Groundwater contamination associated with a potential nuclear waste repository at Yucca Mountain, USA

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Abstract

The groundwater contamination originating from a potential nuclear waste repository at Yucca Mountain, USA, is evaluated in a three-dimensional flow transport simulation. The model has 833,079 elements and includes both the saturated and unsaturated zone. Vertical grid spacing is 20 m in the saturated zone and 40 m in the unsaturated zone. Spacing in the x and y directions is 250 m in both the saturated and unsaturated zone. The simulation period is 1,000,000 years. Three scenarios with different saturation values (0.056, 0.1 and 0.18) for Dirichlet conditions at the top of the model and different permeabilities for the total model are calculated. The results differ from previous calculations conducted with a combination of one-dimensional models for the saturated zone and uncoupled models for the unsaturated zone. Since one-dimensional models produce averaged values for the three-dimensional space, they necessarily produce a relatively low radioactive dose. In contrast, the peak dose for the 250 x 250 x 20-m cells in the three-dimensional space is relatively high but closer to the risk an individual is exposed to within a reasonably small area.

Keywords Nuclear waste · Groundwater contamination · Numerical model

Introduction

The candidate repository for nuclear waste at Yucca Mountain, USA (Fig. 1), is conceived for waste storage above the water table. Modelling potential groundwater contamination is a challenging task if the contaminant source is located above the water table. The models published to date consist of a combination of a three-dimensional (3D) transport model for the unsaturated zone and an uncoupled one-dimensional (1D) model for the saturated zone (DOE 2009). This combination has the disadvantage of relying on a large number of assumptions that are difficult to verify.

Groundwater contamination is a 3D process. Integrating the saturated and unsaturated zone in a single 3D model drastically reduces the number of assumptions required. In other words, transparency and reproducibility are significantly improved.

Study area

The 1057.5-km² model (Fig. 2) is located in an area where explosive magmatism dominated the geologic history during the Miocene (Table 1; DOE 2007a). The sequence of pyroclastic rocks with subordinate flows is approximately 1500 m thick (Applegate 2006). The pre-volcanic formations consist of Late Proterozoic through Palaeozoic folded and faulted sedimentary rocks as well as Middle Proterozoic metamorphic and igneous rocks. Late Tertiary and Quaternary deposits consist of alluvial sediments and minor basaltic flows (Fig. 3). The horizontal boundaries are the UTM Zone 11 x coordinates 533,000–563,000 and y coordinates 4,046,500–4,081,750. The southwest corner of the model is located 1 km northeast of the Nevada-California state boundary.

The repository

The 6.3-km² repository should be located at an altitude of 1050–1250 m a.s.l. in an area where the water table is 740–940 m a.s.l. or 25–750 m below the topographic surface (Fig. 4; DOE 2007b). The Nuclear Waste Policy Act of 1982 (DOE 2004) specifies that the first US repository cannot exceed the equivalent of 70,000 metric tons of heavy metal

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Fig. 1 Location of the Yucca Mountain project, USA

(MTHM, including uranium and other radioactive heavy metals) until a second repository is operational. The statutory limit is still valid today and corresponds to 11,629 waste containers (Table 1; DOE 2007c).

Model setup

The model mesh is a hybrid mesh consisting of a dual-permeability sub-mesh for the volcanic rock units and a single-continuum (single porosity) sub-mesh for the non-

volcanic units. All elements are interconnected. Flow occurs between all elements. The mesh has 833,079 elements. The top of the grid is the topographic surface (730–1640 m a.s.l.), and the bottom is located at 200 m a.s.l.

The primary mesh with 470,250 elements, consisting of the single-continuum sub-mesh and the fracture continuum of the dual-continuum sub-mesh, is regular horizontally and irregular vertically. The node spacing in the x and y directions is 250 m. The layers of the mesh are aligned parallel to the initial water table except for the top and bottom layers (Fig. 5). The initial water table of the base case (Fig. 4c) is the modelled “potentiometric surface” of DOE (2007a). The initial water table of the sensitivity case (Fig. 4d) is derived by kriging the measured water level data of DOE (2007a). The layers above the reference horizons are 40 m thick except for the top layer. There are 101 contaminant injection cells 320 m above the initial water table characterising the 6.3-km² repository. Below the reference horizons, there are 22 layers, each of which is 20 m thick except for the bottom layer.

In order to facilitate the comparison with previous models, preference is given to published mean values for input data, except for permeability, which is better represented by median values. When mean values do not exist,

Fig. 2 Map with hydrogeologic units (Table 1) of the Yucca Mountain model. Traces of cross sections (Fig. 3; solid black lines) and the repository outline (solid red line) are also shown

Table 1 Hydrogeologic units and hydraulic properties of the Yucca Mountain region

Unit ID	Unit name	Age	Zone ^a	Permeability (m ²)				Matrix			Porosity (–)	
				Fracture/single continuum				Fracture/ single continuum			Fracture/ single continuum	
				x	y	z	x	y	z	x	y	z
28	Young Alluvial Aquifer	Pliocene-Holocene	1	2.0×10^{-11}	2.0×10^{-11}	2.0×10^{-12}	–	–	–	–	0.3	–
28	Young Alluvial Aquifer	Pliocene-Holocene	2	9.8×10^{-13}	9.8×10^{-13}	9.8×10^{-14}	–	–	–	–	0.3	–
27	Young Alluvial Confining Unit	Pliocene-Holocene	1	2.0×10^{-11}	2.0×10^{-11}	2.0×10^{-12}	–	–	–	–	0.3	–
27	Young Alluvial Confining Unit	Pliocene-Holocene	2	9.9×10^{-15}	9.9×10^{-15}	9.9×10^{-16}	–	–	–	–	0.3	–
26	Older Alluvial Aquifer	Pliocene-Holocene	1	2.0×10^{-11}	2.0×10^{-11}	2.0×10^{-12}	–	–	–	–	0.3	–
26	Older Alluvial Aquifer	Pliocene-Holocene	2	1.5×10^{-13}	1.5×10^{-13}	1.5×10^{-14}	–	–	–	–	0.3	–
24	Limestone Aquifer	Cenozoic, undivided	5	9.8×10^{-14}	9.8×10^{-14}	9.8×10^{-14}	–	–	–	–	0.01	–
23	Lava Flow Unit	Cenozoic, undivided	5	8.9×10^{-14}	8.9×10^{-14}	8.9×10^{-15}	–	–	–	–	0.08	–
21	Volcanic and Sedimentary Units	Cenozoic, undivided	5	8.7×10^{-13}	8.7×10^{-13}	8.7×10^{-14}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.25
20	Timber Mountain Volcanic Aquifer	Miocene	3	9.5×10^{-14}	4.7×10^{-13}	4.7×10^{-14}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.15
20	Timber Mountain Volcanic Aquifer	Miocene	4	9.5×10^{-14}	9.5×10^{-14}	9.5×10^{-15}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.15
19	Paintbrush Volcanic Aquifer	Miocene	3	6.4×10^{-14}	3.2×10^{-13}	3.2×10^{-14}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.15
19	Paintbrush Volcanic Aquifer	Miocene	4	6.5×10^{-14}	6.5×10^{-14}	6.5×10^{-15}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.15
18	Calico Hills Volcanic Unit	Miocene	3	2.4×10^{-13}	1.2×10^{-12}	1.2×10^{-13}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.25
18	Calico Hills Volcanic Unit	Miocene	4	2.4×10^{-13}	2.4×10^{-13}	2.4×10^{-14}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.25
17	Wahmonie Volcanic Unit	Miocene	3	9.8×10^{-14}	4.9×10^{-13}	4.9×10^{-14}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.25
17	Wahmonie Volcanic Unit	Miocene	4	9.8×10^{-14}	9.8×10^{-14}	9.8×10^{-15}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.25
16	Crater Flat-Prow Pass Aquifer	Miocene	3	3.1×10^{-12}	1.5×10^{-11}	1.5×10^{-12}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.23
16	Crater Flat-Prow Pass Aquifer	Miocene	4	3.1×10^{-12}	3.1×10^{-12}	3.1×10^{-13}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.23
15	Crater Flat-Bullfrog Confining Unit	Miocene	3	5.2×10^{-14}	2.6×10^{-13}	2.6×10^{-14}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.18
15	Crater Flat-Bullfrog Confining Unit	Miocene	4	5.2×10^{-14}	5.2×10^{-14}	5.2×10^{-15}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.18
14	Crater Flat-Tram Aquifer	Miocene	3	9.4×10^{-13}	4.7×10^{-12}	4.7×10^{-13}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.21
14	Crater Flat-Tram Aquifer	Miocene	4	9.4×10^{-13}	9.4×10^{-13}	9.3×10^{-14}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.21
12	Older Volcanic Units	Oligocene-Miocene	3	9.8×10^{-16}	4.9×10^{-15}	4.9×10^{-16}	10^{-17}	10^{-17}	10^{-17}	10^{-17}	0.01	0.21
12	Older Volcanic Units	Oligocene-Miocene	4	9.8×10^{-16}	9.8×10^{-16}	9.8×10^{-17}	10^{-17}	10^{-17}	10^{-17}	10^{-17}	0.01	0.21
11	Lower Volcanic and Sedimentary Units	Cenozoic, undivided	3	1.1×10^{-14}	5.5×10^{-14}	5.5×10^{-15}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.21
11	Lower Volcanic and Sedimentary Units	Cenozoic, undivided	4	1.1×10^{-14}	1.1×10^{-14}	1.1×10^{-15}	10^{-15}	10^{-15}	10^{-15}	10^{-15}	0.01	0.21
9	Lower Carbonate Aquifer (thrust)	Cambrian-Devonian	5	5.6×10^{-12}	5.6×10^{-12}	5.6×10^{-12}	–	–	–	–	0.01	–
8	Lower Carbonate Aquifer (thrust)	Proterozoic-Cambrian	5	9.8×10^{-19}	9.8×10^{-19}	9.8×10^{-19}	–	–	–	–	0.18	–
6	Upper Clastic Confining Unit	Devonian-Mississippian	5	9.8×10^{-16}	9.8×10^{-16}	9.8×10^{-16}	–	–	–	–	0.18	–
5	Lower Carbonate Aquifer	Cambrian-Devonian	5	9.7×10^{-15}	9.7×10^{-15}	9.7×10^{-15}	–	–	–	–	0.01	–
4	Lower Carbonate Aquifer	Proterozoic-Cambrian	5	9.7×10^{-17}	9.7×10^{-17}	9.7×10^{-17}	–	–	–	–	0.18	–
3	Crystalline Confining Unit	Middle Proterozoic	5	1.0×10^{-16}	1.0×10^{-16}	1.0×10^{-16}	–	–	–	–	0.00001	–
40	Fortymile Fault		5	1.4×10^{-10}	1.4×10^{-10}	1.4×10^{-10}	–	–	–	–	0.18	–
41	Bare Mountain Fault		5	9.9×10^{-16}	9.9×10^{-16}	9.9×10^{-16}	–	–	–	–	0.18	–
42	Crater Flat Fault		5	9.7×10^{-17}	9.7×10^{-17}	9.7×10^{-17}	–	–	–	–	0.18	–
43	Highway 95 Fault		5	1.0×10^{-14}	1.0×10^{-14}	1.0×10^{-14}	–	–	–	–	0.18	–
44	Solitario Canyon Fault		5	5.0×10^{-16}	5.0×10^{-16}	5.0×10^{-16}	–	–	–	–	0.18	–
46	Stage Coach Fault		5	4.7×10^{-16}	4.7×10^{-16}	4.7×10^{-16}	–	–	–	–	0.18	–
47	Windy Wash Fault		5	4.8×10^{-16}	4.8×10^{-16}	4.8×10^{-16}	–	–	–	–	0.18	–

^a 1 = Inside alluvial zone

2 = Outside alluvial zone

3 = Inside anisotropic zone

4 = Outside anisotropic zone

5 = Total mesh

Fig. 3 Vertical cross sections of the Yucca Mountain model (traces in Fig. 2) with hydrogeologic units (legend shows stacking order). The water table (black solid line) and the repository (red solid line) are also shown

“calibrated” values, “expected” values, “base case” values and “conceptual” model data are used in decreasing order of priority.

Hydraulic properties and transport parameters

The permeabilities of the base case (Table 1) are the “calibrated” values of DOE (2007a). They refer to the “conceptual” isopach model of DOE (2007b), “base case” horizontal anisotropy of DOE (2007d), “conceptual” vertical anisotropy of DOE (2007a), “conceptual” model of vertical faults of DOE (2007a) and further vertical (geometric) subdivisions of DOE (2007a). The sensitive cases use these values multiplied by 0.1 and 10. The remaining hydraulic properties are identical for the base case and sensitivity cases. These are the median value for matrix permeability (DOE 2007e), “expected” values for matrix and single-continuum porosity (DOE 2009) and mean value for fracture porosity (DOE 2007e). The fracture spacing and van Genuchten parameters in Table 2 are the mean value of DOE (2007e).

Transport parameters are identical for the base case and sensitivity cases. These are the mean values for sorption (DOE 2007e) as well as “base-case” values for diffusion and dispersion (DOE 2009).

Computer codes

The flow fields and associated water saturations are calculated with the TOUGH2 code (parallel version 2.01; Zhang et al. 2008). Contaminant transport is calculated with the FEHM code (version 3.3.0; Zyvoloski et al. 2015) using the TOUGH2 flow fields and water saturations (Ho and Robinson 1998). The TOUGH2 output files are converted to FEHM input files with a combination of terminal scripts, text editor and spreadsheet. The FEHM format requirements are documented in Zyvoloski et al. (2015).

The TOUGH2 mesh is calculated with the WINGRIDDER code (Pan 2007) and subsequently adapted to requirements of the FEHM code with the LaGrit program (online manual; <http://lagrit.lanl.gov>).

Flow model

Boundary conditions and initialisation

During the one-year initialisation step, the lateral volume elements have a large volume (10^{10} m^3). The top elements have an infinite volume (10^{52} m^3) during initialisation and subsequent flow field calculation. The infinite volume elements impose Dirichlet conditions, i.e., the thermodynamic parameters of these elements do not change at all.

Fig. 4 Yucca Mountain model: **a** topographic surface (m a.s.l.); **b** depth of the base case water table below the topographic surface (m); **c** base case water table (m a.s.l.); **d** sensitivity case water table (m a.s.l.). The outline of the repository is also shown (solid red line). The scale bar corresponds to 10 km

The elements above the initial water table, including the top elements, have a pressure of 10^5 MPa and a saturation dependent on the permeability model (see above); the appropriate saturation value is determined by a trial-and-error procedure (see below).

The pressure of the initial saturated zone at the beginning of the initialisation step is 10^5 MPa plus the depth below the

water table (m) multiplied by 10^4 MPa/m. The permeability is set at a high value (10^{-12} m²) for all elements in order to achieve an efficient fine tuning of the pressure.

Flow field calculation

Saturation and pressure at the end of the initialisation step are used as initial conditions for the flow field calculation. The lateral boundary elements are replaced by infinite volume elements (10^{52} m³), and the initial permeabilities are replaced by the actual values (see above).

At the end of the one-year simulation period, the flow field approaches a steady state. The optimal saturation value is found by trial and error. This is the value that produces a water table closest to the initial position (Figs. 6 and 7). The optimal saturation values are 0.1 for the case with the “calibrated” permeability values of DOE (2007a), 0.056 for a high-permeability sensitivity case and 0.18 for a low-permeability sensitivity case. The optimal saturation values are identical for both types of initial water table (modelled “potentiometric surface” or water table derived by kriging of the measured water level data; see above).

Fig. 5 Block diagram of the Yucca Mountain model showing nodal positions. Twenty-fold vertical exaggeration (z direction)

Table 2 Set-up of the Yucca Mountain model

General properties	
Simulation period (a)	1,000,000
Model length/width (m)	35,250/30,000
Model height (m)	1400
Model temperature (°C)	25
Rock grain density (kg/m ³)	2800
Residual liquid saturation (–)	0
Residual gas saturation (–)	0
Fracture spacing (m)	13
van-Genuchten parameter for two-phase flow α [fracture, single continuum] (1/Pa)	1.5×10^{-3}
van-Genuchten parameter for two-phase flow m [fracture, single continuum] (–)	0.63
van-Genuchten parameter for two-phase flow α [matrix] (1/Pa)	1.0×10^{-4}
van-Genuchten parameter for two-phase flow m [matrix] (–)	0.27
FEHM parameter for colloid transport SLOPE_KF (–)	1
FEHM parameter for colloid transport CINT_KF (–)	0.95
Number of simultaneous contaminant sources (–)	101
Repository	
Capacity (MTHM) ^a	70,000
Number of waste containers (–)	11,629
Initial inventory	
Am-241 (Bq)	8.67×10^{18}
Am-243 (Bq)	7.66×10^{16}
C-14 (Bq)	2.03×10^{14}
Cl-36 (Bq)	3.54×10^{13}
Cs-135 (Bq)	1.56×10^{15}
I-129 (Bq)	9.55×10^{13}
Np-237 (Bq)	1.00×10^{15}
Pa-231 (Bq)	1.01×10^{13}
Pu-239 (Bq)	8.33×10^{17}
Pu-240 (Bq)	1.44×10^{18}
Pu-242 (Bq)	6.40×10^{15}
Ra-226 (Bq)	3.43×10^9
Se-79 (Bq)	2.15×10^{14}
Tc-99 (Bq)	4.02×10^{16}
Th-230 (Bq)	1.01×10^{12}
U-233 (Bq)	1.10×10^{14}
U-234 (Bq)	3.41×10^{15}
U-236 (Bq)	7.67×10^{14}
U-238 (Bq)	9.04×10^{14}
Half-life	
Am-241 (a) ^b	4.33×10^2
Am-243 (a) ^c	7.37×10^3
C-14 (a)	5.71×10^3
Cl-36 (a)	3.01×10^5
Cs-135 (a)	2.3×10^6
I-129 (a)	1.57×10^7
Np-237 (a) ^b	2.14×10^6
Pa-231 (a)	3.28×10^4
Pu-239 (a) ^c	2.41×10^4
Pu-240 (a) ^d	6.56×10^3
Pu-242 (a) ^e	3.75×10^5

Table 2 (continued)

Ra-226 (a) ^f	1.60×10^3
Se-79 (a)	2.90×10^5
Tc-99 (a)	2.13×10^5
Th-230 (a) ^f	7.54×10^4
U-233 (a) ^b	1.59×10^5
U-234 (a) ^f	2.46×10^5
U-236 (a) ^d	2.34×10^7
U-238 (a) ^c	4.47×10^9
Distribution coefficient	
Am (mL/g)	5500
C (mL/g)	0
Cs (mL/g)	728
Cl (mL/g)	0
I (mL/g)	0
Np (mL/g)	0.69
Pa (mL/g)	5500
Pu (mL/g)	100
Se (mL/g)	14.3
Tc (mL/g)	0
Th (mL/g)	5500
U (mL/g)	2
Diffusivity	
All radionuclides (m ² /s)	5×10^{-11}
Dispersivity	
Longitudinal, all radionuclides (m)	10
Transverse, horizontal, all radionuclides (m)	0.05
Transverse, vertical, all radionuclides (m)	0.0005
Biodose conversion factor	
Am-241 (Sv/a:Bq/m ³)	8.34×10^{-7}
Am-243 (Sv/a:Bq/m ³)	8.88×10^{-7}
C-14 (Sv/a:Bq/m ³)	1.39×10^{-9}
Cl-36 (Sv/a:Bq/m ³)	8.09×10^{-9}
Cs-135 (Sv/a:Bq/m ³)	1.45×10^{-8}
I-129 (Sv/a:Bq/m ³)	1.29×10^{-7}
Np-237 (Sv/a:Bq/m ³)	2.74×10^{-7}
Pa-231 (Sv/a:Bq/m ³)	2.44×10^{-6}
Pu-239 (Sv/a:Bq/m ³)	9.55×10^{-7}
Pu-240 (Sv/a:Bq/m ³)	9.51×10^{-7}
Pu-242 (Sv/a:Bq/m ³)	9.07×10^{-7}
Ra-226 (Sv/a:Bq/m ³)	3.78×10^{-6}
Se-79 (Sv/a:Bq/m ³)	2.42×10^{-8}
Tc-99 (Sv/a:Bq/m ³)	1.12×10^{-9}
Th-230 (Sv/a:Bq/m ³)	1.08×10^{-6}
U-233 (Sv/a:Bq/m ³)	8.97×10^{-8}
U-234 (Sv/a:Bq/m ³)	8.19×10^{-8}
U-236 (Sv/a:Bq/m ³)	7.67×10^{-8}
U-238 (Sv/a:Bq/m ³)	7.87×10^{-8}

^a Metric tons heavy metal (uranium and other radioactive heavy metal)^b Decay sequence: Am-241, Np-237, U-233^c Decay sequence: Am-243, Pu-239^d Decay sequence: Pu-240, U-236^e Decay sequence: Pu-242, U-238^f Decay sequence: U-234, Th-230, Ra-226

Transport simulation

The flow fields and associated water saturations calculated with TOUGH2 are fed into the FEHM transport model (see above). Contaminant transport is calculated with the particle tracking macro of the FEHM code. Particle

injection takes place in 101 cells in the repository area 320 m above the initial water table. The injection rate is proportional to the near-field release (engineered barrier system release; DOE 2009) shown in Fig. 8. Particle injection starts in the simulation year 300 and ends in the simulation year 1,000,000.

Fig. 6 Maps showing the saturation at the end of the one-year initialisation step at the initial lowermost unsaturated layer and the initial topmost saturated layer for the base case as well as sensitivity

cases with low and high permeabilities; the reference water table is the base-case water table (see text for explanation). The outline of the repository is also shown (solid black line)

Two types of particles are injected. The particles representing aqueous species are subjected to sorption, which takes place only in the single-continuum sub-mesh and matrix continuum of the dual-continuum sub-mesh. The particles representing contaminants irreversibly attached to colloids are subjected to neither sorption nor filtration.

Radioactive dose

The radioactive dose D (Sv/a) is calculated with the biodose conversion factor (BDCF), representing the all-pathway dose (DOE 2007f) to a hypothetical “reasonably maximally

exposed individual” (RMEI). The dose is calculated according to the equation

$$D = \sum X_i B_i \quad (1)$$

where X_i is the concentration (Bq/L) of the radionuclide i in the saturated zone where the depth of the water table below the topographic surface is less than 200 m, and B_i is the BDCF (Sv/a:Bq/L) of the radionuclide i .

The peak dose is the relevant parameter for the various flow fields (Figs. 9 and 10). The reference limits are the US generic regulatory limit (0.15 mSv/a; GAO 2000) or the local limits (0.15 mSv/a < 10,000 years and 1 mSv/a > 10,000 years; NRC 2014).

Fig. 7 Vertical cross section D-D’ (trace in Fig. 2) of the Yucca Mountain model showing the saturation at the end of the one-year initialisation step for the base case (see text for explanation). The water table at the beginning of the initialisation step is also shown (solid black line)

Fig. 8 Annual near-field release (Bq/a) from defective waste containers in the Yucca Mountain repository from year 300 to year 1,000,000 (DOE 2009)

Base case

The topmost layer of the saturated zone usually has the highest concentrations of contaminants (Fig. 11). The dose reaches the 0.15 mSv/a limit in the simulation year 4000 and the 1 mSv/a limit in the simulation year 8100. The maximum peak dose is approximately 4.7 mSv/a towards the end of the simulation period at 1,000,000 a.

Fig. 9 Peak radioactive dose (Sv/a) of the topmost layer of the saturated zone for the base case as well as sensitivity cases with high and low permeabilities from year 1000 to year 1,000,000 (base-case water table). The reference dose is the total “mean” dose of DOE (2009). The US generic regulatory limit (solid black line; equivalent to the local regulatory limit for <10,000 a) and the local regulatory limit for >10,000 a (dotted brown line) are also shown

Sensitivity cases

The sensitivity tests investigate the relationship between mesh discretisation and contaminant migration. In addition, the tests address two of the greatest uncertainties in the Yucca Mountain project (Gelhar 2006):

- the location of the water table;
- the permeabilities of the rocks in the contaminant-transport zone.

The sensitivity case with an initial water table derived by kriging of the measured water level data differs significantly from the base case with an initial water table that corresponds to the modelled “potentiometric surface” of DOE (2007a). This is especially evident in the northern part of the model, where the water table is located more than 400 m below the topographic surface (Fig. 10). In contrast, the peak dose where the water table is less than 200 m below the topographic surface (southern part of the model) plotted versus time is not much different (not shown).

Reducing the permeability expands the time span for reaching the regulatory limits but increases the maximum peak dose towards the end of the simulation period. In contrast, increasing the permeability shortens the time span for reaching the regulatory limits but reduces the maximum peak dose.

In the low-permeability sensitivity case, the 0.15-mSv/a limit is reached in the simulation year 9400, and the 1-mSv/a limit is reached in the year 19,000; the maximum peak dose towards the end of the simulation period is 8.5 mSv/a. In the high-permeability case, the 0.15-mSv/a limit is reached in the year 5000; the maximum peak dose towards the end of the simulation period is 0.53 mSv/a.

Fig. 10 a–i Maps of the topmost layer of the saturated zone with radioactive dose (Sv/a) in the simulation year 4000, 8000 and 1,000,000 for the base-case water table and base-case permeabilities as well as the base-case water table and sensitivity-case permeabilities (low

and high permeabilities). j Map of the topmost layer of the saturated zone with radioactive dose (Sv/a) in the simulation year 1,000,000 for the sensitivity-case water table and base-case permeabilities. The outline of the repository is also shown (solid black line)

Increasing or decreasing the discretisation of the mesh in the unsaturated zone has a minor influence on contaminant migration because transport occurs mainly in one direction (vertical). In contrast, grid geometry has a strong influence in the saturated zone. Due to the restrictions of the one-processor codes FEHM and LaGrit, it is not possible to calculate a grid with a finer discretisation than that of the base case (20 m vertically and 250 m horizontally). Therefore, the reverse procedure is used in order to show the effect of discretisation.

Using a sensitivity-case mesh with 500-m horizontal spacing (instead of 250-m base-case spacing) results in a peak dose of 2 mSv/a at the end of the 1,000,000-year simulation period (not shown). The corresponding base case value (for a grid with 250-m horizontal spacing) is 4.7 mSv/a (see above). Extrapolating this result to a finely discretised mesh with 125-m horizontal spacing implies

that the peak dose would not be larger than the base-case value multiplied by 4.7/2, i.e. ≤ 11 mSv/a.

Summary and conclusion

Calderas with pyroclastic deposits originating from high-viscosity siliceous magma together with deformed pre-eruption country rock constitute extremely heterogeneous geological systems. High-permeability zones alternate with low-permeability zones horizontally over relatively short distances. The conceptual hydrogeological model of DOE (2007a, 2007b) simulates the geological heterogeneity albeit based on relatively little drill hole data (Gelhar 2006).

The 1D contaminant transport model of DOE (2009) translates the geological heterogeneity into statistical parameters. However, probabilistic 1D procedures can hardly reproduce

Fig. 11 Maps of the topmost layer of the saturated zone, 60 m below the topmost layer of the saturated zone and 120 m below the topmost layer of the saturated zone with radioactive dose (Sv/a) for the base case in the simulation years 4000, 8000 and 1,000,000; the reference water table is the base-case water table. The outline of the repository is also shown (solid black line)

the geological variability of the 3D space. Thus, the 1D model may be a very imperfect representation of the geological variability, implying a considerable risk of underestimating the radioactive hazard for the maximally exposed individual. This situation is a particular challenge for the regulating agency. Ambiguities can only be avoided if the biodose conversion factor is linked to the water volume in the model cells, e.g., the 250 x 250 x 20-m cells used in this paper.

The standard procedure for calculating the radioactive dose is using a simulation period of one million years (e.g. SKB 2006; Nykyri et al. 2008; DOE 2009). This long period is due to the long half-life of the major pollutants. It comes as no surprise that the peak radioactive dose calculated with the 3D flow transport model is higher than that calculated with the 1D model towards the end of the simulation period (Fig. 9). The difference may be exacerbated by the fact that the reference 1D model uses a dual-permeability model for the unsaturated zone and a dual-porosity model for the saturated zone. Dual-porosity rock has unconnected matrix elements, as opposed to dual-permeability rock with interconnected matrix elements. Contaminant transport between a fracture and the matrix in dual-porosity rock is possible by diffusion only, not by advection (fluid flow) because the matrix holds only stagnant water. Apart from being unphysical, this model configuration may produce a stronger retention of contaminants in the saturated zone than the alternative with identical physical properties in

the saturated and unsaturated zones. As opposed to dual-permeability systems, dual-porosity systems are extremely difficult to simulate. Large models, such as the one in this paper, would have to be simplified, requiring additional sub-models (Schwartz 2012). It is beyond the scope of this paper to evaluate the possible impact of a dual-porosity concept or mixed dual-porosity/dual-permeability concept.

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References

- Applegate D (2006) The mountain matters. In: Macfarlane AM, Ewing RC (eds) *Uncertainty underground: Yucca Mountain and the Nation's high-level nuclear waste*. MIT Press, Cambridge, Massachusetts, U.S.A., pp 105–130
- DOE (2004) Nuclear Waste Policy as Amended. US Department of Energy
- DOE (2007a) Saturated zone site-scale flow model. US Department of Energy (DOE) MDL-NBS-HS-000011 REV 03

- DOE (2007b) Hydrogeologic framework model for the saturated zone site-scale flow and transport model. US Department of Energy (DOE) MDL-NBS-HS-000024 REV 01
- DOE (2007c) Initial radionuclide inventories. US Department of Energy (DOE) DOC.20070801.0001
- DOE (2007d) Site-scale saturated zone transport. US Department of Energy (DOE) MDL-NBS-HS-000010 REV 03
- DOE (2007e) Calibrated unsaturated zone properties. US Department of Energy (DOE) ANL-NBS-HS-000058 REV 00
- DOE (2007f) Biosphere model report. US Department of Energy (DOE) DOC.20070830.0007
- DOE (2009) Yucca Mountain repository license application safety analysis report. US Department of Energy (DOE) RW-0573 Rev. 1
- GAO (2000) Radiation standards. US General Accounting Office (GAO) GAO/RCED-00-152
- Gelhar LW (2006) Contaminant transport in the saturated zone at Yucca Mountain. In: Macfarlane AM, Ewing RC (eds) *Uncertainty underground: Yucca Mountain and the nation's high-level nuclear waste*. MIT Press, Cambridge, Massachusetts, U.S.A., pp 237–254
- Ho CK, Robinson BA (1998) Flow and transport calculations of Yucca Mountain using TOUGH2 and FEHM. International High-Level Radioactive Waste Management Conference, Las Vegas, U.S.A., 11–14 May 1998
- NRC (2014) Safety evaluation report related to disposal of high-level radioactive wastes in a geologic repository at Yucca Mountain, Nevada, volume 3, Repository safety after permanent closure. US Nuclear Regulatory Commission (NRC) NUREG-1949, Vol. 3
- Nykyri M, Nordman H, Marcos N, Löfman J, Poteri A, Hautajärvi A (2008) Radionuclide release and transport - RNT-2008. Posiva Report 2008–06, Olkiluoto, Finland
- Pan L (2007) WINGRIDDER version 3.0. Lawrence Berkeley National Laboratory. University of California, Berkeley, U.S.A
- Schwartz MO (2012) Modelling radionuclide transport in large fractured-media systems: the example Forsmark, Sweden. *Hydrogeol J* 20: 673–687
- SKB (2006) Long-term safety for KBS-3 repositories at Forsmark and Laxemar - a first evaluation. SKB Technical Report TR-06-09, Stockholm, Sweden
- Zhang K, Wu YS, Pruess K (2008) User's guide for TOUGH2-MP - a massively parallel version of the TOUGH2 code. Report LBNL-315E, Earth Sciences Division, Lawrence Berkeley National Laboratory. University of California, Berkeley, U.S.A.
- Zyvoloski GA, Robinson BA, Dash ZV, Kelkar S, Viswanathan HS, Pawar RJ, Stauffer PH (2015) User manual for the FEHM application version 3.3.0. Los Alamos National Laboratory, Los Alamos, U.S.A.