Chapter 7
Tables

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Part 3

Table 7-1. Summary of Data Tracking Numbers (DTNs) and Q Status of Source Data Used in TSPA-VA Calculations.

Type of Data Used	General Description	DTN	QA Status
Matrix Sorption Distribution Coefficients	Neptunium K_d	LAIT831341AQ96.001	Q
		LA000000000106.001	Q
	Plutonium K_d	LAIT831341AQ96.001	Q
	Uranium K_d	LAIT831341AQ96.001	Q
	All Other K_ds and K_d distributions	MO9807SPATBDOC.000	NQ
Matrix Diffusion Coefficients	Rock-Beaker Matrix Diffusion Laboratory Measurements	LAIT831362AQ95.001	Q
	UFA Matrix Diffusion Laboratory Measurements	LAIT831362AQ95.002	Q
	Matrix Diffusion Distributions	MO9807SPATBDOC.000	NQ
Fracture Aperture	DLS 0+60 to 4+00	GS950508314224.002	Q
	DLS 4+00 to 8+00	GS950808314224.004	Q
	DLS 8+00 to 10+00	GS951108314224.005	Q
	DLS 10+00 to 18+00	GS960408314224.002	Q
	DLS 18+00 to 26+00	GS960608314224.006	Q
	DLS 26+00 to 30+00	GS960608314224.007	Q
	DLS 35+00 to 40+00	GS960808314224.011	Q
	DLS 40+00 to 45+00	GS960708314224.010	Q
	DLS 45+00 to 50+00	GS960808314224.013	Q
	SD-12	SNF29041993002.071	Q
	NRG-7a	SNF29041993002.015	Q
	NRG-7a	SNF29041993002.048	Q
	Air-permeability	GS960908312232.013	Q
	Fracture aperture and distribution	MO9807SPATBDOC.000	NQ
Dispersivity	Distribution of dispersion length scale for fracture and matrix continua.	MO9807SPATBDOC.000	NQ
Aqueous/Colloid Partitioning Coefficient	Distribution of bulk partition coefficient for aqueous plutonium on colloids.	MO9807SPATBDOC.000	NQ

Table 7-2. Summary of Codes, Input/Output Files, and DTNs Associated with Technical Figures. All calculations were performed using a Sun Ultra Sparc computer and UNIX operating system unless otherwise noted.

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-4	One-dimensional dispersion comparison	FEHM V2.00	control.test1 problem1-1.dat control.test2 problem1-2.dat control.test3 problem1-3.dat control.test4 problem1-4.dat control.test5 problem1-5.dat oned24.geom	problem1-1.fin problem1-2.fin problem1-3.fin problem1-4.fin problem1-5.fin	LABR831371 DQ98.001	NQ
7-5	One-dimensional dispersion comparison	FEHM V2.00	control.test1 problem1-1.dat control.test1a problem1-1a.dat control.test1b problem1-1b.dat oned24.geom	problem1-1.fin problem1-1a.fin problem1-1b.fin	LABR831371 DQ98.001	NQ
7-6	One-dimensional solution with matrix diffusion	FEHM v2.00	control.2-1 problem2-1.dat control.2-2 problem2-2.dat control.2-3 problem2-3.dat control.2-4 problem2-5.dat oned24.geom	problem2-1.fin problem2-2.fin problem2-3.fin problem2-4.fin	LABR831371 DQ98.001	NQ
7-8	Two-dimensional dispersion comparison	FEHM v2.00	control.pt1 permc_pt1.dat control.pt2 permc_pt2.dat control.cd cd_pt2.dat twod64x64.geom permconst.ini	permc_pt1.fin permc_pt2.fin cd_pt2.trc	LABR831371 DQ98.001	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-9	Transient flow; water mass flow rates	FEHM v2.00	multiple simulation control file: fehmn.msim.8-31 (change name to fehmn.msim to run) control file: control.ptrk.8-31 (change name to control.ptrk to run) grid file: 2d97.grid fehm .stor file:2dgrid97.stor zone list file: 2dgrid.zone zone list file: flow.zone zone list file: zones.repo main data file: pu1.dat restart file: fl41f.ini macro files: dpdp_lbl_2d.macro rlp6541_2d.macro pres_lbl_2d.macro rock_lbl_2d.macro flnt_infil_2d97f.flow particle tracking macro files: ptrk.pu_base1 ptrk.pu_base2 ptrk.pu_base3 ptrk.pu_base4 ptrk.pu_base5 ptrk.pu_base6 ptrk.pu_base7 ptrk.pu_base8 ptrk.pu_base9 ptrk.pu_base10 post-processing code: process1_fuj	pu.temp.1 pu.temp.2 pu.temp.3 pu.temp.4 pu.temp.5 pu.temp.6 pu.temp.7 pu.temp.8 pu.temp.9 pu.temp.10	LABR831371 DQ98.001	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-10 7-11 7-12	Transient flow; matrix saturations Transient flow; matrix saturations Transient flow; Np mass flux	FEHM v2.00	control file: control.3x data file: fl3x.dat grid file: 2d97.grid fehm .stor file:2dgrid97.stor zone list file:2dgrid.zone zone list file: flow.zone restart file: fl41f.ini macro files: dpdp_lbl_2d.macro rlp6541_2d.macro pres_lbl_2d.macro rock_lbl_2d.macro flnt3x.flow control file: control.flup data file: fl41fup.dat grid file: 2d97.grid fehm .stor file:2dgrid97.stor zone list file:2dgrid.zone zone list file: flow.zone restart file: flp3x.ini macro files: dpdp_lbl_2d.macro rlp6541_2d.macro pres_lbl_2d.macro rock_lbl_2d.macro flnt_infil_2d97f.flow control file:control.p3x data file: flp3x.dat grid file: 2d97.grid fehm .stor file:2dgrid97.stor zone list file:2dgrid.zone zone list file: flow.zone restart file: fl41f.ini macro files: dpdp_lbl_2d.macro rlp6541_2d.macro pres_lbl_2d.macro rock_lbl_2d.macro flntp3x.flow	fl3x.out fl41fup.out flp3x.out	LABR831371 DQ98.001	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-13 7-14 a) and b)	Transient flow; Np mass flux Water table change; mass flux	FEHM v2.00	control file: control.ptrk1 data file: np1.dat grid file: 2d97.grid fehm .stor file:2dgrid97.stor zone list file: 2dgrid.zone zone list file: flow.zone zone list file: zones.repo restart file: flp3x.ini macro files: dpdp_lbl_2d.macro rlp6541_2d.macro pres_lbl_2d.macro rock_lbl_2d.macro flntp3x.flow ptrk.release30k control file: control.ptrk2 data file: np2.dat grid file: 2d97.grid fehm .stor file:2dgrid97.stor zone list file: 2dgrid.zone zone list file: flow.zone zone list file: zones.repo restart file: fl41f.ini macro files: dpdp_lbl_2d.macro rlp6541_2d.macro pres_lbl_2d.macro rock_lbl_2d.macro flnt_infil_2d97f.flow ptrk.release30k control file: control.ptrk3 data file: np1-5000.dat grid file: 2d97.grid fehm .stor file:2dgrid97.stor zone list file: 2dgrid.zone zone list file: flow.zone zone list file: zones.repo restart file: flp3x.ini macro files: dpdp_lbl_2d.macro rlp6541_2d.macro pres_lbl_2d.macro rock_lbl_2d.macro flntp3x.flow ptrk.release30k	np1.out np2.out np1-5000.out np2-jump.out	LABR831371 DQ98.001	NQ
			control file: control.ptrk4 data file: np2-res5k.dat grid file: 2d97.grid fehm .stor file:2dgrid97.stor zone list file: 2dgrid.zone zone list file: flow.zone zone list file: zones.repo restart file: np1-5000.ini macro files: dpdp_lbl_2d.macro rlp6541_2d.macro pres_lbl_2d.macro rock_lbl_2d.macro flnt_infil_2d97f.flow ptrk.rel30k-res5k			

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-15 a) and b)	Water table change; accumulative breakthrough	FEHM v2.00	control file: control.ptrk.8-37 (change name to control.ptrk to run) grid file: 2d97.grid fehm .stor file:2dgrid97.stor zone list file: 2dgrid821.zone zone list file: flow821.zone zone list file: zones.repo main data file: np1.dat.8-37 (change name to np1.dat to run) restart file: fl41f821.ini macro files: dpdp_lbl_2d.macro rip6541_2d.macro pres_lbl_2d.macro rock_lbl_2d.macro flnt_infil_2d97f.flow particle tracking macro files: ptrk.np_base1 ptrk.np_base2 ptrk.np_base3 ptrk.np_base4 ptrk.np_base5 ptrk.np_base6 ptrk.np_base7 ptrk.np_base8 ptrk.np_base9 ptrk.np_base10 post-processing code: process1_fuj	np.temp1	LABR831371 DQ98.001	NQ
7-18	Radionuclide release from NW repository region	RIP 5.19.01 FEHMN 1.0	FEHMN input[1] R1PULSE.RP	R1PULSE.RP (also .BAK, .BPF, .BSR, .BTF, .BTR, .OUT)	MO9807MW DRIP00.000	NQ
7-19	Radionuclide release from NE repository region	RIP 5.19.01 FEHMN 1.0	FEHMN input[1] R2PULSE.RP	R2PULSE.RP (also .BAK, .BPF, .BSR, .BTF, .BTR, .OUT)	MO9807MW DRIP00.000	NQ
7-20	Radionuclide release from CC repository region	RIP 5.19.01 FEHMN 1.0	FEHMN input[1] R3PULSE.RP	R3PULSE.RP (also .BAK, .BPF, .BSR, .BTF, .BTR, .OUT)	MO9807MW DRIP00.000	NQ
7-21	Radionuclide release from SE repository region	RIP 5.19.01 FEHMN 1.0	FEHMN input[1] R4PULSE.RP	R4PULSE.RP (also .BAK, .BPF, .BSR, .BTF, .BTR, .OUT)	MO9807MW DRIP00.000	NQ
7-22	Radionuclide release from SC repository region	RIP 5.19.01 FEHMN 1.0	FEHMN input[1] R5PULSE.RP	R5PULSE.RP (also .BAK, .BPF, .BSR, .BTF, .BTR, .OUT)	MO9807MW DRIP00.000	NQ
7-23	Radionuclide release from SW repository region	RIP 5.19.01 FEHMN 1.0	FEHMN input[1] R6PULSE.RP	R6PULSE.RP (also .BAK, .BPF, .BSR, .BTF, .BTR, .OUT)	MO9807MW DRIP00.000	NQ
7-24	Radionuclide release from all repository regions	RIP 5.19.01 FEHMN 1.0	FEHMN input[1] PULSETOT.RP	PULSETOT.RP (also .BAK, .BPF, .BSR, .BTF, .BTR, .OUT)	MO9807MW DRIP00.000	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-27[2] 7-28[2]	3-D transport, Flint (96) infiltration, different matrix diffusion coefficients and a constant release period of 1,000 years.	FEHMN: xfehmn96 0507	/base3d/simus/np/contrelease/R1000y/ mdif1e-11/kd0.0_1000.trn mdif1e-12kd0.0_1000.trn mdif1e-13/kd0.0_1000.trn mdif1e-14/kd0.0_1000.trn mdif1e-30/kd0.0_1000.trn fehmn.files ptrk	/base3d/simus/np/contrelease/R1000y/ mdif1e-11/kd0.0_1000.out mdif1e-12kd0.0_1000.out mdif1e-13/kd0.0_1000.out mdif1e-14/kd0.0_1000.out mdif1e-30/kd0.0_1000.out	MO9807MW DOSEHM.000	NQ
7-29[2] 7-30[2]	2-D transport, Flint(96) infiltration, different matrix diffusion coefficients and a release period of 1,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/R1000y/ mdif1e-11/kd0.0_1000.trn mdif1e-12kd0.0_1000.trn mdif1e-13/kd0.0_1000.trn mdif1e-14/kd0.0_1000.trn mdif1e-30/kd0.0_1000.trn fehmn.files ptrk	/base2d/simus/np/flint_i/R1000y / mdif1e-11/kd0.0_1000.out mdif1e-12kd0.0_1000.out mdif1e-13/kd0.0_1000.out mdif1e-14/kd0.0_1000.out mdif1e-30/kd0.0_1000.out	MO9807MW DOSEHM.000	NQ
7-33[2] 7-34[2]	2-D transport, Flint(96) infiltration, different matrix diffusion coefficients and a release period of 5,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/R5000y/ mdif1e-11/kd0.0_5000.trn mdif1e-12kd0.0_5000.trn mdif1e-13/kd0.0_5000.trn mdif1e-14/kd0.0_5000.trn mdif1e-30/kd0.0_5000.trn fehmn.files ptrk	/base2d/simus/np/flint_i/R5000y / mdif1e-11/kd0.0_5000.out mdif1e-12kd0.0_5000.out mdif1e-13/kd0.0_5000.out mdif1e-14/kd0.0_5000.out mdif1e-30/kd0.0_5000.out	MO9807MW DOSEHM.000	NQ
7-35[2] 7-36[2]	2-D transport, Flint(96) infiltration, different matrix diffusion coefficients and a release period of 10, 000 years	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/R10000y/ mdif1e-11/kd0.0_10000.trn mdif1e-12kd0.0_10000.trn mdif1e-13/kd0.0_10000.trn mdif1e-14/kd0.0_10000.trn mdif1e-30/kd0.0_10000.trn fehmn.files ptrk	/base2d/simus/np/flint_i/R10000y/ mdif1e-11/kd0.0_10000.out mdif1e-12kd0.0_10000.out mdif1e-13/kd0.0_10000.out mdif1e-14/kd0.0_10000.out mdif1e-30/kd0.0_10000.out	MO9807MW DOSEHM.000	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-31[2] 7-32[2]	Plots of peak mass flow rate and peak mass arriving time vs. matrix diffusion coefficient, respectively, for different release periods.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/R*y/ midf1e-11/kd0.0_*..trn midf1e-12/kd0.0_*..trn midf1e-13/kd0.0_*..trn midf1e-14/kd0.0_*..trn	/base2d/simus/np/flint_i/peak_time	MO9807MW DOSEHM.000	NQ
7-37[2] 7-38[2]	2-D transport, 1/3 of Flint(96) infiltration, different matrix diffusion coefficients and a release period of 1,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i3/R1000y/ mdif1e-11/kd0.0_1000.trn mdif1e-12kd0.0_1000.trn mdif1e-13/kd0.0_1000.trn mdif1e-14/kd0.0_1000.trn mdif1e-30/kd0.0_1000.trn fehmn.files ptrk	/base2d/simus/np/flint_i3/R1000y/ mdif1e-11/kd0.0_1000.out mdif1e-12kd0.0_1000.out mdif1e-13/kd0.0_1000.out mdif1e-14/kd0.0_1000.out mdif1e-30/kd0.0_1000.out	MO9807MW DOSEHM.000	NQ
7-39[2] 7-40[2]	Plots of peak mass flow rate and peak mass arriving time vs. matrix diffusion coefficient, respectively, for different release periods under 1/3 of the Flint (96) infiltration rate.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i3/R*y/ midf1e-11/kd0.0_*..trn midf1e-12/kd0.0_*..trn midf1e-13/kd0.0_*..trn midf1e-14/kd0.0_*..trn	/base2d/simus/np/flint_i3/peak_time	MO9807MW DOSEHM.000	NQ
7-41[2] 7-42[2]	2-D transport, 3 times of Flint(96) infiltration, different matrix diffusion coefficients and a release period of 1,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_ix3/R1000y/ mdif1e-11/kd0.0_1000.trn mdif1e-12kd0.0_1000.trn mdif1e-13/kd0.0_1000.trn mdif1e-14/kd0.0_1000.trn mdif1e-30/kd0.0_1000.trn fehmn.files ptrk	/base2d/simus/np/flint_ix3/R1000y/ mdif1e-11/kd0.0_1000.out mdif1e-12kd0.0_1000.out mdif1e-13/kd0.0_1000.out mdif1e-14/kd0.0_1000.out mdif1e-30/kd0.0_1000.out	MO9807MW DOSEHM.000	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-43[2] 7-44[2]	Plots of peak mass flow rate and peak mass arriving time vs. matrix diffusion coefficient, respectively, for different release periods under 3 times of the Flint (96) infiltration rate.	FEHMN: xfehm960507	/base2d/simus/np/flint_ix3/ R1000y/mdif1e*/kd0.0_1000.trn R5000y/mdif1e*/kd0.0_5000.trn R10000y/mdif1e*/kd0.0_10000.trn	/base2d/simus/np/flint_ix3/peak_time	MO9807MW DOSEHM.000	NQ
7-45[2] 7-46[2]	2-D transport, Flint(96) infiltration, different matrix adsorption coefficients, no matrix diffusion, and a release period of 1,000 years.	FEHMN: xfehmn960507	/base2d/simus/np/flint_i/R1000y/ mdif1e-30/kd0.0_1000.trn mdif1e-30kd1.0_1000.trn mdif1e-30/kd2.5_1000.trn mdif1e-30/kd10.0_1000.trn mdif1e-30/kd50.0_1000.trn mdif1e-30/kd100.0_1000.trn fehmn.files ptrk	/base2d/simus/np/flint_i/R1000y/ mdif1e-30/kd0.0_1000.out mdif1e-30kd1.0_1000.out mdif1e-30/kd2.5_1000.out mdif1e-30/kd10.0_1000.out mdif1e-30/kd50.0_1000.out mdif1e-30/kd100.0_1000.out	MO9807MW DOSEHM.000	NQ
7-47[2] 7-48[2]	2-D transport, Flint(96) infiltration, different matrix adsorption coefficients, no matrix diffusion, and a release period of 10,000 years.	FEHMN: xfehmn960507	/base2d/simus/np/flint_i/R10000y/ mdif1e-30/kd0.0_10000.trn mdif1e-30kd1.0_10000.trn mdif1e-30/kd2.5_10000.trn mdif1e-30/kd10.0_10000.trn mdif1e-30/kd50.0_10000.trn mdif1e-30/kd100.0_10000.trn fehmn.files ptrk	/base2d/simus/np/flint_i/R10000y/ mdif1e-30/kd0.0_10000.out mdif1e-30kd1.0_10000.out mdif1e-30/kd2.5_10000.out mdif1e-30/kd10.0_10000.out mdif1e-30/kd50.0_10000.out mdif1e-30/kd100.0_10000.out	MO9807MW DOSEHM.000	NQ
7-49[2] 7-50[2]	Plots of peak mass flow rate and peak mass arriving time vs. matrix adsorption coefficient, respectively, for different release periods under the Flint (96) infiltration rate.	FEHMN: xfehmn960507	/base2d/simus/np/flint_i/ R1000y/mdif1E-30/kd*_1000.trn R5000y/mdif1E-30/kd*_1000.trn R10000y/mdif1E-30/kd*_1000.trn	/base2d/simus/np/flint_i/ R1000y/mdif1E-30/pkmasstime R5000y/mdif1E-30/pkmasstime R10000y/mdif1E-30/pkmasstime	MO9807MW DOSEHM.000	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-51[2] 7-52[2]	2-D transport, Flint(96) infiltration, different fracture surface retardation coefficients, no matrix diffusion or matrix adsorption, a release period of 1,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/R1000y/mdif 1E-30/kd0.0_1000_ka/ ka0.0.trn ka50.trn ka100.trn ka500.trn ka100.trn fehmn.files ptrk	/base2d/simus/np/fli nt_i/R1000y/mdif1E-30/kd0.0_1000_ka/ ka0.0.out ka50.out ka100.out ka500.out ka100.out	MO9807MW DOSEHM.000	NQ
7-53[2] 7-54[2]	2-D transport Flint(96) infiltration, different fracture surface retardation coefficients, no matrix diffusion or matrix adsorption, a release period of 10,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/R10000y/md if1E-30/kd0.0_10000_ka/ ka0.0.trn ka50.trn ka100.trn ka500.trn ka100.trn fehmn.files ptrk	/base2d/simus/np/fli nt_i/R10000y/mdif1 E- 30/kd0.0_10000_ka/ ka0.0.out ka50.out ka100.out ka500.out ka100.out	MO9807MWD 0SEHM.000	NQ
7-55[2] 7-56[2]	Plots of peak mass flow rate and peak mass arriving time vs. fracture surface retardation factors, respectively, for different release periods under the Flint (96) infiltration rate.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/ R1000y/mdif1E- 30/kd0.0_1000_ka/ka*.trn R5000y/mdif1E- 30/kd0.0_5000_ka/ka*.trn R10000y/mdif1E- 30/kd0.0_10000_ka/ka*.trn	/base2d/simus/np/fli nt_i/ R1000y/mdif1E- 30/kd0.0_1000_ka/p ktime R5000y/mdif1E- 30/kd0.0_1000_ka/p ktime R10000y/mdif1E- 30/kd0.0_1000_ka/p ktime	MO9807MW DOSEHM.000	NQ
7-57[2] 7-58[2]	The combined effects of matrix diffusion and matrix adsorption. Flint (96) infiltration, matrix kd=0.5 in CHnz, different matrix diffusion coefficients, a release period of 1,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/R1000y/ mdif1E-11/kd0.5_100.0trn mdif1E-12/kd0.5_100.0trn mdif1E-13/kd0.5_1000.trn mdif1.E14/kd0.5_1000.trn mdif1E-30/kd0.5_1000.trn	/base2d/simus/np/fli nt_i/R1000y/ mdif1E- 11/kd0.5_1000.out mdif1E- 12/kd0.5_1000.out mdif1E- 13/kd0.5_1000.out mdif1.E- 14/kd0.5_1000.out mdif1E- 30/kd0.5_1000.out	MO9807MW DOSEHM.000	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-59[2] 7-60[2]	The combined effects of matrix diffusion and matrix adsorption. Flint (96) infiltration, matrix kd=2.5 in CHnz, different matrix diffusion coefficients, a release period of 1,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/R1000y/ mdif1E-11/kd2.5_100.0trn mdif1E-12/kd2.5_100.0trn mdif1E-13/kd2.5_1000.trn mdif1.E14/kd2.5_1000.trn mdif1E-30/kd2.5_1000.trn	/base2d/simus/np/flint_i/R1000y/ mdif1E-11/kd2.5_1000.out mdif1E-12/kd2.5_1000.out mdif1E-13/kd2.5_1000.out mdif1.E-14/kd2.5_1000.out mdif1E-30/kd2.5_1000.out	MO9807MW DOSEHM.000	NQ
7-61[2] 7-62[2]	The combined effects of matrix diffusion and matrix adsorption. Flint (96) infiltration, matrix kd=10 in CHnz, different matrix diffusion coefficients, a release period of 1,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/R1000y/ mdif1E-11/kd10_100.0trn mdif1E-12/kd10_100.0trn mdif1E-13/kd10_1000.trn mdif1.E14/kd10_1000.trn mdif1E-30/kd10_1000.trn	/base2d/simus/np/flint_i/R1000y/ mdif1E-11/kd10_1000.out mdif1E-12/kd10_1000.out mdif1E-13/kd10_1000.out mdif1.E-14/kd10_1000.out mdif1E-30/kd10_1000.out	MO9807MW DOSEHM.000	NQ
7-63[2] 7-64[2]	The combined effects of matrix diffusion and matrix adsorption. Flint (96) infiltration, matrix kd=2.5 in CHnz, different matrix diffusion coefficients, a release period of 10,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/R10000y/ mdif1E-11/kd2.5_1000.0trn mdif1E-12/kd2.5_1000.0trn mdif1E-13/kd2.5_10000.trn mdif1.E14/kd2.5_10000.trn mdif1E-30/kd2.5_10000.trn	/base2d/simus/np/flint_i/R10000y/ mdif1E-11/kd2.5_10000.out mdif1E-12/kd2.5_10000.out mdif1E-13/kd2.5_10000.out mdif1.E-14/kd2.5_10000.out mdif1E-30/kd2.5_10000.out	MO9807MW DOSEHM.000	NQ
7-65[2] 7-66[2]	Plots of peak mass flow rate and peak mass arriving time vs. matrix adsorption coefficient under the condition of matrix diffusion coefficient of 1.E-11 m^2/sec, respectively. The Flint (96) infiltration rate was applied. Different release periods.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/ R1000y/mdif1E-11/kd*_1000.trn R5000y/mdif1E-11/kd*_5000.trn R10000y/mdif1E-11/kd*_10000.trn	/base2d/simus/np/flint_i/ R1000y/mdif1E-11/pktime R5000y/mdif1E-11/pktime R10000y/mdif1E-1/pktime	MO9807MW DOSEHM.000	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-67[2] 7-68[2]	The combined effects of matrix diffusion and matrix adsorption. 1/3 of Flint (96) infiltration, matrix kd=2.5 in CHnz, different matrix diffusion coefficients, a release period of 1,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i3/R1000y/ mdif1E-11/kd2.5_100.0trn mdif1E-12/kd2.5_100.0trn mdif1E-13/kd2.5_1000.trn mdif1.E14/kd2.5_1000.trn mdif1E-30/kd2.5_1000.trn	/base2d/simus/np/flint_i3/R1000y/ mdif1E-11/kd2.5_1000.out mdif1E-12/kd2.5_1000.out mdif1E-13/kd2.5_1000.out mdif1.E-14/kd2.5_1000.out mdif1E-30/kd2.5_1000.out	MO9807MW DOSEHM.000	NQ
7-69[2] 7-70[2]	The combined effects of matrix diffusion and matrix adsorption. 1/3 of Flint (96) infiltration, matrix kd=10 in CHnz, different matrix diffusion coefficients, a release period of 1,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i3/R1000y/ mdif1E-11/kd10_100.0trn mdif1E-12/kd10_100.0trn mdif1E-13/kd10_1000.trn mdif1.E14/kd10_1000.trn mdif1E-30/kd10_1000.trn	/base2d/simus/np/flint_i3/R1000y/ mdif1E-11/kd10_1000.out mdif1E-12/kd10_1000.out mdif1E-13/kd10_1000.out mdif1.E-14/kd10_1000.out mdif1E-30/kd10_1000.out	MO9807MW DOSEHM.000	NQ
7-71[2] 7-72[2]	Plots of peak mass flow rate and peak mass arriving time vs. matrix adsorption coefficient under the condition of matrix diffusion coefficient of 1.E-11 m^2/sec, respectively. 1/3 of Flint (96) infiltration rate, different release periods.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i3/ R1000y/mdif1E-11/kd*_1000.trn R5000y/mdif1E-11/kd*_5000.trn R10000y/mdif1E-11/kd*_10000.trn	/base2d/simus/np/flint_i3/ R1000y/mdif1E-11/pktime R5000y/mdif1E-11/pktime R10000y/mdif1E-1/pktime	MO9807MW DOSEHM.000	NQ
7-73[2] 7-74[2]	The combined effects of matrix diffusion and matrix adsorption. 3 times of Flint (96) infiltration, matrix kd=2.5 in CHnz, different matrix diffusion coefficients, a release period of 1,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_ix3/R1000y/ mdif1E-11/kd2.5_100.0trn mdif1E-12/kd2.5_100.0trn mdif1E-13/kd2.5_1000.trn mdif1.E14/kd2.5_1000.trn mdif1E-30/kd2.5_1000.trn	/base2d/simus/np/flint_ix3/R1000y/ mdif1E-11/kd2.5_1000.out mdif1E-12/kd2.5_1000.out mdif1E-13/kd2.5_1000.out mdif1.E-14/kd2.5_1000.out mdif1E-30/kd2.5_1000.out	MO9807MW DOSEHM.000	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-75[2] 7-76[2]	The combined effects of matrix diffusion and matrix adsorption. 3 times of Flint (96) infiltration, matrix kd=10 in CHnz, different matrix diffusion coefficients, a release period of 10,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_ix3/R1000y/ mdif1E-11/kd10_10000.trn mdif1E-12/kd10_10000.trn mdif1E-13/kd10_10000.trn mdif1.E14/kd10_10000.trn mdif1E-30/kd10_10000.trn	/base2d/simus/np/flint_ix3/R1000y/ mdif1E-11/kd10_10000.out mdif1E-12/kd10_10000.out mdif1E-13/kd10_10000.out mdif1.E-14/kd10_10000.out mdif1E-30/kd10_10000.out	MO9807MW DOSEHM.000	NQ
7-77[2] 7-78[2]	Plots of peak mass flow rate and peak mass arriving time vs. matrix adsorption coefficient under the condition of matrix diffusion coefficient of 1.E-11 m^2/sec, respectively. 3 times of Flint (96) infiltration rate, different release periods.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_ix3/ R1000y/mdif1E-11/kd*_1000.trn R5000y/mdif1E-11/kd*_5000.trn R10000y/mdif1E-11/kd*_10000.trn	/base2d/simus/np/flint_ix3/ R1000y/mdif1E-11/pktime R5000y/mdif1E-11/pktime R10000y/mdif1E-1/pktime	MO9807MW DOSEHM.000	NQ
7-79[2]	Comparison of rock parameters on the influence of radionuclide transport in the UZ. Rock parameter set was from LANL milestone (Robinson, et. Al., 1997) Table 15-3. Different combinations of transport parameters were tested. Flint (96) infiltration map was used. Source release period was 5,000 years.	FEHMN: xfehmn96 0507	/base2d/simus/np/flint_i/R5000y/ mdif1E-30/kd0.0_5000.trn mdif1E-11/kd0.0_5000.trn mdif1E-30/kd2.5_5000.trn mdif1E-11/kd2.5_5000.trn	/base2d/simus/np/flint_i/R5000y/ mdif1E-30/kd0.0_5000.out mdif1E-11/kd0.0_5000.out mdif1E-30/kd2.5_5000.out mdif1E-11/kd2.5_5000.out	MO9807MW DOSEHM.000	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-80[2]	Comparison of rock parameters on the influence of radionuclide transport in the UZ. Rock parameter set was from LANL milestone (Robinson, et. Al., 1995). Combinations of transport parameters were tested. Flint (96) average infiltration was used. Source release period was 5,000 years.	FEHMN: xfehmn96 0507	/base96/inf_4/contrelease/simus/np/R5000y mdif1E-30/kd0.0_5000.trn mdif1E-11/kd0.0_5000.trn mdif1E-30/kd2.5_5000.trn mdif1E-11/kd2.5_500.0trn	/base96/inf_4/contrelease/simus/np/R5000y mdif1E-30/kd0.0_5000.out mdif1E-11/kd0.0_5000.out mdif1E-30/kd2.5_5000.out mdif1E-11/kd2.5_500.out	MO9807MW DOSEHM.000	NQ
7-81[3] 7-82[3]	Long term average, no matrix diffusion, mean alpha model for Tc	FEHMN: xfehmn97 1001p	/lta/mdif1.E-30/ meankd.trn ptrk fehmn.files[5]	/lta/mdif1.E-30/ meankd.out spec_4	MO9807MW DOSEHM.000	NQ
	Long term average, D_f=3.2E-11 m^2/sec, mean alpha model for Tc	FEHMN: xfehmn97 1001p	/lta/mean_mdif/ meankd.trn ptrk.mean fehmn.files[5]	/lta/mean_mdif/ mean.out_mean spec_4_mean		
	Present day infiltration, no matrix diffusion, mean alpha model for Tc	FEHMN: xfehmn97 1001p	/present/mean_mdif/ meankd.trn ptrk.mean fehmn.files[4]	/present/mean_mdif/ meankd.out spec_3		
	Present day infiltration, D_f=3.2E-11 m^2/sec, mean alpha model for Tc	FEHMN: xfehmn97 1001p	/present/mean_mdif/ meankd.trn ptrk.mean fehmn.files[4]	/present/mean_mdif/ meankd.out spec_4		
	Super pluvial, no matrix diffusion, mean alpha model for Tc	FEHMN: xfehmn97 1001p	/sp/mean_mdif/ meankd.trn ptrk.mean fehmn.files[6]	/sp/mean_mdif/ meankd.out spec_3		
	Super pluvial, D_f=3.2E-11 m^2/sec, mean alpha model for Tc	FEHMN: xfehmn97 1001p	/sp/mean_mdif/ meankd.trn ptrk.mean fehmn.files[6]	/sp/mean_mdif/ meankd.out spec_4		

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-83[3] 7-84[3]	Long term average, mean kd, D_f=1.6E-10 m^2/sec, mean alpha model for Np	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Mean.trn, Ptrk.mean Fehmn.files[5]	/lta/Mean_mdif/ Mean.out_mean Spec_1_mean	MO9807MW DOSEHM.000	NQ
	Present day infiltration, mean kd, D_f=1.6E-10 m^2/sec, mean alpha model for Np	FEHMN: xfehmn97 1001p	/present/mean_dif/ meankd.trn ptrk.mean fehmn.,files[3]	/present/mean_mdif/ meankd.out spec_1		
	Super pluvial infiltration, mean. kd, D_f=1.6E-10 m^2/sec, mean alpha model for Np	FEHMN: xfehmn97 1001p	/sp/mean_mdif/ meankd.trn ptrk.mean fehmn.files[6]	/sp/mean_mdif/ meankd.out spec_1		
7-85[3] 7-86[3]	Long term average, min. kd, no matrix diffusion, mean alpha model for Np	FEHMN: xfehmn97 1001p	/lta/Mdif1E-30/ Mimkd.trn, ptrk, fehm.files[5]	/lta/Mdif1E-30/ Mimkd.out, spec_1	MO9807MW DOSEHM.000	NQ
	Long term average, mean kd, no matrix diffusion, mean alpha model for Np	FEHMN: xfehmn97 1001p	/lta/Mdif1E-30/ Meankd.trn, ptrk, fehmn.files[5]	/lta/Mdif1E-30/ Meankd.out, spec_1		
	Long term average, max. kd, no matrix diffusion, mean alpha model for Np	FEHMN: xfehmn97 1001p	/lta/Mdif1E-30/ Maxkd.trn, ptrk, fehmn.files[5]	/lta/Mdif1E-30/ Maxkd.out, spec_1		
	Long term average, min kd, D_f=1.6E-10 m^2/sec. mean alpha model for Np	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Mimkd.trn,, ptrk, fehmn.files[5]	/lta/Mean_mdif/ Mimkd.out, spec_1		
	Long term average, mean kd, D_f=1.6E-10 m^2/sec, mean alpha model for Np	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Mean.trn, Ptrk.mean Fehmn.files[5]	/lta/Mean_mdif/ Mean.out_mean Spec_1_mean		
	Long term average, max kd, D_f=1.6E-10 m^2/sec, mean alpha model for Np	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Maxkd.trn Ptrk Fehmn.files[5]	/lta/Mean_mdiif/ Maxkd.out Spec_1		

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-87[3] 7-88[3]	Long term average, mean kd, mean ks, D_f=1.6E-10 m^2/sec, mean alpha model for Pu	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Mean.trn, Ptrk.mean Fehmn.files[5]	/lta/Mean_mdif/ Mean.out_mean Spec_2_mean	MO9807MW DOSEHM.000	NQ
	Present day infiltration, mena kd, mean kc, D_f=1.6E-10 m^2/sec, mean alpha model for Pu	FEHMN: xfehmn97 1001p	/present/mean_mdif/ meankd.trn ptrk.mean fehmn.files[4]	/present/mean_mdif/ meankd.out spec_2		
	Super pluvial, mean kd, mean kc, D_f=1.6E-10 m^2/sec, mean alpha model for Pu	FEHMN: xfehmn97 1001p	/sp/mean_mdif/ meankd.trn ptrk.mean fehmn.files[6]	/sp/mean_mdif/ meankd.out spec_2		
7-89[3] 7-90[3]	Long term average, min. kd, mean kc, no matrix diffusion, mean alpha model for Pu	FEHMN: xfehmn97 1001p	/lta/mdif1E-30/ Mimkd.trn, ptrk, fehm.files[5]	/lta/mdif1E-30/ Mimkd.out, spec_2	MO9807MW DOSEHM.000	NQ
	Long term average, mean kd, mean kc, no matrix diffusion, mean alpha model for Pu	FEHMN: xfehmn97 1001p	/lta/Mdif1E-30/ Meankd.trn, ptrk, fehmn.files[5]	/lta/Mdif1E-30/ Meankd.out, spec_2		
	Long term average, max. kd, mean kc, no matrix diffusion, mean alpha model for Pu	FEHMN: xfehmn97 1001p	/lta/Mdif1E-30/ Maxkd.trn, ptrk, fehmn.files[5]	/lta/Mdif1E-30/ Maxkd.out, spec_2		
	Long term average, min kd, mean kc, D_f=1.6E-10 m^2/ sec. mean alpha model for Pu	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Mimkd.trn, ptrk, fehmn.files[5]	/lta/Mean_mdif/ Mimkd.out, spec_2		

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
	Long term average, mean kd, mean ks, D_f=1.6E-10 m^2/sec, mean alpha model for Pu	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Mean.trn, Ptrk.mean Fehmn.files[5]	/lta/Mean_mdif/ Mean.out_mean Spec_2_mean		
	Long term average, max kd, mean kc, D_f=1.6E-10 m^2/sec, mean alpha model for Pu	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Maxkd.trn Ptrk Fehmn.files[5]	/lta/Mean_mdif/ Maxkd.out Spec_2		
7-91[3] 7-92[3]	Long term average, mean kd, mean ks, D_f=1.6E-10 m^2/sec, mean alpha model for Pu	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Mean.trn, Ptrk.mean Fehmn.files[5]	/lta/Mean_mdif/ Mean.out_mean Spec_2_mean	MO9807MW DOSEHM.000	NQ
	Long term average, mean kd, max. kc=10, D_f=1.6E-10 m^2/sec, mean alpha model for Pu	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Mean.trn, Ptrk.kcmax Fehmn.files[5]	/lta/Mean_mdif/ Mean.out Spec_2_kcmax		
	Long term average, mean kd, no ks, D_f=1.6E-10 m^2/sec, mean alpha model for Pu	FEHMN: xfehmn97 1001p	/lta/mean_mdif/ mean.trn, ptrk.meankd0kc pehmn.files[5]	/lta/mean_mdif/ mean.out_meankd0 kc eaeipu_meankd0kc		
7-93[3] 7-94[3]	Long term average, mean kd, D_f=1.6E-10 m^2/sec, mean permeability dkm weeps model for Np	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Mean.trn, Ptrk.mean Fehmn.files[7]	/lta/Mean_mdif/ Mean.out_mean Spec_1_mean	MO9807MW DOSEHM.000	NQ
	Long term average, D_f=3.2E-11 m^2/sec, mean permeability dkm weeps model for Tc	FEHMN: xfehmn97 1001p	/lta/mean_mdif/ meankd.trn ptrk.mean fehmn.files[7]	/lta/mean_mdif/ mean.out_mean spec_4_mean		

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
	Long term average, mean kd, mean kc, D_f=1.6E-10 m^2/sec, mean permeability dkm weeps model for Pu	FEHMN: xfehmn97 1001p	/lta/Mean_mdif/ Meankd.trn Ptrk.mean Fehmn.files[7]	/lta/Mean_mdiif/ Meankd.out Spec_2_mean		
7-95[3] 7-96[3]	Long term average infiltration, kd was turned on only in one unit at a time. Mean alpha model and constant release over 10,000 years at the repository	FEHMN: xfehmn97 1001p	/trans/base97/base3d/base_tspa/EXDKM/EaEi/step_noxfm/R10000/lta/mdif1.E-10/ zkd0vkd0dkd0_np.trn zkd4vkd0dkd0_np.trn zkd0vkd1dkd0_np.trn zkd0vkd0dkd1_np.trn zkd4vkd1dkd1_np.trn fehmn.files ptrk[5]	/base3d/base_tspa/EXDKM/EaEi/step_noxfm/R10000/lta/mdif1.E-10/ zkd0vkd0dkd0_np.fin.output zkd4vkd0dkd0_np..fin.output zkd0vkd1dkd0_np.fin.output zkd0vkd0dkd1_np.fin.output zkd4vkd1dkd1_np.fin.output	MO9807MWDOSEHM.000	NQ
7-97[3] 7-98[3]	Long term average infiltration, no adsorption, no matrix diffusion, but with different fracture dispersivity for the mean alpha model.	FEHMN: xfehmn97 1001p	/trans/base97/base3d/base_tspa/EXDKM/EaEi /pulse/nf/lta/mdif1.E-30/ zkd0vkd0dkd0disp15.trn zkd0vkd0dkd0disp25.trn zkd0vkd0dkd0disp50.trn zkd0vkd0dkd0disp75.trn zkd0vkd0dkd0..trn fehmn.files ptrk[5]	/base3d/base_tspa/EXDKM/EaEi/pulse/nf/lta/mdif1.E-30 zkd0vkd0dkd0disp15.fin.output zkd0vkd0dkd0disp25.fin.output zkd0vkd0dkd0disp50.fin.output zkd0vkd0dkd0disp75.fin.output zkd0vkd0dkd0..fin.output	MO9807MWDOSEHM.000	NQ
7-99	Travel times from the potential repository to the water table; nondiffusing, nonsorbing tracers	FEHM v2.00	fehmn.msim.cc fehmn.msim.ne fehmn.msim.nw fehmn.msim.sc fehmn.msim.se fehmn.msim.sw control.base base1.dat fmQb.dpdp fmQb.grid fmQb.rock fmQb.stor fmQb.zone fmQb.zone6b fmmnaqbf2master.ini.Z repo.cc repo.ne repo.nw repo.sc repo.se repo.sw ptrk_file ptrk.partial.water[5]	final_times.lta.cc final_times.lta.ne final_times.lta.nw final_times.lta.sc final_times.lta.se final_times.lta.sw	LABR831371DQ98.001	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-100	Travel times from the potential repository to the water table; Pu	FEHM v2.00	fehmn.msim.cc fehmn.msim.ne fehmn.msim.nw fehmn.msim.sc fehmn.msim.se fehmn.msim.sw control.base base1.dat fmQb.dpdp fmQb.grid fmQb.rock fmQb.stor fmQb.zone fmQb.zone6b fmmnaqbf2master.ini.Z repo.cc repo.ne repo.nw repo.sc repo.se repo.sw ptrk_file ptrk.partial.water[5]	final_times.pu.lta.cc final_times.pu.lta.ne final_times.pu.lta.nw final_times.pu.lta.sc final_times.pu.lta.se final_times.pu.lta.sw	LABR831371D Q98.001	NQ
7-101	Transport pathways from the potential repository to the water table	FEHM v2.00	fehmn.msim.cc fehmn.msim.ne fehmn.msim.nw fehmn.msim.sc fehmn.msim.se fehmn.msim.sw control.base base1.dat fmQb.dpdp fmQb.grid fmQb.rock fmQb.stor fmQb.zone fmQb.zone6b fmmnaqbf2master.ini.Z repo.cc repo.ne repo.nw repo.sc repo.se repo.sw ptrk_file ptrk.partial.pu[5]	final_results.lta.cc final_results.lta.ne final_results.lta.nw final_results.lta.sc final_results.lta.se final_results.lta.sw	LABR831371D Q98.001	NQ
7-102 7-103	Np speciation in J-13 water at 25 C Np fraction as a cation versus temperature and fluid composition	FEHM v2.00	script file: ph_script (this file runs FEHMN multiple times with different pHs to obtain the speciation information necessary for Figures 76 and 77 control file: fehmn.files	phout3 phout4 phout5 phout6 phout7 phout8 phout9 phout10	LABR831371D Q98.001	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-104	Np Kd as a function of Na^+ concentration	FEHM v2.00	executable file: simplesolve.f (solves the ion exchange reaction between zeolites, sodium, and 237-Np in a batch system) input files: nap002.in nap005.in nap01.in nap03.in nap1.in (Each input file contains a different value for sodium concentration, the x-axis of the figure. For example, nap002.in contains a sodium concentration of 0.002 mol/L. Note that the initial 237-Np conc. in these runs is 3e-5 which is the solubility of 237-Np in J-13 water @ 25 C.) The Tait et al. 1996 data: file: tait.in	nap002.out nap005.out nap01.out nap03.out nap1.out (These output files contain the Kd, the y-axis for each Na concentration)	LABR831371DQ98.001	NQ
7-105	The effects of CO_2 degassing on pH	FEHM v2.00	grid file: tri_final.fehmn fehm .stor file: tri_final.stor zone list file: mat.zone zone list file: topbot.zone main data file:h3_4mmy.dat common macro files: rlp.original rock.prop cond.prop flow.4mmy ngas.topo hflx.heat control file: control.h3_4mmy_degass restart file: h2_4mmy.ini_degass tracer file:ph7.trac.3_degass chemistry file: npchemph7.rxn_degass	h3_4mmy.trc_degass h3_4mmy.out_degass	LABR831371DQ98.001	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-106	Influence of pH on Np breakthrough	FEHM v2.00	grid file: tri_final.fehmn fehm .stor file: tri_final.stor zone list file: mat.zone zone list file: topbot.zone main data file:h3_4mmy.dat common macro files: rlp.original rock.prop cond.prop flow.4mmy ngas.topo hflx.heat Input files unique to Figure 11-16: The effect of pH 5000 yr carrier plume control file: control.h2_4mmy_5000yr, control.h3_4mmy_5000yr restart file: h1_4mmy.ini_5000yr, h2_4mmy.ini_5000yr tracer file: ph8.trac.2_5000yr, ph8.trac.3_5000yr chemistry file: npchemph8.rxn_5000yr 500 yr carrier plume control file: control.h3_4mmy_500yr restart file: h2_4mmy.ini_500yr tracer file:ph8.trac.3_500yr chemistry file: npchemph8.rxn_500yr	h3_4mmy.trc_degass h3_4mmy.out_degass h2_4mmy.out_500yr h3_4mmy.out_5000yr	LABR831371D Q98.001	NQ
7-107	Influence of transient infiltration and chemical conditions on Np breakthrough	FEHM v2.00	grid file: tri_final.fehmn fehm .stor file: tri_final.stor zone list file: mat.zone zone list file: topbot.zone main data file:h3_4mmy.dat common macro files: rlp.original rock.prop cond.prop flow.4mmy ngas.topo hflx.heat control file: control.h3_1mmy_climate restart file: h2_1mmy.ini_climate chemistry file: ph8.trac.3_climate tracer file: npchemph8.rxn_climate	h3_4mmy.out_climate	LABR831371D Q98.001	NQ
7-109	One-dimensional breakthrough curves; steady flow	FEHM v2.00	half.dat one.dat five.dat ten.dat twenty.dat st35.dat st57.dat repo1.dat	sprsht.636a sprsht.636b sprsht.636c sprsht.636d	LABR831371D Q98.001	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-110	Fracture/matrix flux distributions; station 35	FEHM v2.00	inf1.dat inf10.dat	sprsht.638	LABR831371D Q98.001	NQ
7-111	Fracture/matrix flux distributions; station 57	FEHM v2.00	inf1.dat inf10.dat	sprsht.638	LABR831371D Q98.001	NQ
7-112	Breakthrough curve and fracture/matrix flux distribution; station 35	FEHM v2.00	file half.dat one.dat five.dat ten.dat inf5.dat	sprsht.640	LABR831371D Q98.001	NQ
7-113	Saturation profiles for repository column	FEHM v2.00	ten.dat inf10.dat	sprsht.641	LABR831371D Q98.001	NQ
7-114	Transient and steady flow breakthrough curves; station 35	FEHM v2.00	tena.dat cont.tena tenb.dat cont.tenb tenfltss.dat cont.fltss tr10510a.dat cont.10510a inf5.dat cont.10510b tenflttr.dat cont.flttr	sprsht.642	LABR831371D Q98.001	NQ
7-115	Transient and steady flow breakthrough curves; station 57	FEHM v2.00	tena.dat cont.tena tenb.dat cont.tenb tenfltss.dat cont.fltss tr10510a.dat cont.10510a inf5.dat cont.10510b tenflttr.dat cont.flttr	sprsht.643	LABR831371D Q98.001	NQ
7-116	Transient and steady flow breakthrough curves; repository column	FEHM v2.00	tena.dat cont.tena tenb.dat cont.tenb tenfltss.dat cont.fltss tr10510a.dat cont.10510a inf5.dat cont.10510b tenflttr.dat cont.flttr	sprsht.644	LABR831371D Q98.001	NQ
7-117	Breakthrough curves at potential repository	FEHM v2.00	tr20510a.dat cont.20510a tr20510b.dat cont.20510b tr20510flt.dat cont.20510a tr50510a.dat cont.50510a	sprsht.645	LABR831371D Q98.001	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-118	Comparison of breakthrough curves for 10-day and 90-day transients	FEHM v2.00	tr10510a.dat cont.10510a tr10510b.dat cont.10510b tr10510flt.dat cont.10510a tr10590a.dat cont.10590a	sprsht.646	LABR831371D Q98.001	NQ
7-119	Flux at potential repository for transient infiltration	FEHM v2.00	tr10510a.dat cont.10510a tr10510b.dat cont.10510b tr10510flt.dat cont.10510flt	sprsht.647	LABR831371D Q98.001	NQ
7-120 a) b)	Zeolite continuity at different thresholds	X3Dgen v14:30:00 on 11/22/94 by Grid Tm	x3d.input_psets_10pct_m14_m26.Z x3d.input_psets_10pct.Z x3d.input_psets_20pct.Z	outx3dgen_m14_m26_10pct.Z outx3dgen_m1_m13_10pct.Z outx3dgen_m1_m13_20pct.Z	LABR831371D Q98.001	NQ
7-121 b)	Np transport through layered and lensed heterogeneity	FEHM v2.00	control file: control.bg_bp6, control.trans_bp6 data files: bg.dat_bp6, trans.dat_bp6 grid file: grid32.dat control file: control.bg_lp6, control.trans_lp6 data files: bg.dat_bp6, trans.dat_lp6 grid file: grid32.dat control file: control.bg_lp7, control.trans_lp7 data files: bg.dat_bp7, trans.dat_lp7 grid file: grid32.dat control file: control.bg_lp9, control.trans_lp9 data files: bg.dat_bp9, trans.dat_lp9 grid file: grid32.dat	trans.out_bp6 trans.out_lp6 trans.out_lp7 trans.out_lp9	LABR831371D Q98.001	NQ
7-122	Conditional simulation of percent zeolite abundance	RC^2 v Aug 4, 1997 17:32:40	x3d.input	tri_zeol_cond.inp	LABR831371D Q98.001	NQ

Table 7-2. (continued).

Figure	Subject	Code and Version	Input Filename	Output Filename	Data Tracking Number	QA Status
7-123 7-124 7-125	Conditional simulation; effects of matrix sorption Conditional simulation; effects of matrix sorption and infiltration Comparison of 10% zeolite threshold and conditional simulation	FEHM v2.00	multiple simulation control file: fehmn.msim.12-18 control.file: control.ptrk.12-18 grid file: 2dref.grid zone file: 2dref.zone zone file: flow.zone restart file: contzeo.ini macro files: dpdp_lbl_2d.macro (same as in chapter 8) rlp6541_2d.macro pres_lbl_2d.macro rock_lbl_2d.macro flnt_infil_2d97f.flow particle tracking macro files: ptrk.npcase1 ptrk.npcase2 ptrk.npcase3 ptrk.npcase4 post-processing code: process1_fuj	np.temp1 np.temp2 np.temp3 np.temp4	LABR831371DQ98.001	NQ

[1] The following files are FEHMN input for the RIP/FEHM calculations presented in Figures 7.5-2 through 7.5-8.

baserun1.chk	Fehmn.files	fmQb.dpdp	fmQb.zone
baserun1.dat	Ff0300.ini	fmQb.grid	fmQb.zone6
baserun1.his	Ff1300.ini	fmQb.rock	ptrk.expval
baserun1.trc	Ff2300.ini	fmQb.stor	transbase1.dat

[2] Unless specified the preceding directory is: /trans/base97/

[3] Unless specified the preceding directory is /trans/base97/base3d/base_tspa/EXDKM/EaEi/step_noxfm/TBR400k

[4] Flow field used was present-day climate, mean-alpha model computed using TOUGH2; see Table 2-2, DTN: SNT05091597001.007

[5] Flow field used was for long-term-average climate, mean-alpha model computed using TOUGH2; see Table 2-2, DTN: SNT05091597001.007

[6] Flow field used was for superpluvial climate, mean-alpha model computed using TOUGH2; see Table 2-2, DTN: SNT05091597001.007

[7] Flow field used was for long-term-average climate, DKM/Weeps model computed using TOUGH2; see Table 2-2, DTN: SNT05091597001.007

[8] Calculations performed with an Intel, Pentium PII-based PC using the NT 4.0 operating system.

Table 7-3. Sorption Coefficient Distributions (Kd in ml/g) for Unsaturated Zone. Units (Triay et al. 1997; Table 58) (DTN: MO9807SPATBDOC.000).

Element	Rock Type	Minimum (ml/g)	Maximum (ml/g)	Expected Value (ml/g)	Coefficient of Variation*	Distribution Type
Am	D	100	2000			uniform
	V	100	1000	400	0.20	beta
	Z	100	1000			uniform
	Fe	1000	5000			uniform
Pu	D	20	200	100	0.25	beta
	V	50	200	100	0.25	beta
	Z	30	200	100	0.25	beta
	Fe	1000	5000			uniform
U	D	0	4.0	2.0	0.3	beta
	V	0	3.0	1.0	0.3	beta
	Z	0	30.0	7.0	1.0	beta(exp)
	Fe	100	1000			uniform
Np	D	0	6.0	1.0	0.3	beta
	V	0	15.0	1.0	1.0	beta(exp)
	Z	0	12.0	4.0	0.25	beta
	Fe	500	1000			uniform
Ra	D	100	500			uniform
	V	50	100			uniform
	Z	1000	5000			uniform
	Fe	0	500	30	1.0	beta(exp)
Cs	D	20	1000			uniform
	V	10	100			uniform
	Z	500	5000			uniform
	Fe	0	500	30	1.0	beta(exp)
Sr	D	10	50			uniform
	V	0	20			uniform
	Z	500	2000			uniform
	Fe	0	30	10	0.25	beta

Table 7-3. (continued).

Element	Rock Type	Minimum (ml/g)	Maximum (ml/g)	Expected Value (ml/g)	Coefficient of Variation*	Distribution Type
Ni	D	0	500	100	0.33	beta
	V	0	100	50	0.33	beta
	Z	0	500	100	0.33	beta
	Fe	0	1000			uniform
Pb	D	100	500			uniform
	V	100	500			uniform
	Z	100	500			uniform
	Fe	100	1000			uniform
Sn	D	20	200			uniform
	V	20	200			uniform
	Z	100	300			uniform
	Fe	0	5000			uniform
Pa	D	0	100			uniform
	V	0	100			uniform
	Z	0	100			uniform
	Fe	500	1000			uniform
Se	D	0	30	3	1.0	beta(exp)
	V	0	20	3	1.0	beta(exp)
	Z	0	15	2	1.0	beta(exp)
	Fe	0	500	30	1.0	beta(exp)
C	Fe	10	100			uniform

Ac, Sm, Th, Zr, see Am

Cl, Tc, I, Nb, nonsorbing

*Coefficient of variation: COV = $\sigma[x] / E[x]$

Table 7-4. Groundwater Compositions (ppm) of Unsaturated Zone Fluids and Fluids Used in Sorption Studies (DTN: LABR831371DQ98.001).

Species(mg/L)	J-13 Ogard and Kerrisk (1984)	UE25 p#1 Ogard and Kerrisk (1984)	UZ Fluids Yang et al. (1996)
Ca	11.5	87.8(10)*	1-50
Mg	1.8	31.9	0.1-20
Na	45	171	50-200
HCO3	143	698	50-300
PH	6.9	6.7	7-9

*Ca concentration after degassing and precipitation of $CaCO_3$ is shown in parenthesis. The lower value is typical of values in sorption studies (Triay et al. 1996a).

Table 7-5. Solubility of ^{237}Np [Efurd et al. (1996)].

(DTN: LABR831371DQ98.001)			
Temperature,°C	pH 5.9	pH 7	pH 8.5
	(M)		
25	6.5×10^{-4}	3.1×10^{-5}	1.5×10^{-5}
60	9.4×10^{-4}	1.6×10^{-5}	1.7×10^{-5}
90	9.0×10^{-4}	7.9×10^{-6}	5.5×10^{-6}

Table 7-6. Reactions and Log Equilibrium Coefficients for Np Speciation.

(DTN: LABR831371DQ98.001)						
Reaction	0°C	25°C	60°C	100°C	150°C	200°C
$H_2CO_3(aq) \Leftrightarrow HCO_3^- + H^+$	-6.58	-6.34	-6.27	-6.39	-6.72	-7.24
$HCO_3^- \Leftrightarrow CO_3^- + H^+$	10.62	10.33	10.13	10.08	10.20	N/A
$H_2O \Leftrightarrow OH^- + H^+$	-14.93	-14.17	-13.04	-12.26	-11.64	-11.26
$NpO_2^+ + H_2O \Leftrightarrow NpO_2(OH)^0 + H^+$	N/A	8.9	8.2	7.6	7.2	N/A
$NpO_2^+ + 2H_2O \Leftrightarrow NpO_2(OH)_2^- + 2H^+$	N/A	20.2	N/A	18.0	17.0	N/A
$NpO_2^+ + HCO_3^- \Leftrightarrow NpO_2(CO_3)^- + H^+$	6.85	5.73	4.48	3.40	2.39	N/A
$NpO_2^+ + 2(HCO_3^-) \Leftrightarrow NpO_2(CO_3)_2^{3-} + 2H^+$	14.59	13.66	12.57	11.53	10.36	N/A
$NpO_2^+ + 3(HCO_3^-) \Leftrightarrow NpO_2(CO_3)_3^{5-} + 3H^+$	23.58	22.49	21.11	19.59	17.69	N/A

Table 7-7. Transient Model Description.

(DTN: LABR831371DQ98.001)

Model Name	Avg. Annual Infiltration rate (mm/yr)	Frequency of Application (yrs)	Duration (days)
10-1-10	10	1	10
10-1-90	10	1	90
10-5-10	10	5	10
10-5-90	10	5	90
20-5-10	20	5	10

Table 7-8. Properties used for Zeolitic Tuff Sensitivity Study.

(DTN: LABR831371DQ98.001)		
Parameter	**Vitric Tuff**	**Zeolitic Tuff**
Saturated hydraulic conductivity @25°C, (m/s)	4.3×10^{-9}	7.03×10^{-11}
Saturated permeability, $k_{sat\ (m2)}$	4.4×10^{-16}	7.17×10^{-18}
$\alpha_{of\ van\ Genuchten\ model(1/m)}$	0.0267	0.0035
n of van Genuchten model	1.386	1.495
Porosity, ϕ	0.27	0.29

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