

Simulating large scale groundwater flow for waste disposal purposes

Nagyléptékű talajvízáramlás modellezése hulladékelhelyezési célból

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(4 Figures)

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Tárgyszavak: Modellezés, talajvíz áramlás, részecske követés, hulladék lerakás, Kanada

Abstract

Atomic Energy of Canada Limited (AECL) has developed a concept for the disposal of Canada's nuclear fuel waste in a vault, deep (500 m to 1000 m) in low-permeability plutonic rocks of the Canadian Shield. In the concept, the low-permeability rock mass is expected to provide a natural barrier to the release and migration of wastes from the vault. An understanding of groundwater flow can be used to enhance the role of the rock mass as a barrier in the overall disposal system. Therefore, AECL has developed large-scale groundwater flow models of some candidate sites that are used to identify potential vault locations within the sites which have the longest groundwater flow times from prospective disposal vault depths to ground surface.

One candidate site that has been studied by AECL is the Whiteshell Research Area (WRA) in southeastern Manitoba. At this site, a regional groundwater flow model has been developed for a 1050 km² area in order to evaluate alternative locations for a hypothetical nuclear fuel waste disposal vault that maximizes retention of vault contaminants in the rock. A conceptual model of the hydrogeologic conditions was constructed using information obtained from field investigations at the WRA between 1977 and 1994. Simulations of flow were performed using AECL's three-dimensional finite-element code, MOTIF.

First, average values of hydraulic parameters obtained from an analysis of the field data were used in the simulations. Simulated average groundwater recharge did not compare favorably with the recharge rate that was estimated from field data independently. Model calibration was performed by modifying the hydraulic parameters and total dissolved solids distribution of the fluids in a series of consecutive simulations. The simulated recharge rate for the final calibrated model was 4.8 mm/yr. which compared well with the field-based rate of 5 mm/yr. The simulated freshwater heads for this simulation also compared reasonably well with measured heads in the network of boreholes at the WRA. Most of the groundwater flow occurred in local systems between the ground surface and the depth of 2000 m relative to less flow in the intermediate and region systems at greater depth.

A particle tracking code, TRACK3D was used to determine the travel times, pathways and exit locations of particles released from different depth horizons in the groundwater velocity field of the calibrated model. These were used to select a location for a hypothetical nuclear fuel waste disposal vault that maximizes the retention of vault contaminants in long, slow groundwater flow pathways.

Összefoglalás

A Canada Ltd Atomenergia Ügynöksége (Atomic Energy of Canada Limited - AECL) terve szerint Kanada kéieteg nukleáris fűtőelemeit a Kanadai Pajzs mélyen fekvő boltozatának (500–1000 m közötti), kis átérésztőképességű mélységi kőzeteibe vágott üregbe kellene elhelyezni. A tervben a kis átérésztőképességű kőzettömegtől azt várják, hogy természetes módon akadályozza az üregből kiszökő és elvándorló szennyezőanyagokat. A talajvízáramlási rendszer jobb megértése segítheti tisztázni a kőzettömegnek a lerakórendszerben elfoglalt gát szerepét. Ezért az AECL elkészítette néhány számbajövő terület talajvízmodelljét, amelyek alapján azonosíthatók azok a lehetséges telephelyek a kiválasztott területen belül, amikhez a leghosszabb talajvízáramlási idők tartoznak a várható lerakóhelytől a felszínig.

Az egyik AECL által tanulmányozott lehetséges telephely a Whiteshell Kutatóterület (WRA), Manitoba DK-i részén. Ezen a telephelyen modellezték a regionális talajvízáramlást egy 1050 km²-es területre, hogy több szóbjajöhető helyszínt értékeljenek egy leendő elhasznált nukleáris fűtőelem lerakóhely számára, ami maximálisan visszatartja az üregben elhelyezett szennyező anyagot. A hidrogeológiai körülmények/feltételek koncepciói modelljét készítették el, azoknak az adatoknak a felhasználásával, amiket a WRA 1977–1994 közötti terepi megfigyeléseiből nyertek. Az áramlás modellezésére az AECL háromdimenziós véges-változós programját, a MOTIF-ot alkalmazták.

Először a terepi adatok értékeléséből nyert hidraulikus paraméterek átlagos értékeit használták a modellhez. A modellezett átlagos talajvíz utánpótlódás nem hasonlított eléggé a terepi adatokból közvetlenül becsült értékekhez. A modell helyesbítése úgy történt, hogy egy sorozat modellben fokozatosan módosították a folyadékok hidraulikus paramétereit és a teljesen feloldott szilárdanyagok eloszlását. Az utolsó modellben az utánpótlódás mennyisége 4,8 mm/év volt, ami jól egyezett a terepi becslés 5,0 mm/évével. A modellezett édesvíz nyomások ebben az utolsó modellben szintén megfelelő mértékben hasonlítottak a WRA-n telepített kúthálózatban mértékekhez. A vízármlások többsége a helyi rendszerekben a felszín és 2000 m között található a nagyobb mélységben megjelenő átmeneti és regionális rendszerek kis áramlásával szemben.

Egy részecske-követő rendszert, a TRACK3D-t alkalmazták a kalibrált modell talajvíz áramlási felszínének különböző mélységszintjéről induló részecskék áramlási idejének, áramlási útvonalának és kijutási helyének meghatározására. Ezeket az értékeket használták az elméleti nukleáris fűtőelem lerakóhely boltozat megfelelő helyének kiválasztásához, ami maximálja a boltozatban lévő szennyezőanyagok késleltetését hosszú, lassú talajvíz áramlási útvonalakon.

Introduction

As part of the research on a concept for the disposal of Canada's nuclear fuel waste in plutonic rocks of the Canadian Shield, AECL has developed mathematical models to assess the long-term performance of a disposal system. The methodology has been demonstrated in a postclosure assessment case study by applying it to a hypothetical disposal system including a reference vault, a realistic yet hypothetical geosphere, and a biosphere. For the case study, the characteristics of the geosphere were derived from the site-specific information at AECL's Whiteshell Research Area (WRA) in southeastern Manitoba (Fig. 1).

In studying the WRA, a regional model was developed and alternative locations for a hypothetical disposal vault within the simulated regional groundwater flow regime were evaluated to find a location that maximizes the retention of contaminants in the geosphere. This paper summarizes some aspects in the development of the regional flow model, and its use in evaluating alternative locations for the hypothetical disposal vault.

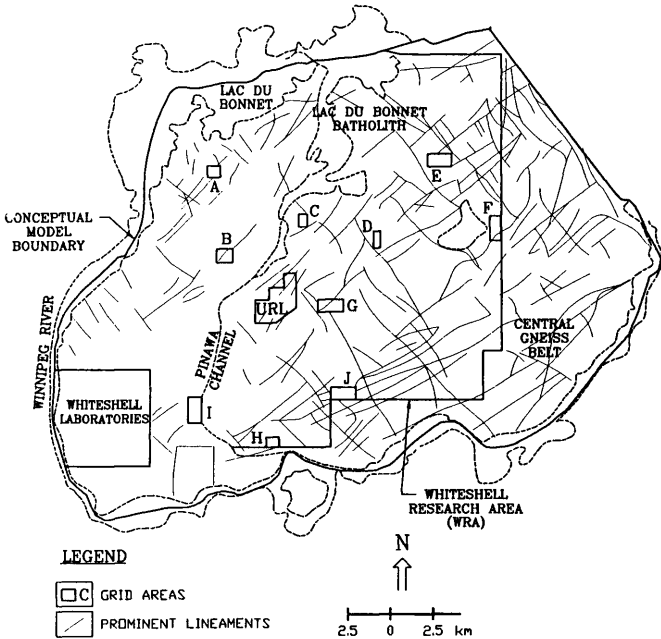


Fig. 1 Map of the Whiteshell research area showing lineaments (fracture zones), model area and locations of deep boreholes (Grid areas)

1. ábra A Whiteshell Kutatási Terület térképe a törés zónákkal, a modell területtel és a mélyfúrások helyével (hálós területek)

Conceptual hydrogeological model of the WRA

The conceptual model of hydrogeological conditions covers an area of about 1050 km² (see Fig. 1), and is bounded on three sides by the Winnipeg River system. The conceptual model was based on surface and subsurface geological, geophysical, geochemical and hydrogeological data in the WRA collected up to 1994. From an analysis of the lineaments (see Fig. 1), a total of seventy-six fracture zones having varying lengths and depths were selected for inclusion in the conceptual model (Fig. 2). The fracture zones strike in different directions, and were assumed from field evidence either to be vertically oriented or to be low dipping with a dip of 25° from the horizontal (except for two with dips of 50° and 10°).

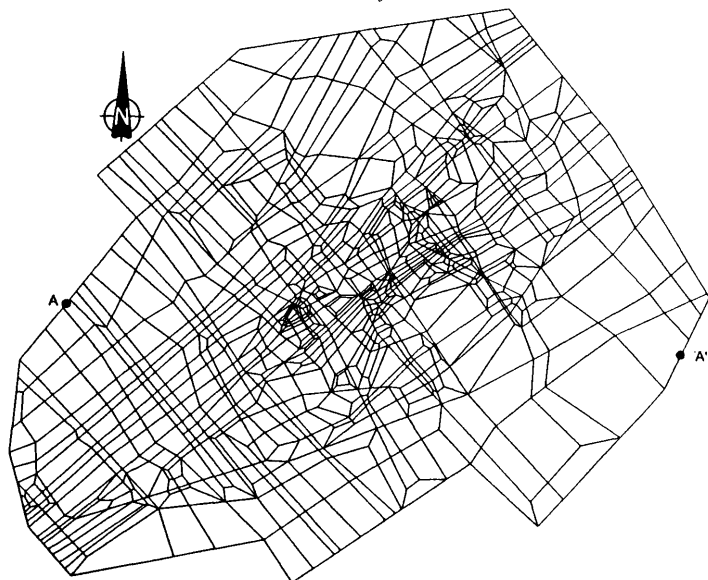


Fig. 2 Geologic Framework, Surface Structure and Finite-Element Mesh of the Whiteshell Research Area. Section A-A' is a Line Joining Point A to Point A'.

2. ábra A Whiteshell Kutatási Terület földtani felépítése, felszíni szerkezete és véges váltós hálójája

Within the WRA, the water table is a subdued replica of the surface topography which has a moderate regional slope of about 0.002 from southeast to northwest. The water table elevation was used as the top boundary condition. The Winnipeg River was assumed to provide stable hydrological boundaries on most sides of the area, except the northeastern part of the model area which is bounded by a major fault referred to as the F-F' fault. Because there is sufficient local topographic relief around it to capture groundwater flow from considerable depth, the Winnipeg River was assumed to be a no-flow hydrogeologic boundary. The major fault along the northeastern part of the area was also assumed to be a no-flow boundary. The bottom boundary of the model at a depth of 4000 m was assumed to be impermeable. Trends in available field permeability data suggest that permeability at this depth could be 10^{-21} m² or lower, essentially impermeable. It was demonstrated that changing these lateral and lower boundary conditions does not affect the convective transport of solutes from the selected locations of a hypothetical vault at 500 m to 1000 m depth to the groundwater discharge locations in the biosphere (OPHORI et al. 1996). These boundary conditions were the same as used in an earlier model of the WRA (DAVISON et al.

1994) except that the elevation of the water table has been substituted for the topographic elevation for the top boundary condition of the model.

Permeability data exist from straddle packer tests and pumping tests in boreholes to depths of 1000 m at the WRA. These data were analysed in detail by STEVENSON et al. (1995). The values of permeability used in the simulation for the rock mass and fracture zones are shown in Table 1. For the rock mass, horizontal permeability decreased from $1 \times 10^{-15} \text{ m}^2$ at the surface to $1 \times 10^{-21} \text{ m}^2$ at a depth of 1000 m. The anisotropy in the rock was represented by assigning vertical permeabilities one order of magnitude higher than horizontal permeabilities between the ground surface and 300 m for the granite, and also between 300 and 1000 m for the gneiss. Below this depth, the rock mass was assigned a constant permeability of $1 \times 10^{-21} \text{ m}^2$. The fracture zones were assumed isotropic with permeability varying from $1 \times 10^{-13} \text{ m}^2$ at the surface to $1 \times 10^{-16} \text{ m}^2$ at a depth of 1000 m. Below 1000 m, the fracture zones were assigned gradually decreasing permeabilities reaching $7.52 \times 10^{-19} \text{ m}^2$ at the bottom of the model (4000 m). The permeability values were derived from the analysis by STEVENSON et al. (1995).

Porosity values were estimated from field and laboratory data by STEVENSON et al. (1996a). These ranged from 0.003 to 0.001 for the rock mass, and from 0.05 to 0.005 for the fracture zones (Table 1).

Flow simulation

For the numerical simulation of groundwater flow using AECL's MOTIF code (GUVANASEN 1984; CHAN et al. 1987), the conceptual model of the rock mass and seventy-six regional fracture zones was discretized into a finite-element mesh. This was done using the PATRAN pre- and post-processor for finite-element codes (PATRAN, 1989). The fracture zones were represented by planar elements of uniform 3 m thickness based on field data. The mesh consisted of a total of 3 323 planar elements, 13 897 solid elements and 15 610 nodes (Fig. 2). The MOTIF code was then used to compute the head and fluid velocity distributions in the model. Details of all the simulation results are presented elsewhere (OPHORI et al. 1996).

Figure 3 is a typical section A-A' (see Fig. 2) showing groundwater flow velocities across the modeled region for a calibrated-model simulation. Flow velocities decrease rapidly in magnitude with depth, becoming insignificant (less than $1 \times 10^{-6} \text{ m/a}$) by a depth of 1000 m. This reduction in velocity is caused by the permeability-depth relationship used in the simulation (see Table 1). Many local flow systems of relatively high groundwater velocities occur near the ground surface of the model (i.e. within 500 m depth). Some local and intermediate systems are continuous to the bottom of the model. The highest point on the topographic divide of this section occurs at about the X coordinate of 5000 m whereas the lowest point is at the X coordinate of -23 000 m. Because these two regions are not linked by a continuous flowline, a regional flow system does not occur along the section in this simulation (TÓTH 1963). A regional flow system may occur along other hydraulic sections (OPHORI et al. 1996), but these large

Hydraulic parameters used in the Calibrated Flow Model

A kalibrált áramlási modellben használt hidraulikus adatok

Table 1 – I. tábla

Rock Mass	Approximate Depth (m)	Horizontal Permeability (m ²)	Vertical Permeability (m ²)	Effective Porosity
Layer 1	0- 100	1.0 x 10 ⁻¹⁵	1.0 x 10 ⁻¹⁴	0.003
2	100- 200	4.46 x 10 ⁻¹⁷	4.46 x 10 ⁻¹⁶	0.003
3	200- 300	5.99 x 10 ⁻¹⁸	5.99 x 10 ⁻¹⁷	0.003
4	300- 400	5.00 x 10 ^{-20**}	5.00 x 10 ^{-20**}	0.003
		7.74 x 10 ^{-19*}	7.74 x 10 ^{-18*}	0.003
5	400- 500	7.74 x 10 ^{-19*}	7.74 x 10 ^{-19*}	0.003
		3.00 x 10 ^{-20**}	3.00 x 10 ^{-20**}	0.003
6	500- 750	3.15 x 10 ^{-19*}	3.15 x 10 ^{-18*}	0.003
		3.15 x 10 ^{-19*}	3.15 x 10 ^{-19*}	0.003
		1.50 x 10 ^{-20**}	1.50 x 10 ^{-20**}	0.003
7	750-1000	3.35 x 10 ^{-20*}	3.35 x 10 ^{-19*}	0.003
		3.35 x 10 ^{-20*}	3.35 x 10 ^{-20*}	0.003
		7.50 x 10 ^{-21**}	7.50 x 10 ^{-21**}	0.003
8	1000-1250	1.36 x 10 ^{-21*}	1.36 x 10 ^{-20*}	0.003
		1.36 x 10 ^{-21*}	1.36 x 10 ^{-21*}	0.003
9	1250-1600	1.0 x 10 ⁻²¹	1.0 x 10 ⁻²¹	0.003
10	1600-2000	1.0 x 10 ⁻²¹	1.0 x 10 ⁻²¹	0.003
11	2000-2500	1.0 x 10 ⁻²¹	1.0 x 10 ⁻²¹	0.003
12	2500-3200	1.0 x 10 ⁻²¹	1.0 x 10 ⁻²¹	0.002
13	3200-4000	1.0 x 10 ⁻²¹	1.0 x 10 ⁻²¹	0.001

Fracture Zones	Approximate Depth (m)	Longitudinal Permeability (m ²)	Transverse Permeability (m ²)	Effective Porosity
Layer 1	0- 100	1.0 x 10 ⁻¹³	1.0 x 10 ⁻¹³	0.05
2	100- 200	1.0 x 10 ⁻¹³	1.0 x 10 ⁻¹³	0.05
3	200- 300	1.0 x 10 ⁻¹³	1.0 x 10 ⁻¹³	0.05
4	300- 400	1.0 x 10 ⁻¹³	1.0 x 10 ⁻¹³	0.05
5	400- 500	1.0 x 10 ⁻¹⁴	1.0 x 10 ⁻¹⁴	0.05
6	500- 750	1.0 x 10 ⁻¹⁵	1.0 x 10 ⁻¹⁵	0.05
7	750-1000	1.0 x 10 ⁻¹⁶	1.0 x 10 ⁻¹⁶	0.05
8	1000-1250	1.56 x 10 ⁻¹⁷	1.56 x 10 ⁻¹⁷	0.046
9	1250-1600	8.44 x 10 ⁻¹⁸	8.44 x 10 ⁻¹⁸	0.041
10	1600-2000	4.61 x 10 ⁻¹⁸	4.61 x 10 ⁻¹⁸	0.035
11	2000-2500	2.58 x 10 ⁻¹⁸	2.58 x 10 ⁻¹⁸	0.028
12	2500-3200	1.37 x 10 ⁻¹⁸	1.37 x 10 ⁻¹⁸	0.018
13	3200-4000	7.52 x 10 ⁻¹⁹	7.52 x 10 ⁻¹⁹	0.005

* Gneiss

* Granite

** Granite under TDS dome

scale flow systems occur below depths of 1000 m in the model where flow magnitudes are so small that molecular diffusion is the dominant transport mechanism. This detailed understanding of flow is required for the selection of the site for the waste disposal vault.

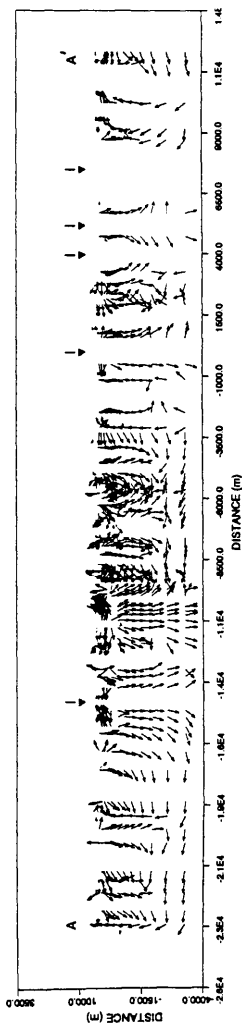


Fig. 3 Hydraulic cross section A-A' through calibrated model. Arrows trace direction of flow and flow pathways

3. ábra A-A' hidraulikus keresztmetszében a kalibrációs modell-területen keresztüli. A nyílak az áramlás irányját és pályáját mutatják. A szelvény nyomvonalát a 2. ábrán látható

The flow model was calibrated using pore fluid pressures measured in the network of boreholes at the WRA, as well as estimates of average groundwater recharge rates determined from experimental sites at the WRA. The recharge rate was used primarily to adjust the value of vertical permeability chosen for the top layer of the model. The lateral permeability and the permeability of the deeper layers in the model do not affect the calculations of recharge rate (OPHORI & CHAN 1994a b, OPHORI 1996, 1999). The mean annual recharge rate was estimated at about 5 mm from field experiments (THORNE 1990, 1992; THORNE & GASCOYNE 1993; THORNE et al. 1991, 1992). This recharge is about 1 percent of the average precipitation of 562 mm at the WRA and is within the range reported for other parts of the Canadian Shield (e.g. THORNE et al. 1994).

Fluid pressures measured in deep boreholes at the WRA were used for adjusting the input parameters in the deeper layers of the model. There were sixteen boreholes with depths of about 1000 m in which fluid pressure had been measured in several packed-off sections (STEVENSON et al. 1996b). These fluid pressures were converted to equivalent freshwater heads and used in the groundwater flow model calibration.

Hypothetical vault location

The results of the final flow model were used in conjunction with AECL's particle tracking code, TRACK3D (NAKKA & CHAN 1994) to evaluate alternative locations for a hypothetical disposal vault. Using the TRACK3D

code, particles were released on a regular grid at different depths into the groundwater velocity field of the calibrated model and tracked to their exit points at surface. The advective travel times of the particles were also determined. Three different particle release depths, 500-, 750- and 1000 m, were analysed in detail.

The travel times of particles released at a depth of 750 m to their exit locations at the ground surface are depicted in Fig. 4. These travel times were used to select a location for a hypothetical disposal vault at a depth of 750 m in the modeled area.

Other aspects that were considered in choosing the location for the hypothetical vault were:

1. the location should have long travel times (minimum 10^6 a),
2. the location should be an area of at least 2 km by 2 km in size containing no regional fracture zones at the depth of the vault,
3. the location should have a reasonable level of field data control (i.e. borehole control within or near the location), and
4. the depth of the hypothetical vault should be within 500 m to 1000 m below groundwater surface.

The selected location for the hypothetical disposal vault is indicated in Figure 4. The site is about 5 km northeast of the location of the Underground Research Laboratory (URL). Details of the selection process are presented in OPHORI et al. (1996) and DAVISON et al. (1996).

Summary

This paper is a summary of the regional groundwater flow simulations performed with a conceptual hydrogeologic model of the Whiteshell Research Area (WRA). The main purpose of the regional flow modeling was to develop a calibrated model of regional groundwater flow of the WRA, and then use the calibrated model to evaluate alternative locations for a hypothetical nuclear fuel waste disposal vault within the flow system.

The MOTIF finite-element code, developed by AECL, was used in the simulations. The conceptual model consisted of seventy-six regional fracture zones which occur in many directions at various angles in the background rock mass. The fracture zones were represented by two-dimensional elements embedded in a three-dimensional element mesh representing the rock mass.

The simulation was performed using average values of hydraulic parameters obtained from field data, and assuming that freshwater occupied the entire modeled region. The model calibration involved a comparison of simulated recharge rates and reference heads to their equivalent values as estimated from field data. A recharge rate of 4.8 mm/a was calculated from the results of the calibrated model. This rate compared favorably with the field estimate of 5.0 mm/a (few percent of precipitation) at the WRA.

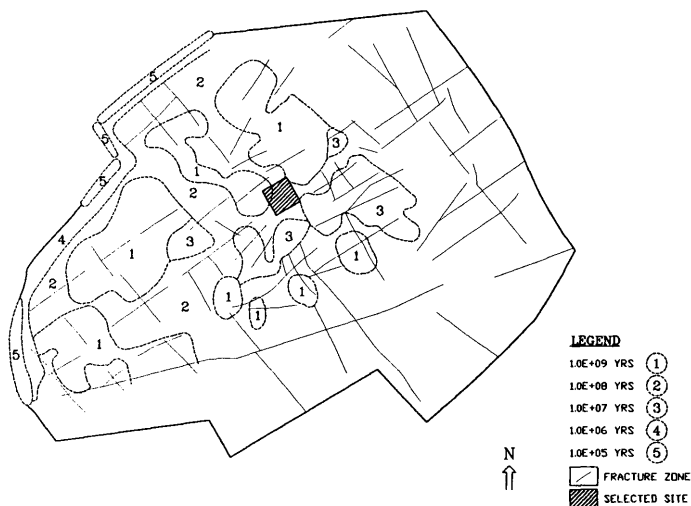


Fig. 4 Travel times of particles released from model depth horizon of 750 m

4. ábra A 750 m-es mélységi modellszintből kiszabadult részecskék vándorlási ideje

A particle tracking code, TRACK3D, was used to calculate advective travel times, pathways and exit locations of particles from various depths in the groundwater velocity field of the calibrated model. Using the travel times, alternative locations were evaluated with the view of selecting a location that maximizes the retention of vault contaminants within the groundwater flow regime. During this evaluation, consideration was focussed on areas of the WRA where subsurface field data were available. The selected location for the hypothetical disposal vault is about 5 km northeast of the URL lease area, where subsurface data exist.

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