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Distribution: w/o encl.
WMHL file
WMHL r/f
WM r/f
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JBMartin
REBrowning
MJBell
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JOBunting
PDR

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WMHL: ~~3104~~.2

AUG 12 1982

MEMORANDUM FOR: Hubert J. Miller, Chief
High-Level Waste Technical
Development Branch
Division of Waste Management

FROM: Malcolm R. Knapp
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Division of Waste Management

SUBJECT: INTERACTIVE BASALT MODEL

Attached is a report from Stewart Silling documenting an interactive model for radionuclide transport in basalt. I have exercised the model and I find that the attached documentation provides all the information which your staff will need to exercise the model. If you or your staff want additional instruction please let me know.

It is extremely important to remember that this is a simplistic model which does not account for much of the complexity and uncertainty of the Hanford Site. I think the model is an excellent tool for developing insight into the behavior of the site, but any specific conclusions must be carefully compared with the results of more sophisticated models.

ORIGINAL SIGNED BY
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Enclosure:
As stated

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DATE	82/08/12					

AN INTERACTIVE MODEL FOR TRANSPORT IN BASALT

This model is an interactive program for performing simple, deterministic calculations of radionuclide discharge at the Hanford site. It allows the user to modify the input parameters easily and immediately see the effect on discharge.

The flow model is a two-pipe network (see Figure 1). One pipe is vertical, representing flow from the repository to an aquifer. The other pipe is horizontal, representing the aquifer which transports material from the site to the accessible environment.

The transport solution used is derived from the BAND model in NWFT/DVM, which is based on an analytic solution by Lester, Jansen, and Burkholder [1]. The discharge is integrated over 10,000 years and is expressed as a fraction of the release limit allowed by the EPA Standard.

The nuclides and their initial inventories are preset. The nuclides are C14, Sr90, Tc99, I129, Sn126, Ni53, Zr93, Cs135, Cs137, Am243, Am241, Pu240, Pu239, Pu238, Np237, and U234. The initial inventories represent the composition of spent fuel.

Most of the remaining parameters in the model can be set by the user. However, each parameter has a "base case" default value which the model assumes unless it is overriden by the user.

The optional parameters are shown in Table 1.

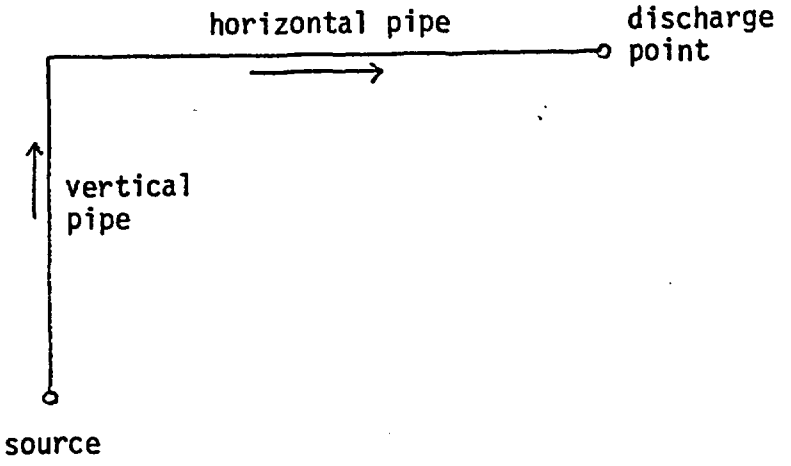

Figure 1. Two pipe network.

Table 1. Parameters

Name	Units	Default	Meaning
KDVC	ml/gm	0	Kd in vertical pipe for carbon
KDVI	ml/gm	2.05E0	Kd in vertical pipe for iodine
KDVTC	ml/gm	1.22E1	Kd in vertical pipe for technecium
KDVFP	ml/gm	3.14E2	Kd in vertical pipe for Sn, Ni, Zr, Cs, and Sr
KDVAM	ml/gm	7.07E3	Kd in vertical pipe for americium
KDVPU	ml/gm	4.84E2	Kd in vertical pipe for plutonium
KDVU	ml/gm	7.21E1	Kd in vertical pipe for uranium
KDVNP	ml/gm	2.05E2	Kd in vertical pipe for neptunium
KDHC	ml/gm	0	Kd in horizontal pipe for carbon
KDHI	ml/gm	1.00E0	Kd in horizontal pipe for iodine
KDHTC	ml/gm	3.16E0	Kd in horizontal pipe for technecium
KDHFP	ml/gm	2.24E0	Kd in horizontal pipe for Su, Ni, Zr, Cs, and Sr
KDHAM	ml/gm	3.16E1	Kd in horizontal pipe for americium
KDHPU	ml/gm	1.00E1	Kd in horizontal pipe for plutonium
KDHU	ml/gm	1.00E1	Kd in horizontal pipe for uranium
KDHNP	ml/gm	7.07E-1	Kd in horizontal pipe for neptunium
SOLC	gm/gm	infinite	Solubility of carbon
SOLI	gm/gm	infinite	Solubility of iodine
SOLTC	gm/gm	1.00E-8	Solubility of technecium
SOLFP	gm/gm	infinite	Solubility of Sn, Ni, Zr, Cs, and Sr
SOLAM	gm/gm	infinite	Solubility of americium
SOLPU	gm/gm	2.50E-10	Solubility of plutonium

(continued)

(Table 1, continued)

Name	Units	Default	Meaning
SOLU	gm/gm	2.00E-5	Solubility of uranium
SOLNP	gm/gm	2.50E-16	Solubility of neptunium
DISP	ft_2	5.00E2	Dispersivity
AREAV	ft^2	8.61E6	Cross-sectional area of vertical pipe
CONDV	ft/da	4.20E-5	Conductivity in vertical pipe
CONDH	ft/da	1.00E2	Conductivity in horizontal pipe
PORV	--	1.20E-2	Porosity in vertical pipe
PORH	--	2.00E-1	Porosity in horizontal pipe
GRADV	ft/ft	1.75E-2	Gradient in vertical pipe
GRADH	ft/ft	5.05E-3	Gradient in horizontal pipe
DISTV	ft	3.25E-3	Length of vertical pipe
DISTH	ft	5.28E3	Length of horizontal pipe
LEACH	yr	1.00E5	Leach time
CANLIFE	yr	1.00E3	Canister life

In order to help account for the fact that vertical flow in basalt is primarily through fractures, a correction proposed by Pepping, Chu, and Siegel [2] is applied to the retardation factor in the vertical pipe. This retardation factor is assumed to be

$$R = 1 + K_d \rho$$

instead of the porous medium expression

$$R = 1 + K_d \rho (1-\phi)/\phi$$

The conductivity in the vertical pipe is an equivalent value which accounts for the series of different resistances in the various layers. The assumed stratigraphy for the site is shown in Figure 2 and the estimated conductivities and porosities are shown in Table 2. The conductivity for the vertical pipe is found as follows:

$$K_{avg} = \frac{\sum_{i=1}^{n} L_i}{\sum_{i=1}^{n} \frac{L_i}{K_i}}$$

where L_i = thickness of layer i
K_i = conductivity of layer i

The average porosity is found similarly:

$$\phi_{avg} = \frac{\sum_{i=1}^{n} L_i}{\sum_{i=1}^{n} \frac{L_i}{\phi_i}}$$

where ϕ_i = porosity of layer i

Using the numerical values shown in Table 2, the average values are found to be as follows:

K_{avg} = 4.2E-5 ft/da
ϕ_{avg} = 0.012

These average values are used as the defaults for the vertical pipe flow parameters. The default values for the horizontal leg are characteristic of the overlying aquifer, layer UA.

The default values for Kd in the vertical pipe are taken from Pepping, Chu, and Siegel [3] and represent the properties of reducing secondary minerals. The Kd values for the horizontal leg are taken from the same source and represent oxidizing sandstone or siltstone. The default solubilities are also taken from this report [4].

Use of the Program

The program operates at the Brookhaven CSCF on either of the 6600 machines, MFA and MFB. It is assumed that the user knows how to dial up and login to one of these machines.

Following the login procedure, execute the following commands:

```
ATTACH,EZHANF,ID=SAS,MR=1.
ETL,400.
EZHANF.
```

i	Layer	Effective Thickness (ft)	Horizontal Hydraulic Conductivity (ft/da)	Vertical Hydraulic Conductivity (ft/da)	Effective Porosity
1	UA	100	1.0E2	1.0E2	1.7E-1
2	J	850	4.5E-1	4.5E-1	1.1E-2
3	I-M	150	1.2E1	1.2E0	1.4E-1
4	H	150	1.0E-1	1.0E-1	1.1E-2
5	G	200	3.2E-2	3.2E-2	1.1E-2
6	F	690	1.0E-4	1.0E-4	1.1E-2
7	I-V	10	1.0E0	1.0E-1	1.4E-1
8	E	690	3.2E-6	3.2E-5	1.1E-2
9	D	60	1.0E-2	1.0E-2	3.5E-2
10	C	50	3.2E-6	3.2E-5	5.0E-3
11	B	150	1.0E-2	1.0E-2	3.5E-2
12	A	150	3.2E-7	3.2E-6	5.0E-3

Table 2. Flow parameters by layer

The program will type some messages and then will await a command. The commands are as follows:

LIST	View the current parameters.
(PARAM)=(VALUE)	Set a parameter to a new numerical value. Parameters are listed in Table 1. Example: CONDV=0.1.
(PARAM)=DEFAULT	Set a parameter to the default value.
ALL=DEFAULT	Set all parameters to their defaults.
RELOAD	Set all parameters to what their values were the last time a GO command was entered. (This is useful in recovering from system aborts.)
GO	Execute the model and print results. Retain the current parameter values following completion.
LONG	Turn on or off the option for printing discharges for each nuclide.
QUIT	Leave the EZHANF program.
HELP	View a writeup on how to use the program.

Error Recovery

Occasionally entry of bad data may cause a system abort, usually as a result of an internal attempt to divide by zero. When this occurs, the user will be returned to Intercom command mode, indicated by an error message and a "COMMAND" prompt. The program may then be restarted by typing the following line:

START.

The program will then load the default values for the parameters. The last set of user-defined parameters (which caused the abort) can be reloaded by typing the following line:

RELOAD

Then the erroneous value can be corrected.

Example

The following output from an interactive session illustrates all the commands. Lines typed by the user are shown in lower case letters, while lines types by the computer are shown in upper case.

Dial up: x28380 for 300 baud

```
BROOKHAVEN INTERCOM 4.7
DATE   08/05/82
TIME   14.38.23.

PLEASE LOGIN
LOGIN,SILLING,7EFB,1349,SUP.

SUP          UPDATED 08/04/82  TODAY IS 08/05/82

        SEE LOGIN FOR IMPORTANT MESSAGES.
 P1  NMSILLING                  PN001349
COMMAND- ATTACH,EZHANF,ID=SAS,MR=1.

 PFN IS
 EZHANF
    CY= 017 SN=SHARE
COMMAND- ETL,400.

COMMAND- EZHANF.

 UPDATE CREATION RUN
 CREATING NEW PROGRAM LIBRARY
 UPDATE COMPLETE.
DEFAULT PARAMETERS LOADED.
READY.

      2.153 CP SECONDS COMPILATION TIME
LIST

KDVC     = 0.              KDVI     = 2.050000E+00
KDVTC    = 1.220000E+01    KDVFP    = 3.140000E+02
KDVAM    = 7.070000E+03    KDVPU    = 4.840000E+02
KDVU     = 7.210000E+01    KDVNP    = 2.050000E+02
KDHC     = 0.              KDHI     = 1.000000E+00
KDHTC    = 3.160000E+00    KDHFP    = 2.240000E+00
KDHAM    = 3.160000E+01    KDHPU    = 1.000000E+01
KDHU     = 1.000000E+01    KDHNP    = 7.070000E-01
SOLC     = 9.999900E+04    SOLI     = 9.999900E+04
SOLTC    = 1.000000E-08    SOLFP    = 9.999900E+04
SOLAM    = 9.999900E+04    SOLPU    = 2.500000E-10
SOLU     = 2.000000E-05    SOLNP    = 2.500000E-16
DISP     = 5.000000E+02    AREAV    = 8.610000E+06
CONDV    = 4.200000E-05    CONDH    = 1.000000E+02
PORV     = 1.200000E-02    PORH     = 2.000000E-01
GRADV    = 1.750000E-02    GRADH    = 5.050000E-03
DISTV    = 3.250000E+03    DISTH    = 5.280000E+03
LEACH    = 1.000000E+05    CANLIFE  = 1.000000E+03

READY.
GO
```

Login

Commands to initiate program.

System messages — may appear in a different order. May take a few minutes.

First user command.

Default parameters.

Execute.

```
 TRAVEL TIME=  1.453789E+05
 AL EPA RATIO= 0.
 DY.
 DV=.03

 UE IS  3.000000E-02
 DY.

 TRAVEL TIME=  2.092515E+02
 AL EPA RATIO= 3.264946E-01
 DY.
 G

 DY.

 TRAVEL TIME=  2.092515E+02
 AL EPA RATIO= 3.264946E-01
 CIOS FOR EACH NUCLIDE:
  14      1.963680E-01
  90      0.
  99      1.272668E-01
 129      2.859417E-03
 135      0.
 137      0.
 126      0.
  59      0.
  93      0.
 243      0.
 241      0.
 240      0.
 239      0.
 238      0.
 237      0.
 234      4.208951E-07

 ADY.
 AM=0

 UE IS  0.
 ADY.

 <
```

Results.

Change vertical conductivity.

Execute.

Results. Note shorter travel time.

Request detailed output.

Execute.

Same parameters, detailed output.

Change K_d for Am.

Execute. (Still uses CONDV=.03)

```
   TRAVEL TIME=  2.092515E+02
 JTAL EPA RATIO= 1.415937E+02
RATIOS FOR EACH NUCLIDE:
 C 14      1.953680E-01
SR 90      0.
TC 99      1.272668E-01
 I129      2.859417E-03
CS135      0.
CS137      0.
SN126      0.
NI 59      0.
ZR 93      0.
AM243      1.174406E+02
AM241      2.382658E+01
PU240      0.
PU239      0.
PU238      0.
NP 37      0.
 U234      4.208951E-07

READY.
DISP=10

VALUE IS   1.000000E+01
READY.

LEACH=1E6

VALUE IS   1.000000E+06
READY.
KDVAM=DEFAULT

VALUE IS   7.070000E+03
READY.
L

READY.
GO

GW TRAVEL TIME=  2.092515E+02
TOTAL EPA RATIO= 3.084537E-02
READY.
ALL=DEFAULT

DEFAULT PARAMETERS LOADED.
READY.
DISTV=150
```

Still gives detailed output.
Note large Am discharge.

Change dispersivity.

Change leach time.

Reset K_d for Am to default.

It tells you what it has been reset to.

Turn off detailed output.

Reset all parameters to default.

Change length of vertical pipe.

```
JE IS 1.500000E+02
DY.
DH=0

JE IS  0.
DY.


THMETIC ERROR  MODE = 02  ADDRESS = 021155
MAND- START.

AULT PARAMETERS LOADED.
DY.
OAD

OAD COMPLETE.
DY.
T

C       = 0.                    KDVI      = 2.050000E+00
TC      = 1.220000E+01          KDVFP     = 3.140000E+02
AM      = 7.070000E+03          KDVPU     = 4.840000E+02
U       = 7.210000E+01          KDVNP     = 2.050000E+02
C       = 0.                    KDHI      = 1.000000E+00
TC      = 3.160000E+00          KDHFP     = 2.240000E+00
AM      = 3.160000E+01          KDHPU     = 1.000000E+01
U       = 1.000000E+01          KDHNP     = 7.070000E-01
C       = 9.999900E+04          SOLI      = 9.999900E+04
TC      = 1.000000E-08          SOLFP     = 9.999900E+04
AM      = 9.999900E+04          SOLPU     = 2.500000E-10
U       = 2.000000E-05          SOLNP     = 2.500000E-16
P       = 5.000000E+02          AREAV     = 8.610000E+06
DV      = 4.200000E-05          CONDH     = 0.
V       = 1.200000E-02          PORH      = 2.000000E-01
DV      = 1.750000E-02          GRADH     = 5.050000E-03
TV      = 1.500000E+02          DISTH     = 5.280000E+03
CH      = 1.000000E+05          CANLIFE   = 1.000000E+03

DY.
DH=25

UE IS  2.500000E+01
DY.


 TRAVEL TIME=  6.732449E+03
AL EPA RATIO= 4.454167E-02
DY.
P
```

Change horiz. conductivity.

System abort.

Restart the program.

Go back to parameters just run.

Bad value - must be changed.

same as before abort

Change horiz. conductivity.

See messages.

```
MMANDS ARE AS FOLLOWS:
  LIST                    LIST THE CURRENT PARAMETERS
  LONG                    TURN ON OR OFF THE OPTION FOR
                            DETAILED OUTPUT
  RELOAD                  RESTORE THE PARAMETERS THAT WERE
                            USED WHEN THE LAST GO COMMAND
                            WAS ENTERED OR WHEN THE LAST
                            ERROR OCCURRED
  GO                      EXECUTE THE TRANSPORT MODEL FOR
                            THE CURRENT LIST OF PARAMETERS.
  (PARAM)=(VALUE)         ASSIGN PARAMETER (PARAM) THE VALUE
                            (VALUE).  (VALUE) MUST BE A NUMBER
                            WHICH OCCUPIES NO MORE THAN 10
                            SPACES TO THE RIGHT OF THE =.
  (PARAM)=DEFAULT         ASSIGN PARAMETER (PARAM) THE
                            DEFAULT VALUE.
  ALL=DEFAULT             ASSIGN ALL PARAMETERS THE DEFAULT
                            VALUES.
  HELP                    VIEW THIS WRITEUP.

RAMETERS ARE AS FOLLOWS: E

  KDVC                     KD FOR CARBON IN VERTICAL LEG (ML/GM)
  KDVI                     "  FOR IODINE
  KDVTC                    "  FOR TECHNECIUM
  KDVAM                    "  FOR AMERICIUM
  KDVPU                    " FOR PLUTONIUM
  KDVU                     " FOR URANIUM
  KDVNP                    " FOR NEPTUNIUM
  KDVFP                    " FOR SR, NI, ZR, CS AND SN
  KDHC                     SIMILAR TO ABOVE BUT FOR HORIZONTAL
                             LEG
  KDHI                     "
  KDTC                     "
  KDHPU                    "
  KDHU                     "
  KDHNP                    "
  KDHFP                    "
  SOLC                     SOLUBILITY FOR CARBON (GM/GM)
```

```
      SOLI                    " FOR IODINE
      SOLTC                   " FOR TECHNICIUM
      SOLAM                   " FOR AMERICIUM
      SOLPU                   " FOR PLUTONIUM
      SOLU                    " FOR URANIUM
      SOLNP                   " FOR NEPTUNIUM
      SOLFP                   " FOR SR, NI, ZR, CS, AND SN
      CONDV                   CONDUCTIVITY IN VERTICAL LEG (FT/DA)
      CONDH                   CONDUCTIVITY IN HORIZONTAL LEG
                                  (FT/DA)
      PORV                    POROSITY IN VERTICAL LEG
      PORH                    POROSITY IN HORIZONTAL LEG
      DISP                    DISPERSIVITY (FT)
      AREAV                   AREA OF VERTICAL PIPE (FT**2)
      GRADV                   VERTICAL GRADIENT (FT/FT)
      GRADH                   HORIZONTAL GRADIENT (FT/FT)
      LEACH                   LEACH TIME OF WASTE (YR)
      CANLIFE                 CANISTER LIFE (YR)
      DISTV                   LENGTH OF VERTICAL LEG (FT)
      DISTH                   LENGTH OF HORIZONTAL LEG (FT)
READY.
QUIT
```

Exit program.

```
      STOP
      040000 MAXIMUM EXECUTION FL.
:       .843 CP SECONDS EXECUTION TIME.
COMMAND- LOGOUT.
```

Logout.

```
CPA       8.745 SEC.          8.745 ADJ.
SYS TIME                     29.775
CONNECT TIME     0 HRS.    13 MIN.
 08/05/82  LOGGED OUT AT 14.51.56.
      <
```

Hang up.

References

1. D. H. Lester, G. Jansen, and H. C. Burkholder, "Migration of Radionuclide Chains Through an Adsorbing Medium," AIChE Symposium Series No. 152 - Adsorption and Ion Exchange, 71, p. 202 (1975).

2. R. E. Pepping, M. S. Y. Chu, and M. D. Siegel, "Technical Assistance for Regulatory Development: A Simplified Repository Analysis in a Reference Basalt Site," draft, pp. 9-11 (1982).

3. Ibid., p. 14.

4. Ibid., p. 15.