous phase are comprised in the term “filtration”. Finally, in Vieno et al. V [2] deals with safety of the repository and it is said that besides providing a protective environment for the canisters, the KBS-3 concept for disposal system ensures that any radionuclides released from canister undergo retention, retardation and dilution by other engineered barriers, in accordance with the multibarrier principle. Moreover, near-stagnant pore water, colloid filtration and retention of radionuclides on buffer pore surfaces ensure slow aqueous diffusive transport. Thus, bentonite prevents advective and colloid-facilitated transport of species and mass transport takes place predominantly by diffusion. Nevertheless, there are examples of analogues scenario with indications of significant colloidal transport from an underground nuclear test, such as at the nuclear test site in Nevada, USA. In this site, it has been reported that radionuclides were detected in a well located 1.3 km from the test site. This cannot be understood in terms of migration of solutes in groundwater. The enhanced migration could potentially be due to colloids, and thus, it is important to consider their potential impact on repository safety (Kurosawa and Ueta K [7]).

Sorption reactions may lead to an enhanced colloid-mediated radionuclide transport over large distances provided the colloids are stable and mobile. The sorption of radionuclides on natural colloids in groundwater may significantly modify their transport behavior through fractured media, since radionuclides bonding to colloids may not be subject to the important retardation mechanisms of matrix diffusion and sorption on the pore surface (Kurosawa and Ueta). A simplified description of the colloid facilitated transport process is shown in Figure 5.3 where a fracture resulting in a water flow at the bentonite-granite boundary, where the colloids may be generated. Radionuclides diffuse through the bentonite buffer and are also released to the fracture water. The radionuclides then are partially in solution, diffusing into the granite matrix or are sorbed on the colloids (Rubel et al. R [4]).
5.3.4 Modeling features

The domain will clearly be modeled in transient regime and it will be considered saturated. Boundary conditions must be applied to the modeled domain. On the basis of the information available about the site, some preliminary hypothesis may be formulated. If we assume that the model is a cubic volume containing the fracture zones, a no-flow bottom conditions will be applied (second type). The lateral borders will probably have a specified head condition (first type). The top surface of the model can be considered as a no-flow boundary or a constant head boundary. This last hypothesis can be verified by water table measurements or empirical linear transformation from topography elevation data (Vieno et al. V [2]), where water table measures were not available (water table=0.56·topography). In the Task 7 Model (Vidstrand and Ahokas V [4]), where effects of pumping in KR24 are analyzed, the top boundary is represented by a transient water table, created through a groundwater recharge.

Another modeling issue is whether or not the salinity should be taken in consideration by means of a coupled (flow and salt transport) model. This parameter is represented by the TDS (Total Dissolved Solids) value and it is related to water density. Salinity is related to the interface between fresh and salt water and to the upcoming of the latter, due to the drawdown of water table during the excavations. According to previous studies (Vieno et al. V [2]), the disturbances in the salinity distribution caused by inflow during the construction
and operation period will mostly cease within a couple of hundred years after the closure of the repository. So, under the hypothesis of simulate only the postclosure situation, we can assume the salt water having the same initial profile used in Vieno et al. V [2], where salt concentration is assumed to depend on the depth only. At the depth of 520 m, it is approximately 20 g/l of TDS. An evolution of the salinity can be modeled considering salt as a solute. It will be characterized by a density value linked to the TDS parameter.

Finally, long term radionuclides transport will be modeled considering them as soluble species. Values for the retardation factor and the decay constant will be assigned according to the radionuclide types and available literature data. According to the ANDRA Report A [4], after repository closure, the release of radionuclides will mainly take place in soluble phase (no radionuclide release in gas form).

### 5.3.5 Interface LaGriT-Hydrogeosphere

Currently in Hydrogeosphere, available mesh element types are 3D rectangular as well as 3D triangular prism for the matrix and 2D rectangular or triangular elements for the fractures. Triangular prisms elements allow more flexibility and adaptivity to fit complicated geometrical domains. To achieve even more flexibility in fitting complex systems, tetrahedral meshes should be included in the numerical code. The numerical model has presently only the capability to perform a subdivision of rectangular prisms into tetrahedral elements to permit discretization of irregular domains (Therrien and Sudicky T [2]). The objective of this work is to directly import in the numerical code a 3D grid generated in external software. It will be necessary to analyze how Hydrogeosphere reads a mesh and how this part of code is built, in order to make the suitable modifications to allow reading an external 3D tetrahedral mesh.

In short, a program to read the ASCII file containing the data of the mesh will be written. Then the required transformations will be executed, in order to produce a compatible input file for Hydrogeosphere. The development of an interface should allow designating tetrahedral element faces as fractures. Fractures are represented by triangulated surfaces. Originally Hydrogeosphere offered discretizing horizontal and vertical fractures. Currently, the code allows modeling of irregular inclined fractures network, where a
quadrilateral or triangular 2D element is superposed or inserted into block elements (Graf [6]). In the new grid version proposed here, the geometrical and topological relation between a tetrahedral element representing the rock matrix and the 2D fracture discretized by triangles, should have the characteristics shown in the Figure 5.4.

![Figure 5.4 – Scheme of the relation between a 3D tetrahedron and a 2D triangular element.](image)

Finally, another important topic concerns the capability to discretize a well. The present Hydrogeosphere method should be improved, as it leads to an irregular geometry of the axe of the well. The linear structure should be preserved, in order to have a more realistic representation as well as a more reasonable solution of the groundwater flow simulations when pumping action is considered.
6. Preliminary achievements: Onkalo 3D Model

The first step necessary to generate the geological model is to create the surfaces. The aim is to build the principal fracture zones. In order to realize this, a long analyze of the huge quantity of data accessible has been done. The aim was to put together boreholes and geophysical information to identify the structure of the fractured medium. Some alternative fractures are presently kept in consideration. Boreholes are not perfectly vertical. Thus coordinates (x,y,z) have been imported by means of the Import Option of a Column Based File. In this way the original well path is preserved.

The following procedure has been used to create the model:

- Analyze available boreholes data files Task Force IB [6].
- 28 deep boreholes have been imported as a curve element in Gocad from an ASCII formatted file.
- Each curve has got some markers to identify the fractures crossing it.
- A PointSet has been created for each intersection borehole-fracture zone.
- A surface has been built from each PointSet.
- Nodes at intersection between boreholes and fracture zones are settled as Control Nodes.

A sample of the model is already been built, using fractures structures that come from the simplified model cited earlier, the TASK 7A Model Version 1.2 (Ahokas and Oskinen A [2]). Nevertheless, these data were not so user-friendly (ACIS .SAT format) and some intermediate transformations were made through Autocad 2004 in order to produce a dxf format file useful for exchange to Gocad. Moreover, once visualized the structures in Gocad, they consisted of volumes. As Hydrogeopshere works with planar structure, the averaged Z coordinate was adopted for nodes having the same X and Y coordinates. The resulting model is shown in Figure 6.1, where wells are represented by the red curved lines. The vertical structure is the fracture zone RH16A, introduced in this simple model for flow modeling purposes (Ahokas and Koskinen A [2], JP-Fintact J [1]). Others fracture zones in Figure 6.1 are R21, RH20A, RH20B_alt, SHGP1. Concerning structures SGP1 and SGP2 of
the Task7A Model, they have not been represented in Figure 6.1 as they have a very small areal extent.

![Figure 6.1 – Model built in Gocad, with data coming from Task 7A data.](image)

Structures shown in figure 6.1 are presently compared with the others described in the Bedrock Model 2003/01, in order to define the final geometry of the fractured medium (see Section 3.2.2). Shape of fracture zones will be attributed following the mainly rectangular shapes adopted in the previous studies carried out by Posiva Oy. Also the statistical analysis and modeling of the Olkiluoto structures (Hellä et al. H [2]) has been examined to have more information available concerning the fracture zones. Once the surfaces will have been geometrically defined, triangulation will be realized through Gocad tools that are based on DSI (e.g. Beautify triangle for equilaterality).

An approach that may be envisaged before transferring the geometry to the mesh generator or before starting meshing operations in the Gocad platform (if finally it will constitute a good and efficient way to provide the mesh generation) is the determination of mutual intersection lines between fractures. This can be realized by means of the Gocad tool “mutual cut among surfaces” available in the Surface mode. It seems be a good procedure in order to have all the relation among different intersecting fractures. Actually, it is important
to ensure an exact fit of finite elements of one surface with the next (Kalbacher et al. K [1]) and to avoid a poor matching between neighbor elements at intersecting surfaces. Gocad cuts intersecting surfaces adding nodes along the cutting line, in order to guarantee connectivity and a right topology at the intersection. Nevertheless, points distribution along the cutting lines might be not good for further mesh generation phase (Figure 6.2). This may produce bad tetrahedra, i.e. not well-shaped, characterizing a low-quality mesh for numerical simulation. Some improvements would be necessary e.g. beautify these borders.

Concerning the LaGriT software, some preliminary tests have been carried out in order to make certain that it may work. TSurf files exported from Gocad have been easily read by the mesh generator software and some simple meshing operations have been realized.
7. Organization

7.1 Framework

This project is carried under the supervision of Dr. René Therrien, professor at the Department of Geology and Geological engineering of Université Laval, Québec. The co-supervisor is Kerry MacQuarrie, Hydrogeologist at the University of New Brunswick. The work is part of the GEOIDE III Phase Project “GeoTopo3D” (project leader Donna Kirkwood, Laval University. Section 1.2), which Dr. René Therrien and Kerry MacQuarrie are part of. I have been working on this research project since September 2005.

7.2 Financing

This GEOIDE project is financed with funds of 17,000 $ per year, for three years, as a scholarship. For this first year I also received 2000 $ from the Laval University, as a grant offered to the new Ph.D. students.

7.3 Schedule

See the scheme in the next page.
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