MULTI-DIMENSIONAL MODELLING OF GROUNDWATER FLOW AND CONTAMINANT TRANSPORT IN FRACTURED CRYSTALLINE ROCK OF THE CHALK RIVER LABORATORIES SITE

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ABSTRACT

Two- and three-dimensional (2-D and 3-D) hydrogeological simulations were performed to assist in the assessment of the suitability of the CRL site for hosting a deep geologic repository to provide safe long-term management of CRL's low- and intermediate-level wastes. The modelled flow domain includes the bedrock of the CRL site and its immediate vicinity with a number of highly permeable major faults/fracture zones explicitly represented. The 2-D modelling indicates that i) a 10-km length scale is sufficiently large, ii) the predicted groundwater flow field is only weakly influenced by in situ depth-dependent natural temperature and salinity at the CRL site, and iii) advection and dispersion, rather than diffusion, are the predominant contaminant transport mechanisms. A 3-D conceptual hydrogeological model, which encompasses a 165-km^2 area, extends to 3 km below surface and includes eight faults/fracture zones, was developed based on a preliminary 3-D geological framework assembled from data available in 2009. Particle tracking analysis for nearly 500 particles released from a 20-km^2 area at 500-m below surface into the predicted groundwater flow field showed that particles from the northeastern two-thirds of the release area would discharge to the Ottawa River while the remaining particles discharge to Maskinonge Lake, with substantially shorter travel times for the former discharge area. Using this and other information the conceptual design team proposed potential footprints for a repository with an approximate area of 1.6 km^2 at either 500 m or 1000 m below surface. Advective transport through the Geosphere (bedrock) was investigated by tracking more than 500 particles from each hypothetical repository. Predicted travel times suggest a moderately strong natural barrier. A network of 10-20 linear segments was constructed to approximate the flowpaths from each hypothetical repository to surface discharge. The network geometries, head values, travel times and corresponding repository sector information were provided to the Postclosure Performance and Safety Assessment team. Sensitivity analyses were performed to investigate the influence of various model input parameters. The head profiles predicted by the Base Case simulations using two codes and the simulation with the best-fit rock-mass permeability available in 2010 were compared to the measured head profiles in four boreholes. Agreement was only poor to fair, indicating that the subsurface head distribution has not yet equilibrated and that uncertainties remain in the conceptual and numerical models, and the site-specific hydrogeological parameters. The simulation using rock-mass permeability fitted to data from three boreholes predicted significantly slower groundwater flow.

1. INTRODUCTION

1.1 Background

Atomic Energy of Canada Limited (AECL) started a 5-year-long pre-project feasibility study in 2006 to assess the suitability of the Chalk River Laboratories (CRL) site for hosting a Geologic Waste Management Facility (GWMF), which is a deep geologic repository to safely and permanently manage CRL's non-fuel wastes, i.e., L&ILW (low- and intermediate-level radioactive wastes). An understanding of the geological, geophysical, geochemical and hydrogeological characteristics of the bedrock (the geosphere) at a potential GWMF site is essential for selecting a favourable location for the repository, designing the repository, and assessing the potential effects of the repository on human health and the natural environment. Numerical modelling of groundwater flow and contaminant transport in the fractured crystalline bedrock of the CRL site and its immediate environ is an integral part of the pre-project geological assessment [1].

1.2 Objectives

The objective of the hydrogeological modelling task [2] is to perform simulations of groundwater flow in the fractured crystalline rock mass in the vicinity of the CRL site, with limited contaminant transport modelling where feasible. Selected simulation results are provided to:

- the conceptual repository design engineers to aid in the selection of the nominal location and geometry of the hypothetical GWMF repository footprint, and
- the performance and safety assessment (P/SA) team to develop the geosphere network model for the preliminary safety assessment.

1.3 Hydrogeological modelling approach and scope

Groundwater flow in the fractured crystalline rock of the Canadian Shield at a depth of 500-m or more below surface (i.e., the potential depths considered for the GWMF) is governed by a combination of factors, including the local and regional topography, the fault/fracture zone (FZ) network interconnectivity, the distribution of hydraulic properties and the hydraulic boundary conditions. Various hydrogeological modelling approaches have been advanced for this type of rock mass, e.g., equivalent porous media (EPM), dual continua and discrete fracture methods. For modelling on a site or large scale (tens of km^3 or more) at a pre-siting stage, the EPM approach is the most practical and is adopted for this work. In this approach, faults/fracture zones are represented as material property zones with very different permeability and porosity from the rest of the rock mass.

The scope of the study involves the following:

- Steady-state EPM flow simulations of a preliminary two-dimensional (2-D) conceptual model of the CRL site and its immediate environs from existing geological and hydraulic property information compiled from pre-2009 studies to provide guidance to the creation of the three-dimensional (3-D) conceptual model;
- Steady-state EPM flow simulations of a preliminary 3-D conceptual model of the CRL site and its immediate environs from existing geological and hydraulic property information compiled mostly from pre-2009 studies (i.e., the Base Case (BC));

- Advective/convective particle-tracking analysis of groundwater flowpaths and travel times for use by the GWMF repository-design team and the P/SA team;
- Parameter sensitivity analysis of the influence of various hydraulic properties and other model input parameters on the predicted groundwater flow field, flowpaths and travel times; and
- Updating the Base Case hydraulic properties with preliminary borehole data recently obtained as part of the pre-project feasibility study and comparing the (admittedly premature) predicted and measured vertical hydraulic head profiles.

All hydrogeological modelling used AECL's MOTIF (Model Of Transport In Fractured/porous media) finite-element computer program [3]. AECL's conservative advective/convective particle-tracking computer program (TRACK3D, [4]) was used to analyze the flow field to estimate the groundwater flow paths and travel times from 500-m or 1000-m below surface to surface or near-surface discharge points. TRACK3D integrates the velocity field in time to estimate the groundwater flowpaths and travel times from subsurface release to a boundary of the model. Other transport processes, e.g., dispersion, diffusion, sorption, radioactive decay and chemical reactions, are not considered by TRACK3D. Selected confirmatory and complementary simulations are also performed with the commercially available COMSOL™[1] computer program.

2. SUMMARY OF TWO-DIMENSIONAL (2-D) MODELLING

A two-dimensional (2-D) nested-model approach was first taken with a 33 km x 2 km regional model and a 10 km x 2 km local model along the vertical section indicated by the red line in Figure 1a [5], both covering a significantly larger area than the CRL property (shown in close-up in Figure 1b) to help to determine the appropriate size of a three-dimensional (3-D) model and to study the influence of model parameters on the predicted flow field. Fifteen faults/fracture zones were explicitly represented (Figure 2). Table 1 lists the permeability and effective porosity adopted for the Base Case for both the 2-D and 3-D hydrogeological modelling in this study. These hydraulic property values are based primarily on the summary in [6] and the authors' hydrogeological modelling experience in other Canadian Shield areas.

In the Base Case simulation, approximately half of the particles released over a large area in the 500-m horizon were predicted to discharge to each of the two major water bodies, the Ottawa River or Maskinonge Lake with travel times in the range 1.9×10^3 to 4.5×10^5 years [7].

[1] COMSOL and COMSOL Multiphysics are registered trademarks of COMSOL AB (www.comsol.com), Tegnérgatan 23, SE-111 40 Stockholm, SWEDEN.

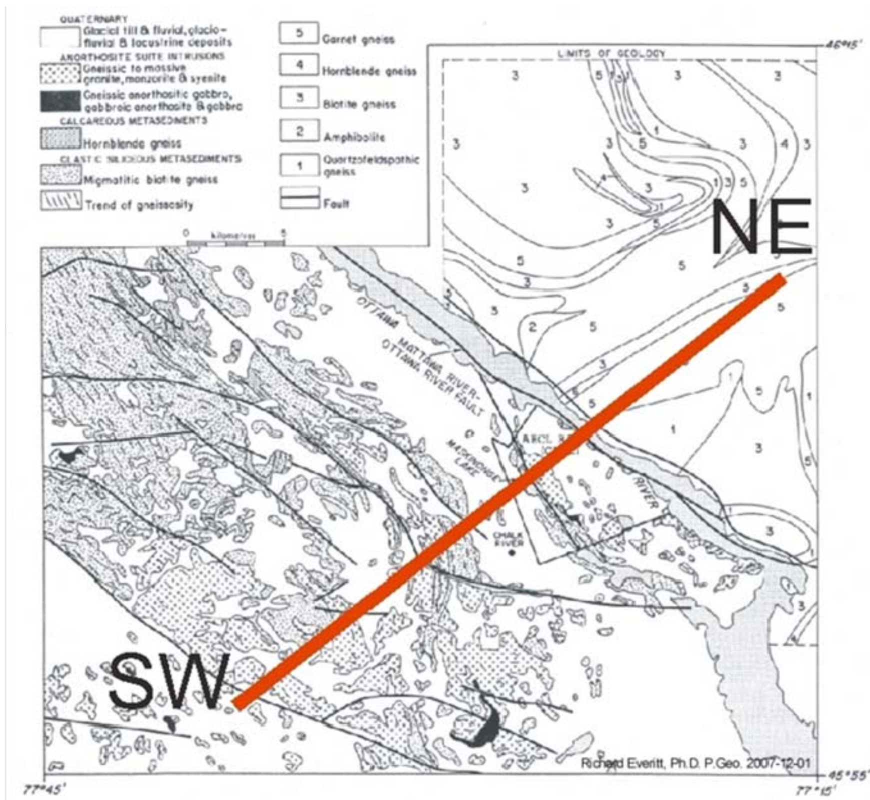

Figure 1a. Location and geological setting of section (red line) comprising the 2-D conceptual model of the CRL region. Geological structure after [5].

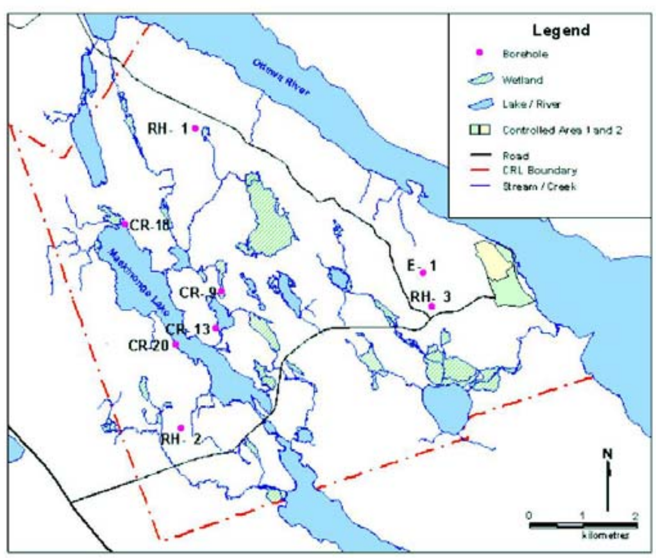

Figure 1b. Map showing surface water bodies and location of some bedrock boreholes prior to the start of the pre-project study.

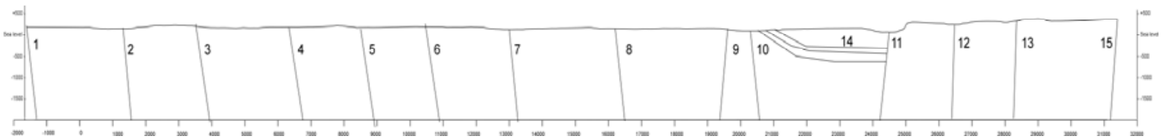

Figure 2. Numbering scheme for faults/fracture zones explicitly represented in the 2-D conceptual regional hydrogeological model.

Table 1. Base case rock mass and fracture zone permeability and porosity distributions in the conceptual hydrogeological model for the CRL region.

Parameter	**Permeability** (m^2)	**Porosity** (%)
Weathered Rock Zone (0- to 50-m depth)	10^{-15}	3%
Moderately Fractured Rock Zone (50- to 150-m depth)	10^{-16}	0.5%
Moderately Fractured Rock Zone (>150-m depth)	10^{-17}	0.1%
Fracture Zones (including faults, fracture zones and dyke zones)	10^{-13}	10%

The sensitivity analyses resulted in the following major findings:

- Neither the regional nor the local model is sensitive to the type of hydraulic boundary conditions prescribed to the vertical/subvertical side boundaries;
- Finer mesh sizes for the regional model did not lead to different hydraulic head distributions, flowpaths or travel times, implying that the element sizes of the first mesh were adequate;
- The permeability values strongly affect both predicted head distribution and water-coincident particle travel paths and travel times, while porosity affects only the particle-tracking results;
- The presence and absence of some major FZs (e.g., the Mattawa fault, the Maskinonge fault[2] or a possible extensive horizontal fault postulated by [5] to underlie the bottom of the model) have significant effects on the predicted flow field;
- Measured natural subsurface temperatures and groundwater salinity at the CRL site have only minor effects on the predicted flow field and particle-tracking results;
- The flow fields of the local model and nine-fold refined regional model are only slightly different, largely attributed to the more detailed representation of the structure from a group of low-dip fractures in the local model; and
- If the local model domain is truncated at the Mattawa fault, a number of particles are predicted to be trapped at depths ranging from a few tens to a few hundreds of metres. This is physically unreasonable considering the high permeability assumed for this fault and a radionuclide-transport model based on this flow field would under-predict the radionuclide release to the Ottawa River.

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[2] The Maskinonge lineament is called the Maskinonge fault for modelling purposes since a dip direction is assumed.

The results suggest that the 10-km extent of the local model is adequate for modelling groundwater flow and advective transport at the CRL site. The very high topographic and hydraulic gradients on the Province of Quebec side northeast of the Ottawa River yielded a south-westward flow towards the Mattawa fault suggesting that this fault should not be modelled as an external boundary.

A special 2-D MOTIF coupled groundwater flow and advective-dispersive/diffusive contaminant transport simulation was performed using a mesh composed of quadrilateral elements for the rock mass and line elements for the fracture zones. The contaminants released as instantaneous mass pulses at six selected points (Pts 1, 6, 12, 18, 24 and 26) from a hypothetical 767-m long repository in the 500-m horizon at approximately 113 m to 880 m from the Maskinonge Fault (FZ10 in Figure 3) were predicted to discharge to surface via this fault. Figure 4 shows the predicted contaminant concentration contours at selected times arising from an instant pulse source at Point 26 at the right end of the repository. This figure illustrates the movement of a hypothetical contaminant plume towards the Maskinonge Fault. It should be noted that the colour scale changes with time as the concentration becomes more dilute. The peak contaminant mass outflow rate at 50 m below surface caused by each individual point-pulse source was predicted to arrive after approximately 20,000 years for the closest point source, which yields the highest mass flow rate to 190,000 years for the farthest, which yields the lowest mass flow rate (Figure 5).

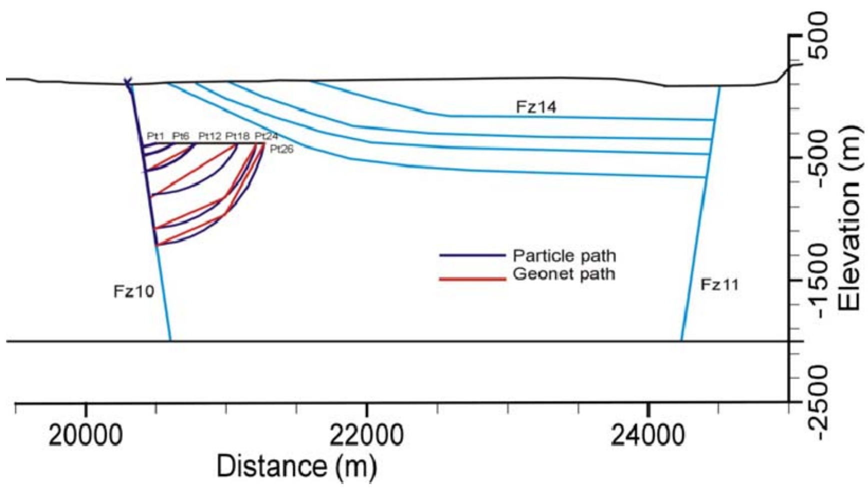

Figure 3. Particle tracks originating from six selected points at approximately 500 m below surface from the local model with line elements representing faults/fracture zones. Also shown are the proposed GEONET paths. All paths go up the Maskinonge Lake Fault (FZ10).

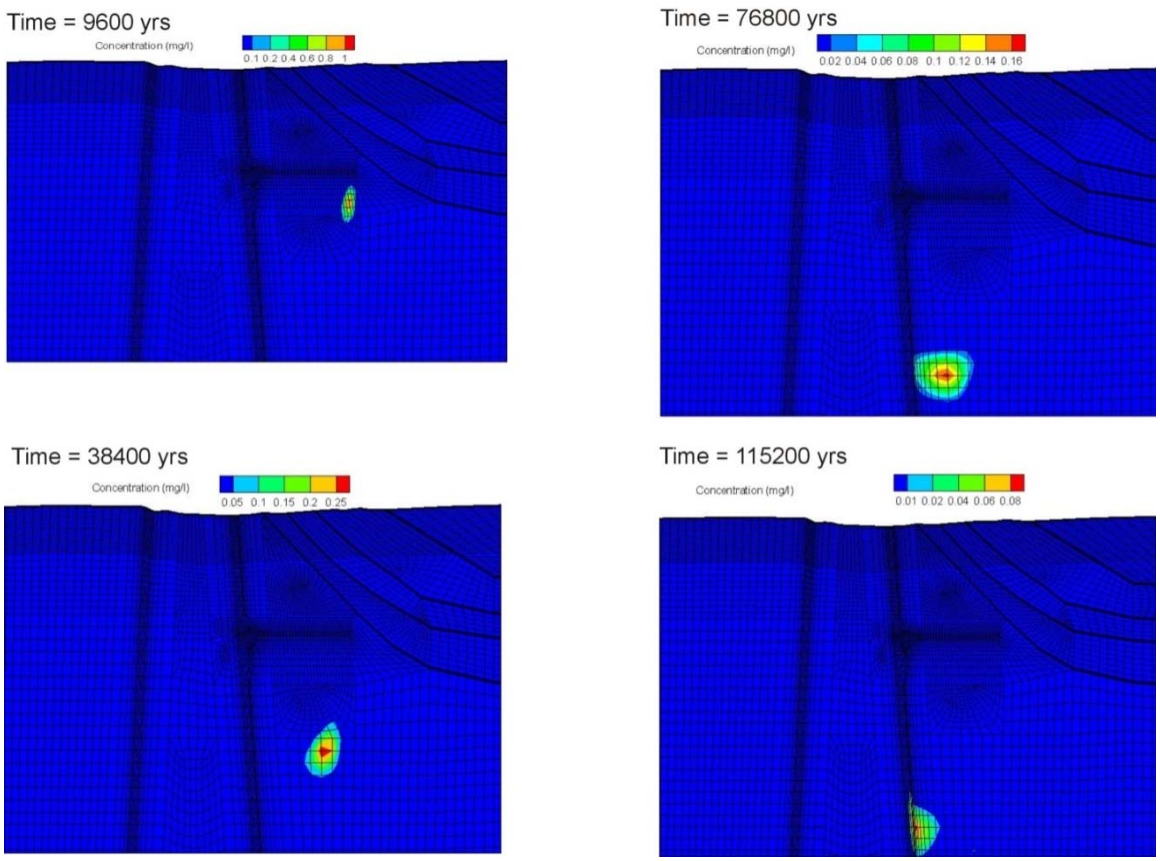

Figure 4. Predicted contaminant concentration contours at selected times after release due to instant pulse source at Point 26.

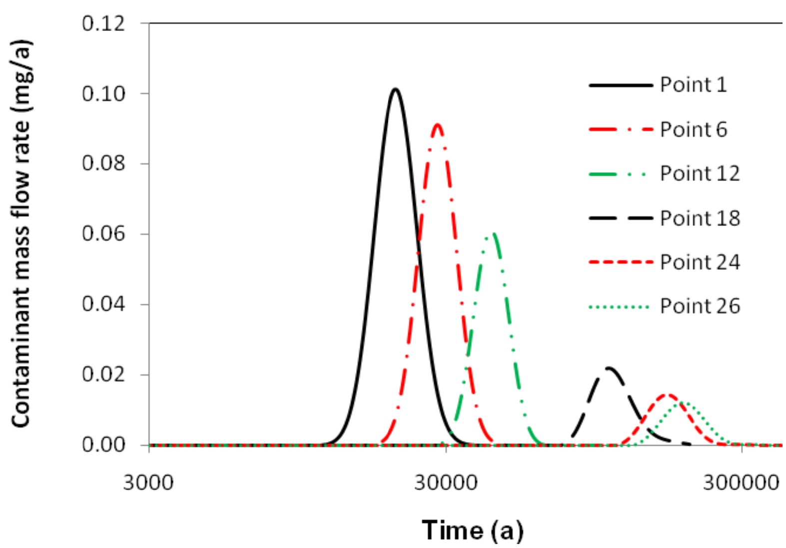

Figure 5. Time evolution of normalized upward contaminant mass flow rate through the Maskinonge Lake Fault at 50 m below ground surface due to pulse source at Points 1, 6, 12, 18, 24 and 26 (see Figure 3 for location).

3. PRELIMINARY 3-D MODELLING [2]

3.1 Version 0 conceptual hydrogeological model

During the summer of 2009 a very preliminary 3D subregional-scale geological framework model, designated Version 0, was assembled of the CRL property and vicinity using geological data available as of June 15 2009 [8]. The Version 0, 3-D preliminary hydrogeological model [2] includes the geometry of the hydrogeological boundaries, structure of major geological features, and spatial distribution of hydraulic properties. The number of potential structures proposed for inclusion in this preliminary conceptual model of the CRL site is deliberately kept low to expedite modelling. It is expected that this Version 0 geological framework model will be modified and/or additional structures included as new information becomes available from the pre-project feasibility investigations, e.g., [9].

Figure 6 depicts (a) a plan view of the Version 0 hydrogeological model geometry showing the proposed model boundaries and surface traces of potentially significant geological structures superimposed on the Google Earth™[3] image of the CRL site and its vicinity and (b) a slightly simplified 3-D isometric view of the structures. The model domain bounded by polygon ABCDEFGHA (Figure 6a) encompasses an area of 165-km^2, includes eight faults/fracture zones and extends from the ground surface to almost 3-km deep. These proposed boundaries are mostly either watershed topographic high divides or local lows or proposed structures with varying degree of confidence.

The Version 0 conceptual structure shown in Figure 6b and the hydraulic properties given in Table 1 together constitute the conceptual hydrogeological model for 3-D Base Case subregional steady-state groundwater flow simulation in this paper.

3.2 Base case finite-element simulation

For 3D finite-element simulations the model domain of the conceptual hydrogeological model shown in Figure 6b was discretized with a mesh using 35,582 nodes comprising 32,458 hexahedron elements. Figure 7 illustrates this finite-element mesh representation. It should be noted that in order to minimize the possibility of round-off errors during numerical simulation, the coordinate origin has been translated. Thus the coordinates shown in Figure 7 and in subsequent figures are in the model coordinate system, rather than in UTM coordinates. In general, prescribed head boundary conditions, equal to the topographic elevations of the site (Figure 8), or water levels of surface water bodies were assigned to the top surface of the model. No-flow boundary conditions were assigned to the sides and bottom of the groundwater flow model. Where a model boundary underlies the surface water (see Figure 6a), however, special considerations were made. Flow boundary conditions assigned to these portions of the side boundaries are as follows:

- BC was assumed to be a no-flow boundary including the portion which coincides with a fault along Cory Lake;
- CD was assumed to be a no-flow boundary including the portion which coincides with a probable extension of the Maskinonge Lake Fault; and

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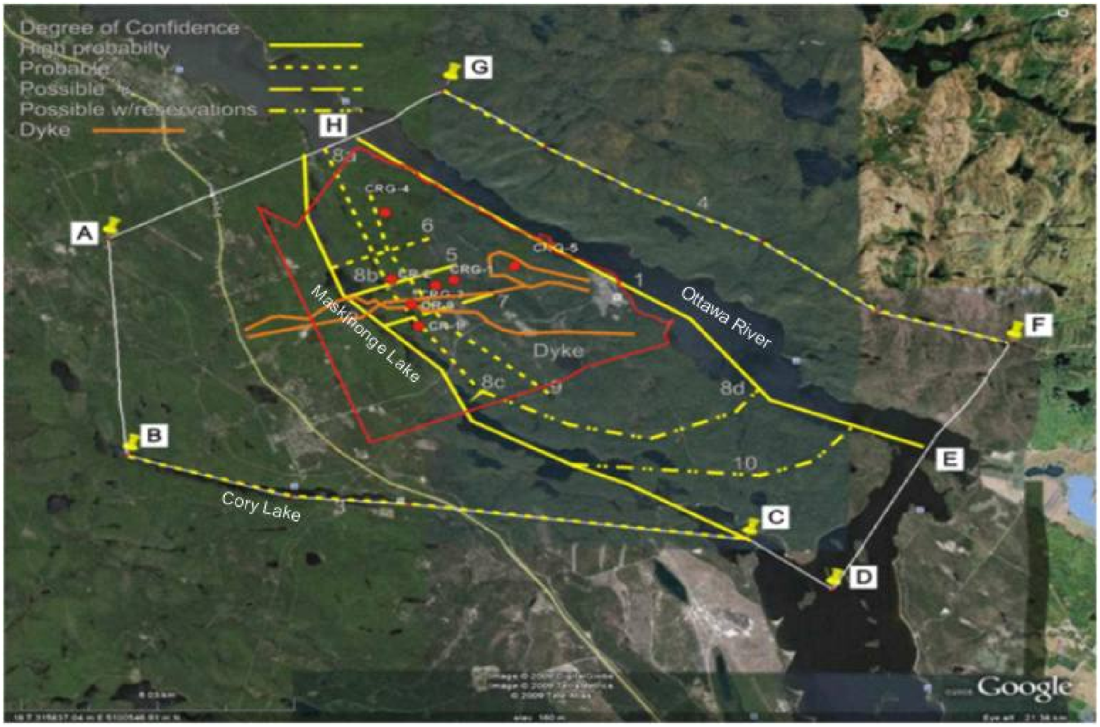
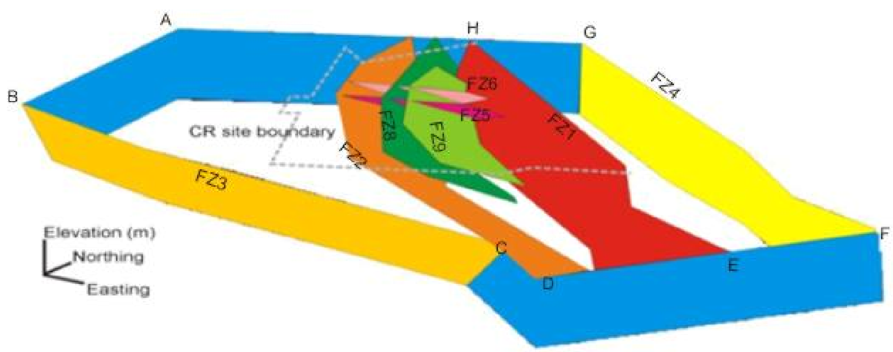
[3] Google Earth is a registered trade mark of Google Inc., 1600 Amphitheatre Parkway, Mountain View, CA 94043.

- Portions of DE, EF, GH and HA, which underlie the Ottawa River, were assumed to be hydrostatic.



(a) Plan View



(b) Isometric Structural Rendition

Figure 6. Preliminary 3-D hydrogeological model structure: (a) plan view superimposed on Google Earth™ view of the CRL area and vicinity and (b) a slightly simplified 3-D isometric rendition.

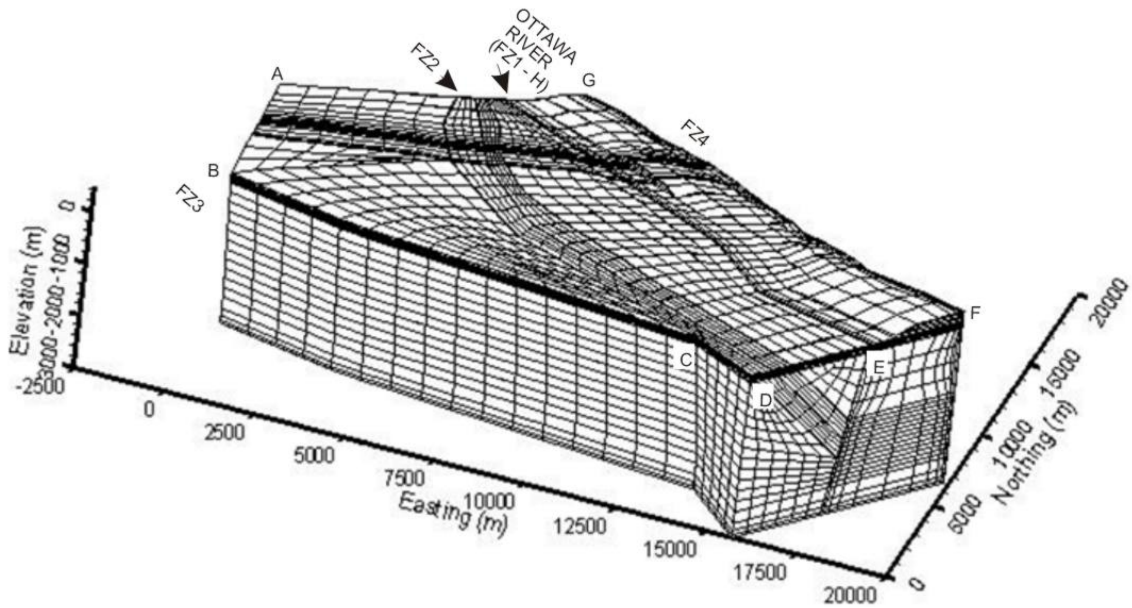


Figure 7. Finite-element mesh representation of the conceptual hydrogeological model shown in Figure 6b.

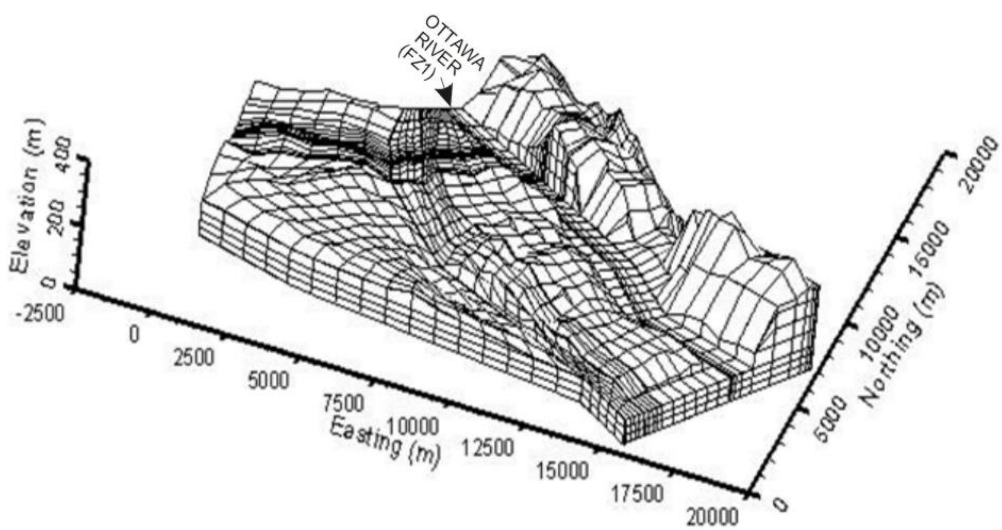


Figure 8. Topography (vertically exaggerated) of the hydrogeological model domain.

3.3 Predicted hydraulic head distribution

Hydraulic head distribution predicted by the Base Case simulation is displayed in Figure 9. Predicted heads range from approximately 110-m amsl (above mean sea level) at and below the Ottawa River to over 300-m amsl at and below the highland area on the northeast shore of the river in the Province of Quebec. Figure 9 shows that, at shallow depths, the small-scale undulations in the land lying between the Ottawa River and the linear chain of lakes to the southwest can be recognized in the predicted hydraulic head distribution. At greater depths (i.e., 500-m or more below surface), the signature of the small-scale topography is gradually damped out.

3.4 Particle tracking analysis

A set of 496 water-coincident particles is released over a ~20-km^2 area at elevation -380-m amsl (~500-m-below surface) into the flow field predicted by the 3-D Base Case simulation. Figure 10 displays the initial locations of these particles with colour coding to represent different intervals of advective transit time[4] for a particle to travel from its initial release at a particular location at elevation -380-m amsl to surface discharge. Grey dashed lines in the figure indicate surface traces of major geological features in the conceptual hydrogeological model of the CRL region. Particles released close to the Mattawa fault and the two ENE striking features travel to surface in a comparatively short time.

Figure 11a shows the initial release points at elevation -380-m amsl for 496 particles into the flow field. The colour coding indicates which fractions discharge to the Ottawa River, Maskinonge Lake or Sturgeon (Chalk) Lake. Particles from ~2/3 of the initial release area discharge to the Ottawa River via the Mattawa fault, while ~1/3 of the particles discharge to Maskinonge Lake or Sturgeon Lake. A few particles discharge to FZ8, which is sub-parallel to the Maskinonge fault. Figure 11b illustrates the relationship between discharge locations and travel times for the 496 particles. Apart from the few particles that discharge directly to the surface via FZ8, the shorter travel times (e.g., $<5.0\times10^2$-5.0×10^3 years) are predicted to be associated with flowpaths that discharge to the Ottawa River. The shortest particle travel path is only a little over 500 m in length, suggesting that the particle travels only tens of metres in moderately fractured rock (MFR) before entering a fault/fracture zone.

3.5 Particle tracking and potential conceptual repository locations

Taking the particle-tracking results, the geometry of major structural features, waste inventory and other factors into consideration, the repository design team [10] proposed potential footprint locations for repositories at depths of 500 and 1000 m (Figure 12[5]). These were adjusted to maintain a waste exclusion distance (WED) of at least 100 m with respect to the significant faults/fracture zones of the CRL site [2]. The WED is the minimum perpendicular distance between a fracture zone and the nearest waste-emplacement area of a repository [11], [12]. Figure 13 shows the adjusted footprints for both a hypothetical 500-m- and 1000-m-deep repository. The east-west vertical section (Figure 14) illustrates the WED separating each potential conceptual repository from the major nearby faults/fracture zones – from the left, the low-dip Maskinonge fault (FZ2 in the 3-D model), Bass Lake fault (FZ8), FZ9 and the subvertical Mattawa fault (FZ1 in the 3-D model).

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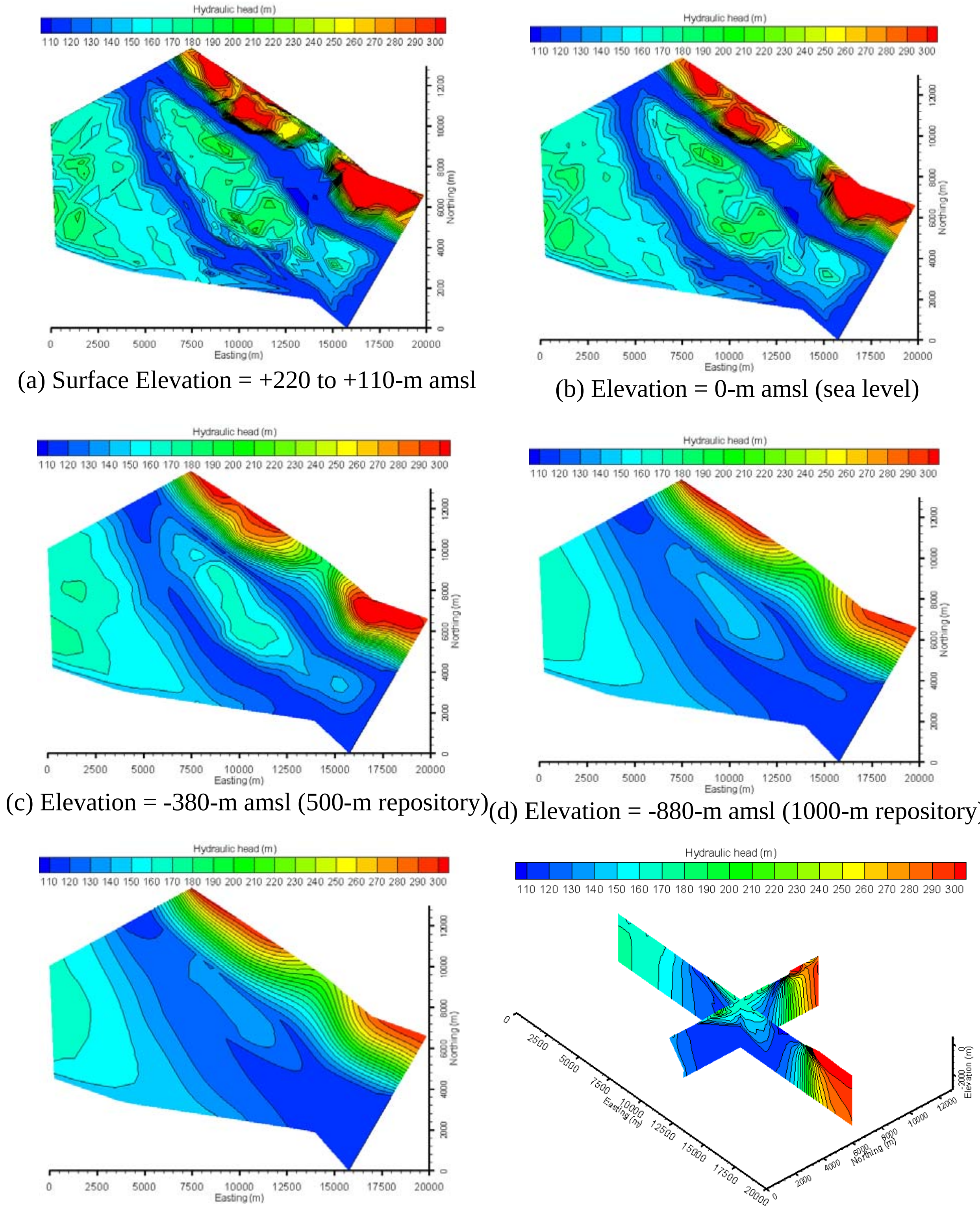
[4] Particle travel time and transit time are synonymous.

[5] The solid black lines are the surface expressions of the fracture zones included in the hydrogeological model.



(a) Surface Elevation = +220 to +110-m amsl

(b) Elevation = 0-m amsl (sea level)

(c) Elevation = -380-m amsl (500-m repository)

(d) Elevation = -880-m amsl (1000-m repository)

(e) Elevation = -1180-m amsl

(f) Isometric

Figure 9. Hydraulic head distributions predicted by base case simulation.

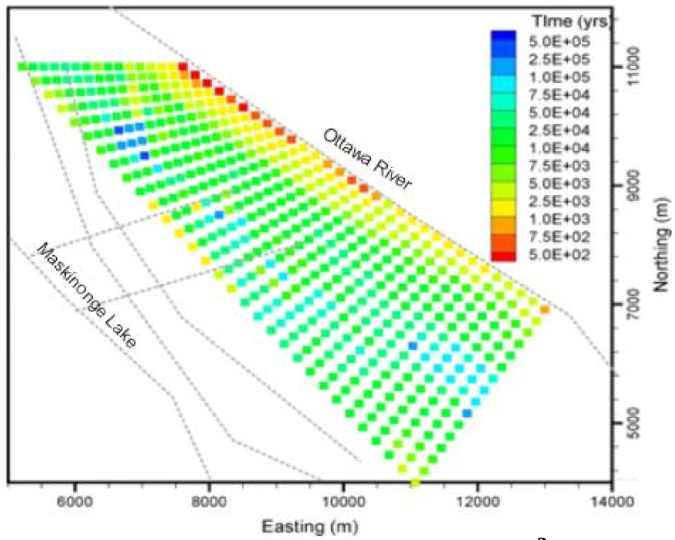
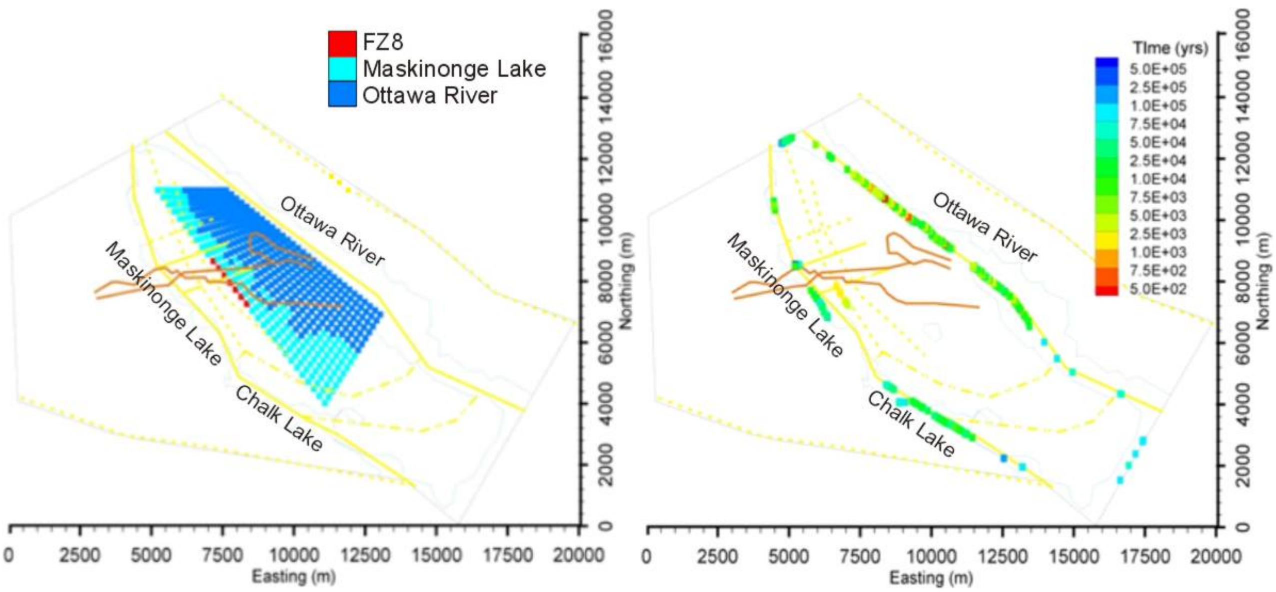


Figure 10. Locations of 496 particles released over a ~20-km^2 area at elevation -380-m amsl (~500-m-below surface) into the flow field predicted by the 3-D Base Case model. Colour shows time for a particle to travel from release at a particular location to surface discharge.



(a) Discharge Locations

(b) Travel Times

Figure 11. Relationship between (a) discharge location and (b) travel time for 496 particles released over a ~20-km^2 area at elevation -380-m amsl into the flow field.

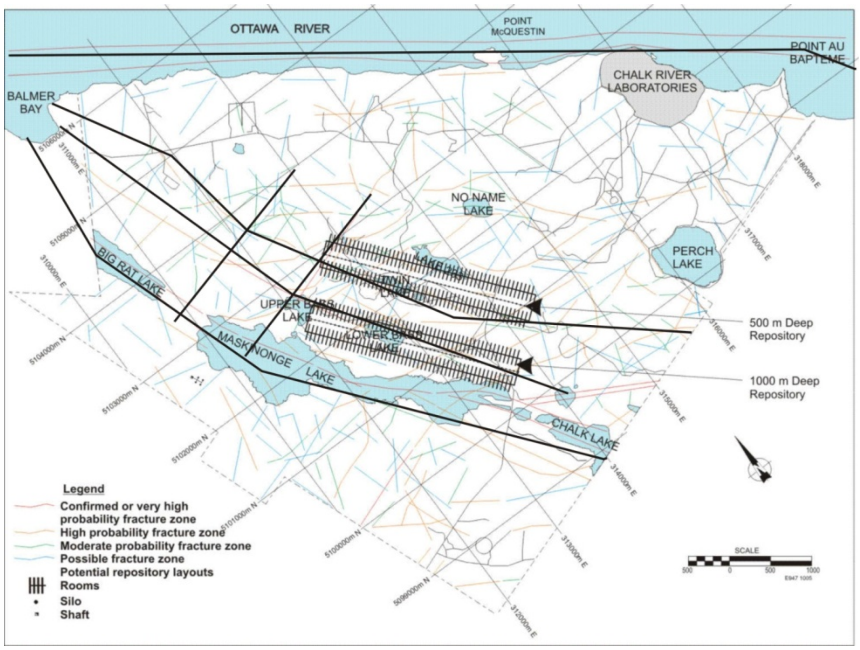
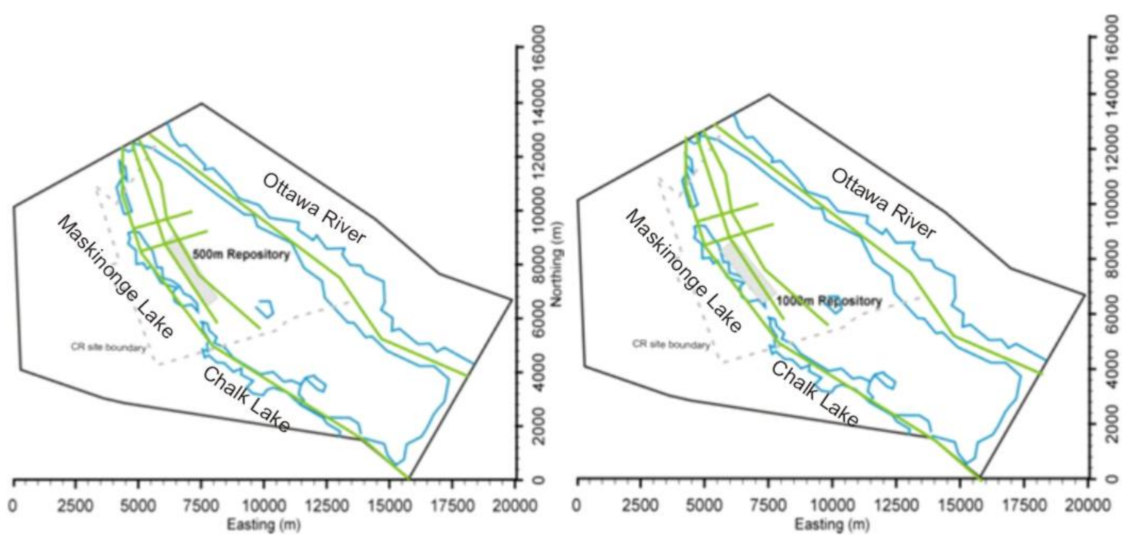


Figure 12. Nominal footprints for the 500- and 1000-m-deep hypothetical repositories, modified from [10].



(a) 500-m-deep Repository (b) 1000-m-deep Repository

Figure 13. Adjusted footprint for the (a) 500-m-deep hypothetical repository and (b) 1000-m-deep hypothetical repository.

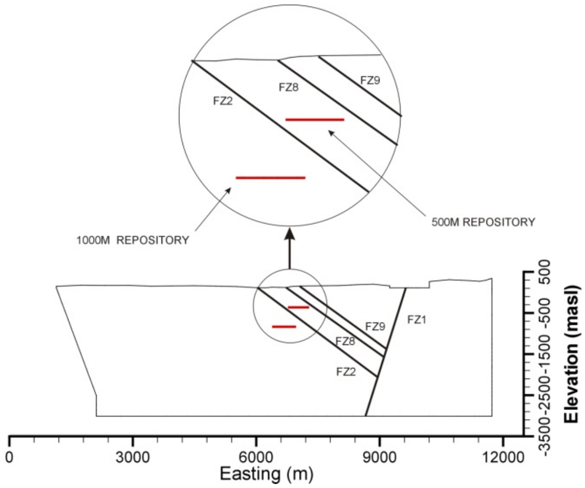


Figure 14. East-west vertical section showing locations of the hypothetical repositories relative to the significant faults/fracture zones of the CRL site.

Figure 15 is a horizontal section at elevation -380-m amsl (~500 m below surface) for a 500-m-deep repository showing the location of the hypothetical repository relative to the Maskinonge fault (FZ2) and the adjacent sub-parallel Bass Lake fault (FZ8). A set of 531 particles is released from the ~1.6-km^2 repository into the predicted Base Case flow field. Most of the particles first descend to elevation -630-m amsl before entering the Maskinonge fault and rising to discharge at surface (i.e., selected particle path lines shown in Figure 16).

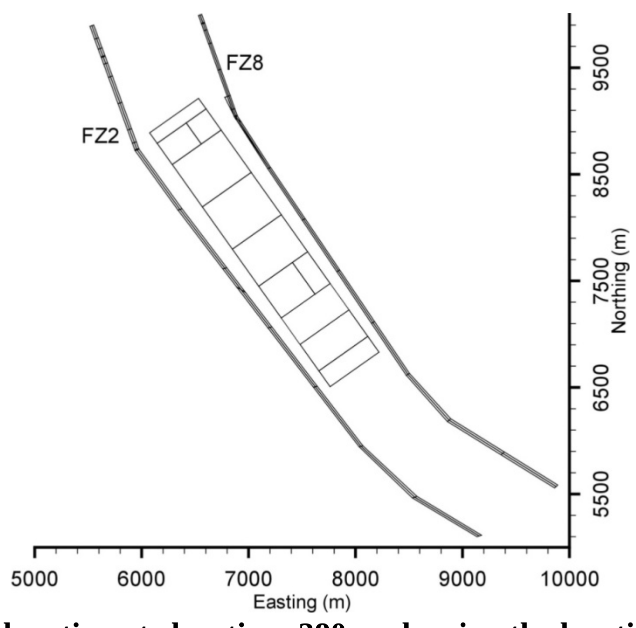
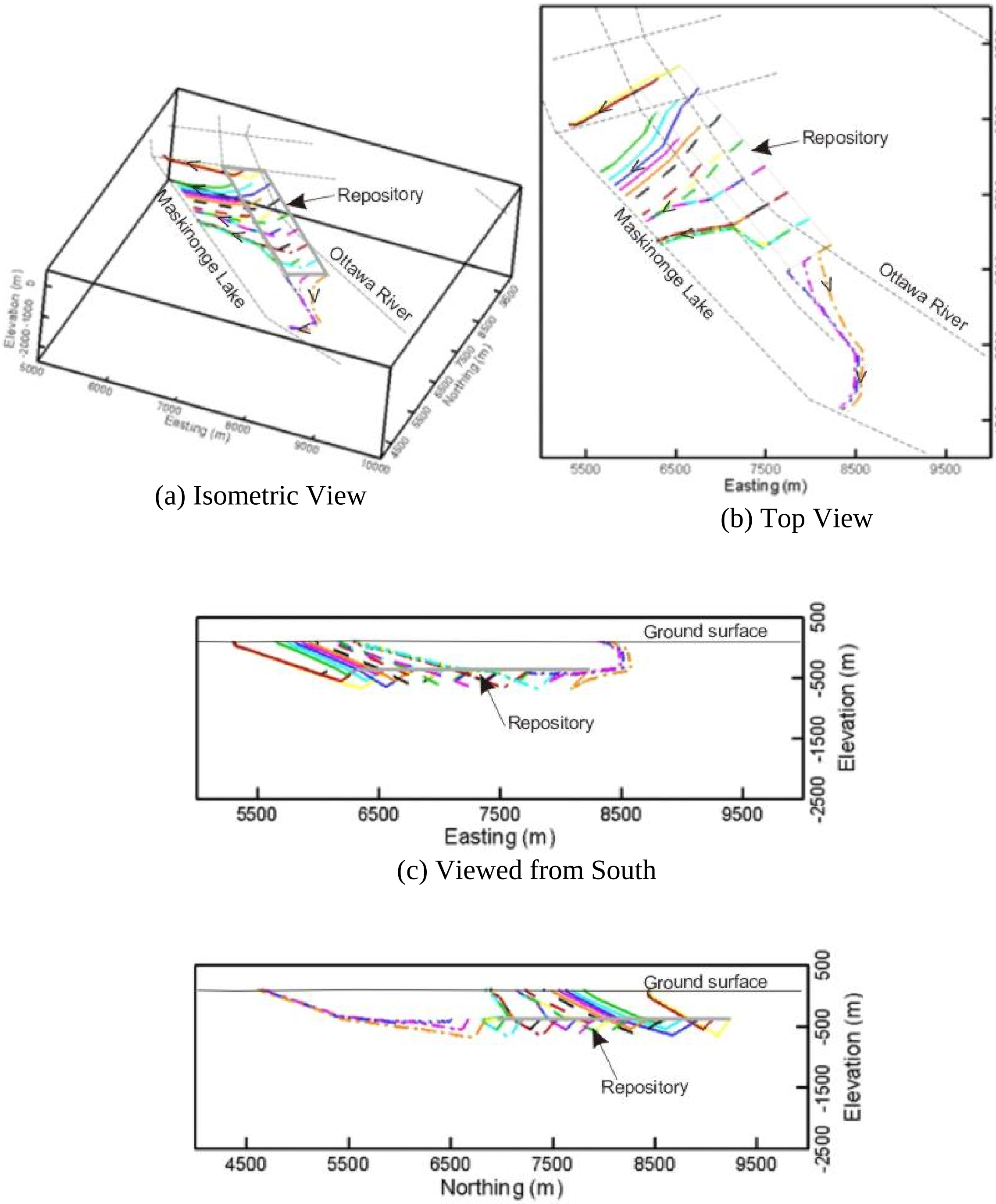


Figure 15. Horizontal section at elevation -380 m showing the location of the 500-m deep repository relative to the Maskinonge lineament (FZ2) and a nearby sub-parallel low-dip fault (FZ8).



(a) Isometric View

(b) Top View

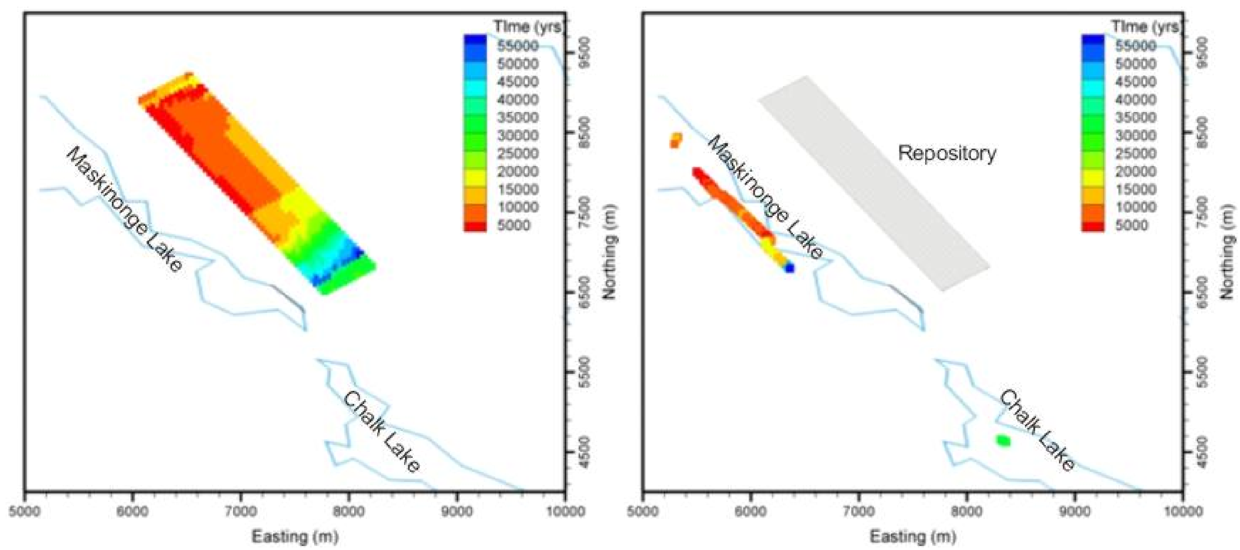
(c) Viewed from South

(d) Viewed from East

Figure 16. Sampled path lines of 531 particles released from the 500-m deep repository into the flow field predicted by the 3-D Base Case model: (a) 3-D isometric view, (b) top view, (c) viewed from the south and (d) viewed from the east.

3.6 Particle-tracking analysis to facilitate development of a geosphere network for the P/SA Model for a 500-m-deep repository

Figure 17 shows the travel times for particles released from the hypothetical 500-m-deep repository and their discharge points (i.e., northwest Maskinonge Lake, central Maskinonge Lake and Sturgeon (Chalk) Lake). Particle travel times were found to range from ~2.2 x 10^3 years to ~5.3 x 10^4 years with a median value of ~1.1 x 10^4 years and travel distances range from ~1,100 m to ~3,500 m with a median value of ~1,700 m. Particles with travel times shorter than 5,000 years were found to originate from a small area (red in Figure 17(a)) of the hypothetical repository.



(a) Released from Repository (b) Discharged at Surface

Figure 17. Travel times for 531 particles (a) released from various portions of the 500-m-deep repository and (b) discharging to various surface locations.

The relationship between initial release and surface discharge locations is shown in Figure 18.

Next particles were grouped according to their travel from the same areas of the repository to the same surface discharge areas in similar time frames based on the results shown in Figures 17 and 18. This grouping reduced the 531 particle path lines to 11 representative paths (Figure 19). Each of these paths was approximated by a small number (i.e., ~10) of concatenated linear segments. The set of 11 paths forms the proposed "network" of advective transport paths for the Geosphere Model of the P/SA system model [13]. Figure 20 illustrates the division of the hypothetical 500-m-deep repository footprint into 11 sectors.

Table 2 provides the advective transit times and transit distances for each of the 11 geosphere transport paths for the preliminary postclosure performance and safety assessment of the hypothetical repository at the CRL site.

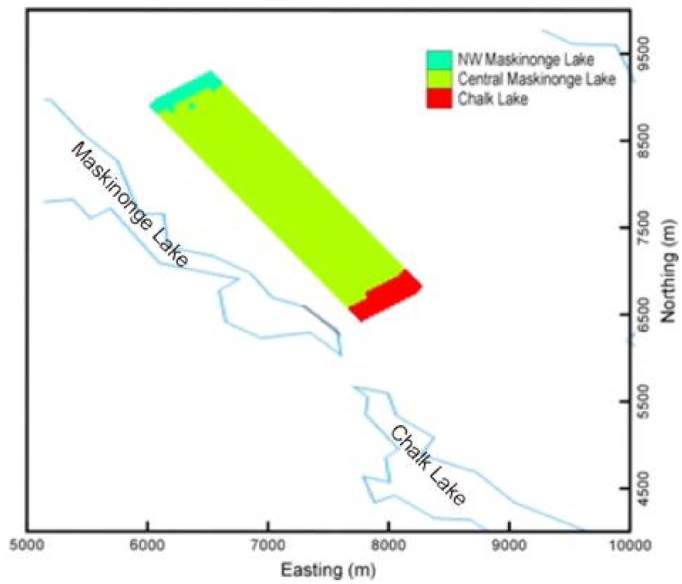


Figure 18. Relationship between initial-release location and surface discharge locations for the 531 particles from a 500-m-deep repository.

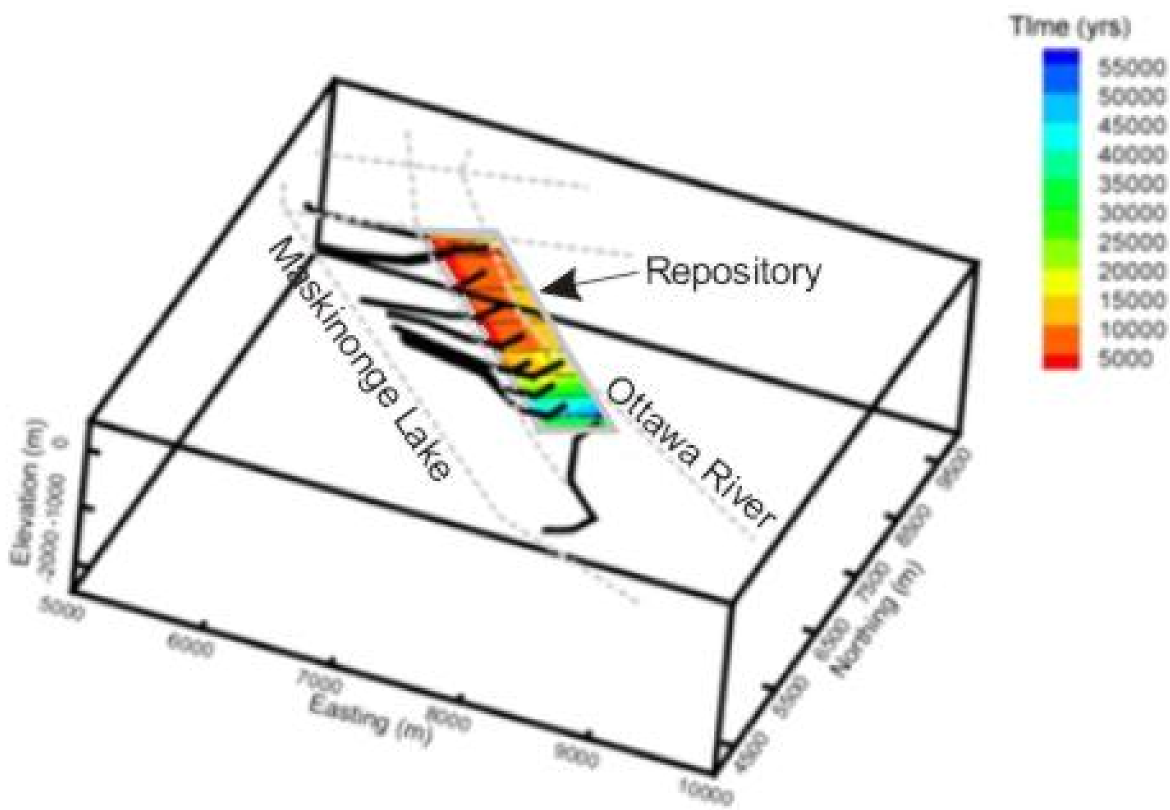


Figure 19. Proposed P/SA geosphere pathways starting from various portions of the 500-m-deep repository.

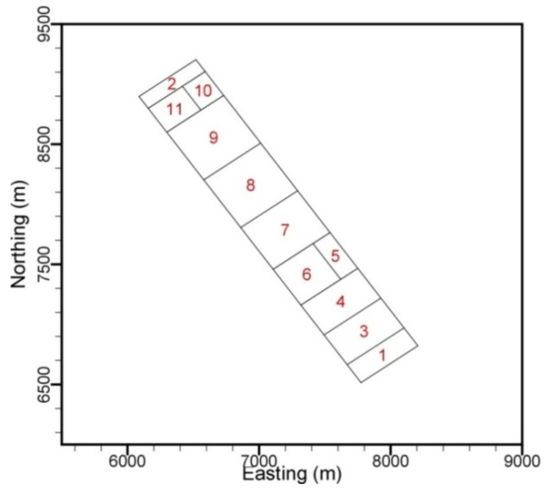


Figure 20. Division of the 500-m-deep repository into 11 sectors.

Table 2. Synopsis of transit times and distances for the 11 particle path lines.

Particle	Transit Time (yrs)	Transit distance (m)	Exit Location	Particle	Transit Time (yrs)	Transit distance (m)	Exit Location
1	30,751	3346	Sturgeon (Chalk)	2	11,027	1723	NW Maskinonge
3	41,724	2396	Maskinonge	4	23,267	2134	Maskinonge
5	17,120	2137	Maskinonge	6	12,487	1747	Maskinonge
7	7,802	1514	Maskinonge	8	8,676	1488	Maskinonge
9	6,736	1526	Maskinonge	10	2,430	1824	Maskinonge
11	5,246	1447	Maskinonge				

3.7 Particle-tracking analysis to facilitate development of a geosphere network for the P/SA Model for a 1000-m-deep repository

The process of particle-tracking analysis and construction of the advective transport paths was repeated for the hypothetical 1000-m-deep repository (at elevation -880 m amsl). Final results are presented in Figure 21, Figure 22 and Table 3.

Salient results can be summarized as follows:

- None of the 539 particles released from the hypothetical 1000-m-deep repository descends below -880-m amsl level before moving upwards first into the moderately fractured rock (MFR) and then into the Maskinonge fault to surface discharge in the Maskinonge Lake area.

- Particle travel times range between ~1.8×10^4 years to 5.7×10^4 years with a median value of 2.5×10^4 years and travel distances range between ~1300 to 2500 m with a median value of 1600 m. In comparison with the hypothetical 500-m-deep repository, the much longer minimum travel time reflects the fact that particles released from the 1000-m-deep repository often travel longer distances in the MFR before entering the fault while the narrower range of travel distances reflect discharge to only one surface area (Maskinonge Lake area).
- The hypothetical 1000-m-deep repository is divided into 21 cell and 21 advective transport paths for use in the Geosphere transport network proposed to the P/SA team.
- For either hypothetical repository the total surface discharge area was predicted to be ~2% of the repository footprint area.

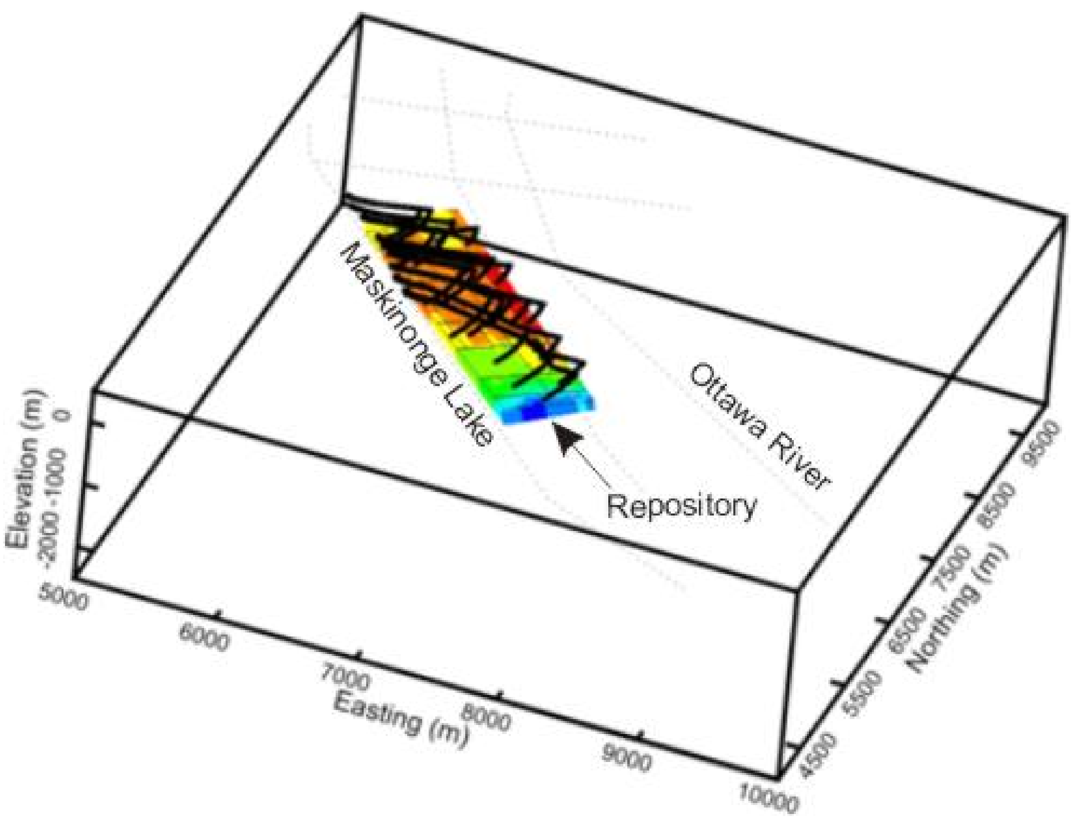


Figure 21. Proposed P/SA geosphere pathways starting from various portions of the 1000-m-deep repository (colour coded to show travel times to surface).

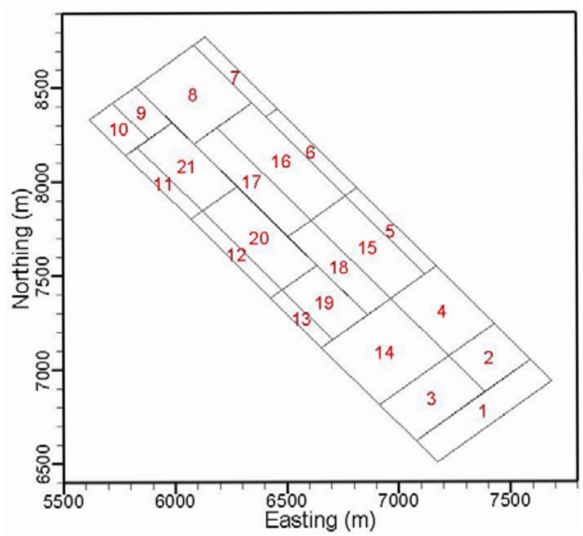


Figure 22. Division of the 1000-m-deep repository into 21 sectors.

Table 3. Synopsis of transit times and distances for the 21 particle path lines.

Particle	Transit Time (yrs)	Transit Distance (m)	Exit Location	Particle	Transit Time (yrs)	Transit Distance (m)	Exit Location
1	51,202	2292	Maskinonge	**2**	39,018	2155	Maskinonge
3	39,246	2115	Maskinonge	**4**	26,350	2043	Maskinonge
5	18,448	1636	Maskinonge	**6**	18,635	1586	Maskinonge
7	24,309	1587	Maskinonge	**8**	27,277	1497	Maskinonge
9	24,905	1408	Maskinonge	**10**	25,268	1385	Maskinonge
11	24,898	1359	Maskinonge	**12**	24,276	1370	Maskinonge
13	25,373	1464	Maskinonge	**14**	30,788	1851	Maskinonge
15	23,027	1614	Maskinonge	**16**	21,604	1518	Maskinonge
17	23,968	1450	Maskinonge	**18**	24,156	1522	Maskinonge
19	24,003	1495	Maskinonge	**20**	23,861	1400	Maskinonge
21	24,148	1388	Maskinonge				

4. SENSITIVITY ANALYSIS

Sensitivity analyses were performed to investigate the influence of natural subsurface temperature distribution (geothermal heat), increased or decreased rock-mass permeability and the presence of two high- or low-permeability dykes.

Results are consistent with the 2-D sensitivity analyses and indicate that:

- The natural geothermal heat at the CRL site will cause little change to the predicted flow field and advective particle travel times;

Increasing (decreasing) the permeability of the rock mass significantly reduces (increases) the particle travel times; and

- Including two high-permeability (low-permeability) dyke zones drastically reduces (increases) the particle travel times.

5. SIMULATING STEADY-STATE GROUNDWATER FLOW AT THE CRL SITE USING DEEP BOREHOLE PERMEABILITY MEASUREMENTS AND COMPARISON WITH MEASURED HEADS

New hydraulic testing data became available in 2010 from the testing that was performed in deep boreholes CRG1, CRG2 and CGR4A during the period 2007-2010 [14] but the results could not be incorporated in time for the P/SA simulations. While the permeability values are reasonably reliable, the hydraulic heads have not necessarily stabilized as discussed below.

5.1 Permeability distribution from interpretation of hydraulic tests

All the permeability values inferred from hydraulic testing in all intervals of the three deep boreholes are displayed in Figure 23, along with the best-fit trend line and the permeability profiles assumed in the Base Case model for the FZs and the rock mass outside the FZs. The interpreted permeability can vary over almost three orders of magnitude from the same type of test in the same borehole within a depth range of a few tens of metres. The best-fit permeability is greater than that assumed for the rock-mass permeability (Table 1) in the Base Case down to a depth of ~540 m, but is less at greater depths, reaching a value in the order of 10^{-19} m^2, which is in realm of the permeability that is associated with sparsely fractured rock.

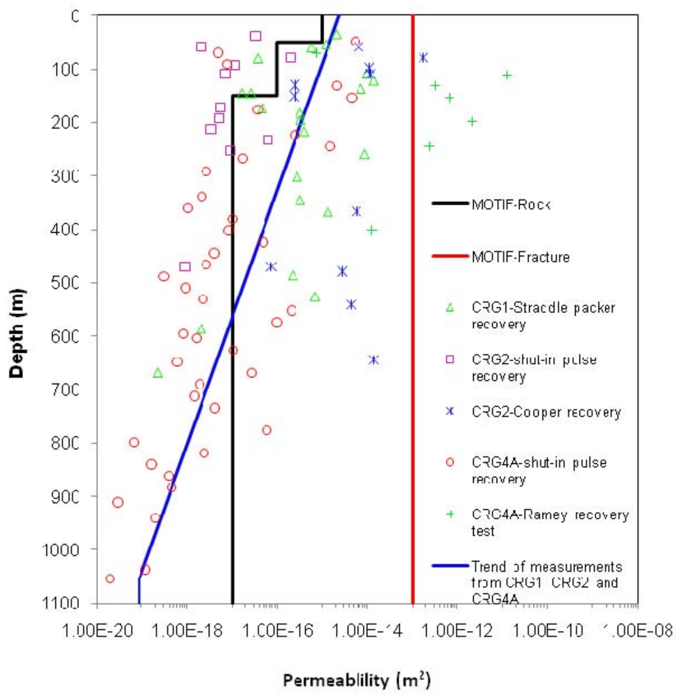


Figure 23. Permeability profiles (Base Case model (black and red lines), field test data from boreholes CRG1, CRG2 and CRG4A (points) and best-fit trend line (blue) to the borehole data).

5.2 Hydraulic head distribution and particle-tracking results from groundwater flow model based on field-determined permeability

A staircase-like approximation for the rock-mass permeability profile (i.e., the blue line in Figure 23) was used in a MOTIF simulation (designated MOTIF CRG124A). Figure 24 shows an isometric view of the predicted head distribution, which is visually similar to that depicted in Figure 9f for the Base Case. Figure 25 displays a sample of path lines a) for 531 particles released from the hypothetical 500-m deep repository into the flow field and b) for 539 particles released from the 1000-m-deep repository. Table 4 lists the summary transit time and transit distance statistics for these repository cases.

These very long particle travel times are much greater than the corresponding Base Case and reflect the nature of the field-based permeability profile and the particle path lines. The particles released from the 500-m-deep repository first descend to ~750-m depth (see Figure 25a) before discharging to surface via the Maskinonge fault. Particles from both hypothetical repositories travel very slowly through a substantial thickness of low-permeability rock (Figure 25a and b).

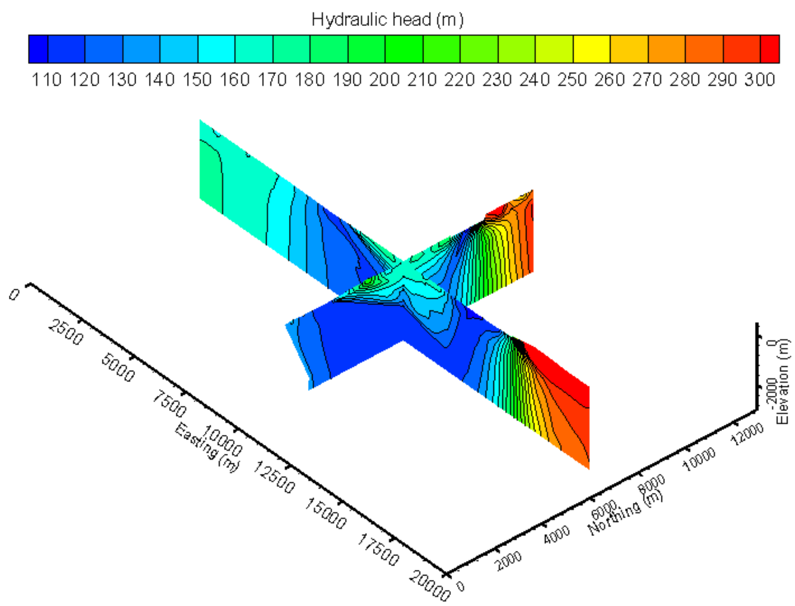
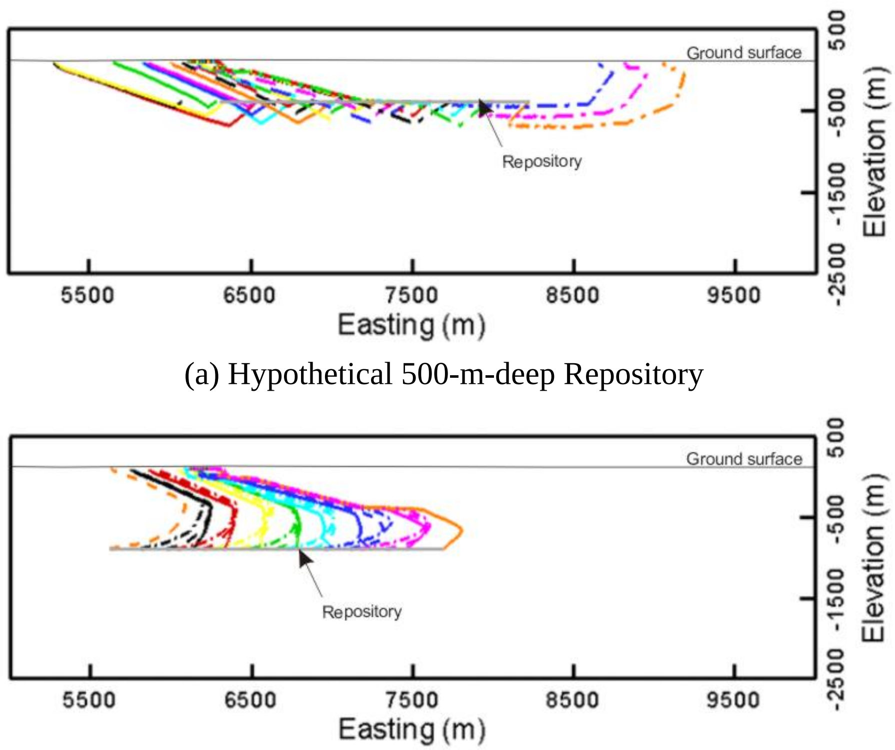


Figure 24. Isometric view of head distribution in vertical sections as modelled with the field-based data.



(a) Hypothetical 500-m-deep Repository

(b) Hypothetical 1000-m-deep Repository

Figure 25. Selected path lines from over 500 particles released from (a) the 500-m-deep repository and (b) the 1000-m-deep repository into the flow field (viewed northward).

Table 4. Summary transit-time and -distance statistics for particles released from two repositories using the best-fit permeability (boreholes CRG1, CRG2 and CRG4A)

Statistics	Transit time (yrs)	Transit distance (m)	Statistics	Transit time (yrs)	Transit distance (m)
500-m Deep Repository			1000-m Deep Repository		
Minimum	1.500E+05	1128	Minimum	1.098E+07	1499
Maximum	1.391E+07	9355	Maximum	5.287E+07	9078
Mean	2.383E+06	3531	Mean	2.277E+07	3248
Median	1.423E+06	1803	Median	1.976E+07	1614
Standard Deviation	2.412E+06	2795	Standard Deviation	8.222E+06	2712

5.3 Preliminary comparison of simulated and measured head profiles

The head profiles predicted by the two Base Case simulations (MOTIF and COMSOL) and the COMSOL CRG124C (i.e., with the best-fit rock-mass permeability in Figure 23) simulation are compared to the measured head profiles in boreholes CR9, CRG1, CRG2 and CRG4A (after Kozak 2011). This comparison (reported in detail in [2]) turns out to be premature. The overall agreement between predicted and measured head profiles is only poor to fair. Plausible reasons for the discrepancies include: i) uncertainties in the conceptual geological and hydrogeological model, ii) uncertainties in permeability distribution, iii) coarseness of the 3-D finite-element flow model mesh and, most importantly, iv) incomplete recovery of the hydraulic heads in the recently installed hydraulic-monitoring system [14] to equilibrium conditions, which is a possible indicator of low-permeability rock-mass zones.

6. SUMMARY AND PRELIMINARY CONCLUSIONS

6.1 Summary

Two- and three-dimensional (2-D and 3-D) hydrogeological simulations were performed to assist in the assessment of the suitability of the CRL site for hosting a deep geologic repository to provide safe long-term management of CRL's low- and intermediate-level wastes. The modelled flow domain includes the bedrock of the CRL site and its immediate vicinity with a number of highly permeable major faults/fracture zones explicitly represented. The 2-D modelling indicates that i) a 10-km length scale is sufficiently large, ii) the predicted groundwater flow field is only weakly influenced by in situ depth-dependent natural temperature and salinity at the CRL site, and iii) based on the assumed flow and transport input parameters, advection and dispersion, rather than diffusion, are the predominant contaminant transport mechanisms.

A 3-D conceptual hydrogeological model, which encompasses a 165-km^2 area, extends to 3 km below surface and includes eight faults/fracture zones, was developed based on a preliminary 3-D geological framework assembled from data available in 2009. The 3-D sub-regional flow domain was discretized with approximately 50, 000 nodes and hexahedron elements for finite-element modelling. As a Base Case simulation, the CRL rock mass was assumed to be layered with permeability decreasing with depth from 10^{-15} m^2 for the weathered rock near surface to 10^{-17} m^2 for moderately fractured rock below 150-m, and porosity decreasing from 3% to 0.1% over these depths. All explicitly modelled faults and fracture zones were assumed to have 10^{-13} m^2 permeability and 10% porosity. A conservative, advective particle-tracking technique was used to estimate the groundwater flowpaths and travel times from two hypothetical repositories (each with a ~1.6 km^2 footprint area) situated 500-m and 1000-m below surface to discharge. Each hypothetical repository was located a 100-m minimum distance (Waste Exclusion Distance) from any major fracture zone in the model. Key findings of the Base Case 3D hydrogeological modelling include: i) particles released from either hypothetical repository discharge either to Maskinonge Lake or Chalk Lake (Sturgeon Lake); ii) advective travel times from the 500-m deep and 1000-m deep hypothetical repositories to surface discharge range from 2.2 x 10^3 to 5.3 x 10^4 years and 1.8 to 5.7 x 10^4 years, respectively; iii) particles with travel times shorter than 5, 000 years for the 500-m deep repository originate from a small fraction of the total hypothetical repository area that could be avoided in future design considerations; and iv) total surface discharge area is 2% or less of either hypothetical repository area.

A network of 10-20 linear segments was constructed to approximate the flow paths from each hypothetical repository to surface discharge. The network geometries, head values, travel times and corresponding repository sector information were provided to the Postclosure Performance and Safety Assessment team for development of the Geosphere Model within the system model.

Sensitivity analyses were performed to investigate the influence of various model input parameters. Results showed: i) increasing (or decreasing) the permeability of the rock mass outside the faults and fracture zones by a factor of 10 from the Base Case drastically reduces (or increases) the particle travel times; ii) including two high-permeability (10^{-13} m^2) dyke zones yields an extremely short minimum particle travel time and a slightly shorter maximum travel time than the Base Case; and iii) including two low-permeability (10^{-19} m^2) dyke zone yields very long particle travel times.

Flow modelling using the best-fit "measured" permeability distribution available in 2010 increases mean and median travel times to over 10^6 years from the 500-m-deep repository and to over 10^7 years from the 1000-m-deep repository. However, predicted and measured head profiles are only in "poor" or "fair" agreement for the limited duration of borehole monitoring.

6.2 Preliminary conclusions

Based on this hydrogeological modelling study the following preliminary conclusions emerge:

- The CRL site as conceptualized using Version 0 of the geological structural framework and the Base Case hydraulic properties would provide a moderately strong natural barrier against transport of radioactive or toxic contaminants from a deep geological repository.
- A number of uncertainties remain in the conceptual and numerical models and the site-specific hydrogeological parameters, which require additional site characterization via drilling, field testing, data interpretation, long-term monitoring and analyses.

- Certain features and processes currently absent from the model (e.g., effects of domestic water-supply wells and coupled thermal-hydraulic-mechanical impacts of future re-glaciation and permafrost evolution) should be included in the next phase of modelling.

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REFERENCES

[1] Baumgartner, P., Beaton, E.D., Chan, T., King-Sharp, K.J., Kitson, C.I., Klimas, S.J., Kozak, E.T., Man, A.G., Stroes-Gascogne, S., Thivierge, R.H., "The suitability of the Chalk River Laboratories site to host a proposed geological waste management facility for CRL's low- and intermediate-level waste: Summary report", Atomic Energy of Canada Limited Report 361101-10260-REPT-002, 2011.

[2] Chan, T., Guo, R., Stanchell, F.W., "Preliminary hydrogeological model of the Chalk River Laboratories region" Atomic Energy of Canada Limited Report 361101-10191-REPT-003, 2011.

[3] Chan, T., Scheier, N.W., Stanchell, F.W., "MOTIF code version 3.2 user's manual", Ontario Hydro Nuclear Waste Management Division Report 06819-REP-01200-0090 R00, 1999.

[4] Nakka, B.W., Chan, T., "A particle-tracking code (TRACK3D) for convective solute transport modelling in the geosphere: Description and user's manual", Atomic Energy of Canada Limited Report AECL-10881, COG-93-216, 1994.

[5] Everitt, R.A., "Conceptual two-dimensional geological model for the Chalk River Laboratories region based on a northeast-southwest vertical section", Atomic Energy of Canada Limited Report 361101-10120-REPT-001, 2007.

[6] Man, A., Baumgartner, P., "Conceptual-design description of a Geological Waste Management Facility located at Chalk River Laboratories for AECL's radioactive wastes", AECL Report 361101-10180-REPT-001, 2008.

[7] Chan, T., Guo, R., Stanchell, F.W., "Two-dimensional hydrogeological model the Chalk River Laboratory site", Atomic Energy of Canada Limited Report 361101-10191-REPT-001, 2011.

[8] McCrank, G., Stanchell, F.W., "Preliminary 3-D sub-regional scale geological model for the CGWMF", Atomic Energy of Canada Limited Report 361101-10120-REPT-009, 2010.

[9] Thivierge, R.H., McCrank, G.F., Sikorsky, R., Janzen, M., Killey, D., King-Sharp, K., Martino, J., Pucciarelli, D., Siddiqui, J., "Preliminary geological synthesis of the Chalk River Laboratories property", Atomic Energy of Canada Limited Report 361101-10120-REPT-010, 2011.

[10] Man, A., Baumgartner, P., Priyanto, D.G., Martino, J.B., "Conceptual-design descriptions and options for a proposed Geologic Waste Management Facility at Chalk River Laboratories", Atomic Energy of Canada Limited Report 361101-10180-REPT-003, 2011.

[11] Chan, T., F.W. Stanchell, F.W., "A numerical study of some effects of nuclear fuel waste vault construction, closure and evolution on convective transport in the geosphere", American Nuclear Society, First Annual International High Level Radioactive Waste Management Conference, Las Vegas, 525-534, 1991.

[12] Davison, C.C., Chan, T., Brown, A., Gascoyne, M., Kamineni, D.C., Lodha, G.S., Melnyk, T.W., Nakka, B.W., O'Connor, P.A., Ophori, D.U., Scheier, N.W., Soonawala, N.M., Stanchell, F.W., Stevenson, D.R., Thorne, G.A., Vandergraaf, T.T., Vilks, P., Whitaker, S.H., "The disposal of Canada's nuclear fuel waste: The geosphere model for postclosure assessment", Atomic Energy of Canada Limited Report AECL-10719, COG-93-9, 1994.

[13] Kitson, C., Goodwin, B.W., "Preliminary postclosure performance and safety assessment for a proposed Geologic Waste Management Facility at Chalk River Laboratories", Atomic Energy of Canada Limited Report 361101-10192-REPT-002, 2011.

[14] Kozak, E.T., "Hydrogeological testing techniques and data from boreholes CR9, CRG1, CRG2 and CRG4A", Atomic Energy of Canada Limited Report 361101-10140-REPT-005, 2011.