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PATH1 Self-Teaching Curriculum: Example Problems for Pathways-to-Man Model

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ABSTRACT

The Pathways-to-Man Model was developed at Sandia National Laboratories to represent the environmental movement and human uptake of radionuclides. This model is implemented by the computer program PATH1. The purpose of this document is to present a sequence of examples to facilitate use of the model and the computer program which implements it. Each example consists of a brief description of the problem under consideration, a discussion of the data cards required to input the problem to PATH1, and the resultant program output. These examples are intended for use in conjunction with the technical report which describes the model and the computer program which implements it (NUREG/CR-1636, Vol 1; SAND78-1711). In addition, a sequence of appendices provides the following: a description of a surface hydrologic system used in constructing several of the examples, a discussion of mixed-cell models, and a discussion of selected mathematical topics related to the Pathways Model. A copy of the program PATH1 is included with the report.

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CHAPTER 1

Introduction

The purpose of this document is to present a sequence of examples to facilitate the use of the Pathways-to-Man Model (Cam78, Hel81b). Each example consists of a brief description of the problem under consideration, a discussion of the data cards required to input the problem to the computer program which implements the model, and the resultant program output.

As the Pathways-to-Man Model and the computer program which implements it are described extensively in a previously published report (Hel81b), such descriptions will not be repeated here. With respect to the preceding document, Chapter 2 provides a conceptual description of the model, Chapter 3 provides an overview of the computer program which inplements the model, and Chapter 4 provides a detailed description of data card structure and arrangement. For the discussions contained in the present report, it is assumed that the reader has access to this document.

Five examples are presented. Chapter 2 contains a relatively simple example which involves one zone and one radionuclide. This example is then expanded in Chapter 3 to include ingestion and inhalation calculations. Chapter 4 presents an example involving three zones and two radionuclides. This example also includes ingestion and inhalation calculations. The example in Chapter 5 uses two zones. However, in contrast to the preceding examples, only two subzones per zone are employed. A decay chain with five radionuclides is considered, but no ingestion or inhalation calculations are performed. Finally, Chapter 6 presents an example with five zones. This example differs from the preceding examples in that nonzero initial values are set for the radionuclide transport equations and the forcing functions for the transport equations are taken to be identically zero. No ingestion or inhalation calculations are performed.

The report ends with a sequence of appendices. Appendix A describes a hypothetical site which was used in a sensitivity analysis involving the Environmental Transport Model and is reprinted from an earlier report

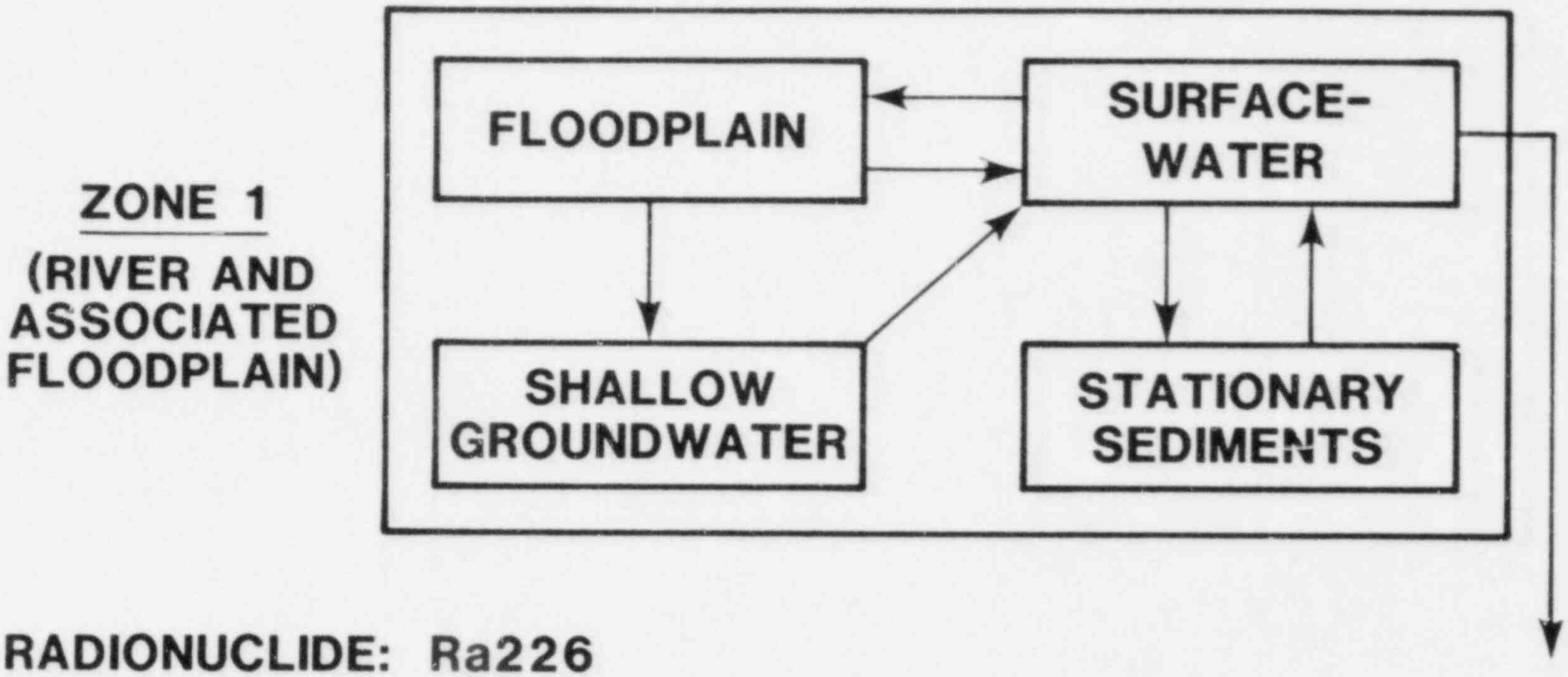
(Hel80, Chapter 2). This site is used as the basis for four of the examples contained in this report. The Environmental Transport Model is the part of the Pathways Model which actually formulates and solves the radionuclide transport equations. Appendix B presents several simple examples of mixed-cell models. These examples are special cases of the type of mathematical model which underlies the Pathways Model and are included to help readers unfamiliar with this type of modeling develop a feeling for the processes involved. Appendix C presents a brief discussion of several mathematical topics associated with the Pathways Model and provides additional references. A microfiche listing of PATH1, the computer program which implements the Pathways Model, is provided at the end of the report.

CHAPTER 2

Example 1

This chapter presents a relatively simple example which illustrates the input data used by PATH1. Specifically, an example involving one zone and one radionuclide is considered. No ingestion or inhalation calculations are performed. This example is expanded in Chapter 3 to include such calculations. The zone considered is the same as that designated zone 1 in a sensitivity analysis of the Pathways Model (Hel80, Chapter 2). This zone corresponds to a stretch of river and the floodplain along the river. Specifically, the surface water subzone consists of a stretch of river and the suspended sediments within the river, the soil subzone consists of an area of floodplain on each side of the river, the sediment subzone consists of the stationary sediments beneath the river, and the groundwater subzone consists of a shallow aquifer beneath the soil subzone which discharges into the surface water subzone. For convenience, the chapter of Helton and Iman (Hel80) which describes this zone is reprinted as Appendix A of the present report. The radionuclide considered is Ra226. This radionuclide is assumed to enter the surface-water subzone at the rate of 1.0 mg/yr.

The general nature of example 1 is indicated in Figure 2-1. Then, the input data to PATH1 associated with this example are listed in Table 2-1, and the location in the user manual (Hel81b) of additional discussion of the card deck presented in Table 2-1 is indicated in Table 2-2. Finally, the model output corresponding to the input in Table 2-1 is listed on microfiche attached at the end of the report.



RADIONUCLIDE: Ra226

NO INGESTION OR INHALATION

Figure 2-1. Example 1.

Table 2-1

Input Data for Example 1

```
C THE DATA READ BY SUBROUTINE DATA1 FOLLOWS. THIS DATA DESCRIBES ZONE 1  CARD   1
C OF A SITE INVOLVING THREE ZONES WHICH WAS USED IN A SENSITIVITY ANAL-  CARD   2
C YSIS OF THE PATHWAYS MODEL. DEFINITION AND/OR DERIVATION OF THE PARA-  CARD   3
C METERS WHICH FOLLOW ARE CONTAINED IN CHAPTER 2 OF HELTON AND IMAN,     CARD   4
C RISK METHODOLOGY FOR GEOLOGIC DISPOSAL OF RADIOACTIVE WASTE: SENSI-    CARD   5
C TIVITY ANALYSIS OF THE ENVIRONMENTAL TRANSPORT MODEL (DECEMBER, 1980). CARD   6
         1                                                              CARD   7
         1                                                              CARD   8
    1.4E12    9.4E12         0         0    2.2E12         0            CARD   9
         0         0         0         0                                CARD  10
    2.0E10    1.1E11    9.8E10         0    4.0E10    1.1E08            CARD  11
         0         0                                                    CARD  12
    2.2E10    3.5E06         0         0    4.0E10    1.1E08            CARD  13
    2.7E08    2.3E08    1.9E13    3.0E09         0         0            CARD  14
         2                                                              CARD  15
    8.7E09    2.3E10         0         0    8.7E08    2.3E09            CARD  16
         0         0                                                    CARD  17
C THE DATA READ BY SUBROUTINE DATA2 FOLLOWS. THIS DATA DESCRIBES RA226.  CARD  18
C CONCENTRATION RATIOS ARE FROM TABLE A-8, P. 1.109-31, AND TABLE C-5,   CARD  19
C P. 1.109-56, OF U. S. NRC REGULATORY GUIDE 1.109 (MARCH, 1976).        CARD  20
         1                                                              CARD  21
         1                                                              CARD  22
     RA226   2.26E02   1.60E03         1                                CARD  23
         2   1.00E00                                                    CARD  24
         1                                                              CARD  25
    5.0E02    5.0E02    5.0E02    5.0E02                                CARD  26
    1.0E00    5.0E02    2.5E02   3.1E-04   8.0E-03   3.4E-02            CARD  27
         1                                                              CARD  28
         0         0   2.67E18         0                                CARD  29
C THE DATA READ BY SUBROUTINE DATA3 FOLLOWS. THIS DATA CONTROLS THE      CARD  30
C OPERATION OF THE DIFFERENTIAL EQUATION SOLVER USED FOR THE RADIONU-    CARD  31
C CLIDE TRANSPORT EQUATIONS.                                            CARD  32
         1                                                              CARD  33
   1.0E-10                                                              CARD  34
   1.0E-20   1.0E-08        21         1                                CARD  35
C THE DATA READ BY SUBROUTINE DATAM FOLLOWS. THIS DATA IS USED BY SUB-   CARD  36
C ROUTINE MANAGE TO CONTROL THE OPERATION OF THE PATHWAYS MODEL.        CARD  37
         1                                                              CARD  38
         1                                                              CARD  39
         1         0    7.5E02         2                                CARD  40
         1         1        -1        -1        -1                      CARD  41
         1         1         0         0         0                      CARD  42
C THE DATA READ BY SUBROUTINE DATA4 FOLLOWS. THIS DATA IS USED BY SUB-   CARD  43
C ROUTINE INGEST TO PERFORM INGESTION CALCULATIONS.                     CARD  44
C NO INGESTION DATA IS READ IN THIS EXAMPLE.                            CARD  45
         0                                                              CARD  46
C THE DATA READ BY SUBROUTINE DATA5 FOLLOWS. THIS DATA IS USED BY SUB-   CARD  47
C ROUTINE INHALE TO PERFORM INHALATION CALCULATIONS.                    CARD  48
C NO INHALATION DATA IS READ IN THIS EXAMPLE.                           CARD  49
         0                                                              CARD  50
C THE DATA READ BY SUBROUTINE ALTER FOLLOWS. THIS DATA IS USED TO DEFINE CARD  51
C AND IMPLEMENT ALTERATIONS TO THE COEFFICIENTS IN THE RADIONUCLIDE      CARD  52
C TRANSPORT EQUATIONS.                                                  CARD  53
         0                                                              CARD  54
```

Table 2-1 (Continued)

```
C THE DATA READ BY SUBROUTINE ADD FOLLOWS. THIS DATA IS USED TO DEFINE        CARD    55
C AND IMPLEMENT ADDITIONAL COEFFICIENTS IN THE RADIONUCLIDE TRANSPORT          CARD    56
C EQUATIONS.                                                                   CARD    57
         0                                                                     CARD    58
C THE DATA READ BY SUBROUTINE REDUCE FOLLOWS. THIS DATA IS USED TO DE-         CARD    59
C FINE AND IMPLEMENT A REDUCTION IN THE NUMBER OF RADIONUCLIDE TRANSPORT       CARD    60
C EQUATIONS.                                                                   CARD    61
         0                                                                     CARD    62
C THE DATA READ BY SUBROUTINE INITIAL FOLLOWS. THIS DATA IS USED TO SET        CARD    63
C THE INITIAL VALUE CONDITIONS FOR THE RADIONUCLIDE TRANSPORT EQUATIONS.       CARD    64
         1                                                                     CARD    65
```

Table 2-2

Discussion of Input Data for Example 1

Cards[a]	Discussion	Sections[b]
1-6	Comments for DATA1	4.2.1.1
7	Option for DATA1	4.2.1.2
8	Number of zones	4.2.2.1
9-10	Description of groundwater subzone	4.2.2.2
11-12	Description of soil subzone	4.2.2.3
13-15	Description of surface-water subzone	4.2.2.4
16-17	Description of sediment subzone	4.2.2.5
18-20	Comments for DATA2	4.3.1.1
21	Option for DATA2	4.3.1.2
22	Number of radionuclides	4.3.2.1
23	Description of decay chain	4.3.2.2
24	Description of decay pattern	4.3.2.3
25-26	Description of distribution coefficients	4.3.2.4
27	Description of concentration ratios	4.3.2.5
28-29	Description of radionuclide input rates	4.3.2.6
30-32	Comments for DATA3	4.4.1.1
33	Option for DATA3	4.4.1.2
34	Minimum coefficient size	4.4.2.1
35	Parameters for GEARB	4.4.2.2
36-37	Comments for DATAM	4.5.1.1
38	Option for DATAM	4.5.1.2
39	Option for MANAGE	4.5.2.1
40	Solution of transport equations	4.5.2.2
41	Subroutine selection for SOL, CONC, INGEST, INHALE, and EXT	4.5.2.3
42	Subroutine options	4.5.2.4
43-45	Comments for DATA4	4.6.1.1
46	Option for DATA4	4.6.1.2
47-49	Comments for DATA5	4.7.1.1
50	Option for DATA5	4.7.1.2
51-53	Comments for ALTER	4.9.1.1
54	Option for ALTER	4.9.1.2
55-57	Comments for ADD	4.10.1.1
58	Option for ADD	4.10.1.2

---

[a] Data card number in Table 2-1.

[b] Location of additional discussion in user manual (Hel81b).

Table 2-2 (Continued)

Cards[a]	Discussion	Sections[b]
59-61	Comments for REDUCE	4.11.1.1
62	Option for REDUCE	4.11.1.2
63-64	Comments for INITIAL	4.12.1.1
65	Option for INITIAL	4.12.1.2

---

[a] Data Card number in Table 2-1.

[b] Location of additional discussion in user manual (Hel81b).

CHAPTER 3

Example 2

This chapter illustrates the ingestion and inhalation calculations performed by PATH1. Specifically, the example presented in Chapter 2 is expanded by the inclusion of ingestion and inhalation calculations. Two ingestion patterns and two inhalation patterns are added.

The general nature of example 2 is indicated in Figure 3-1. Then, the input data to PATH1 associated with this example are listed in Table 3-1, and the location in the user manual (Hel81b) of additional discussion of the card deck presented in Table 3-1 is indicated in Table 3-2. Finally, the model output corresponding to the input in Table 3-1 is listed on microfiche attached at the end of the report.

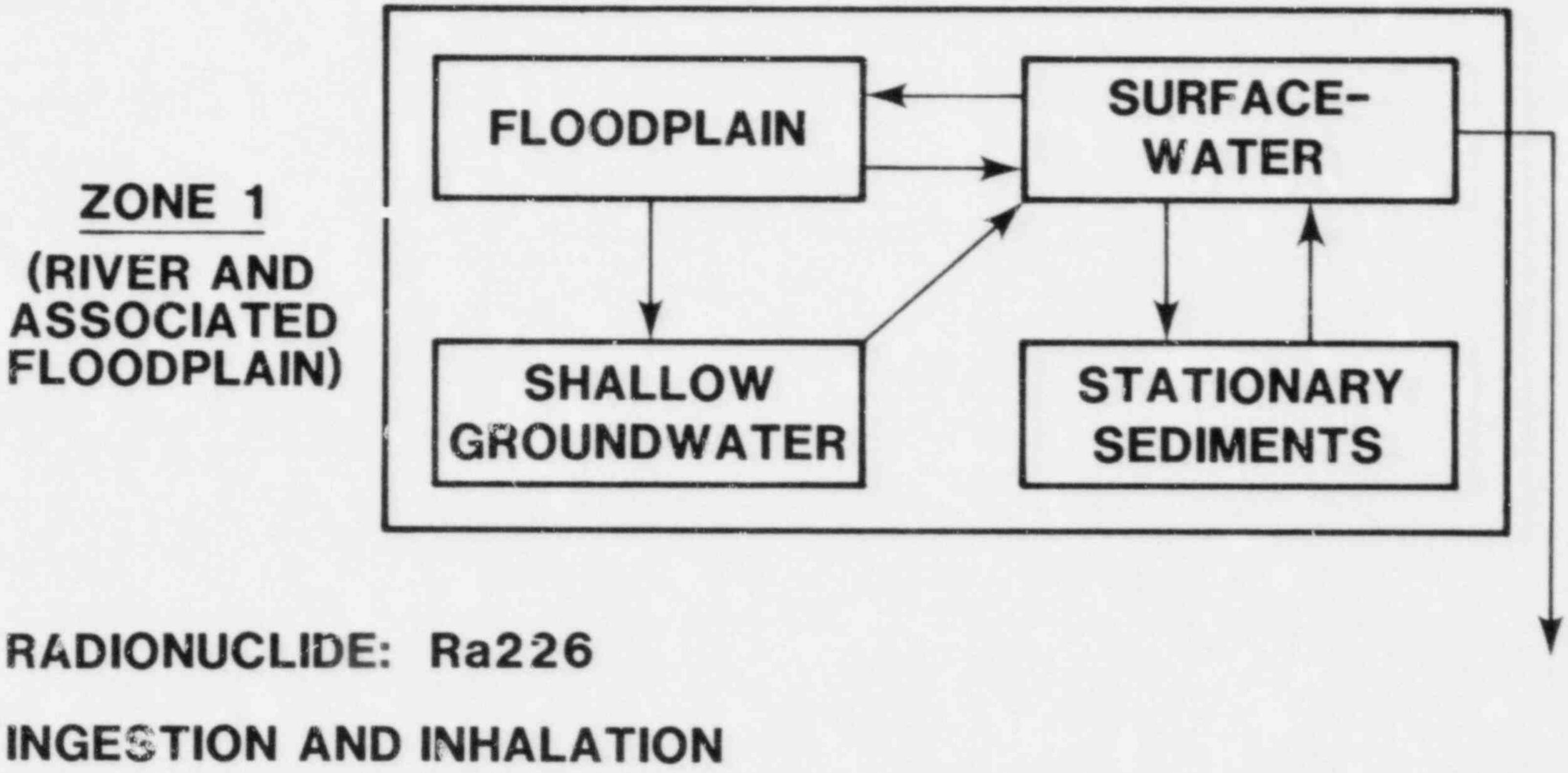


Figure 3-1. Example 2.

Table 3-1

Input Data for Example 2

```
C THE DATA READ BY SUBROUTINE DATA1 FOLLOWS. THIS DATA DESCRIBES ZONE 1         CARD    1
C OF A SITE INVOLVING THREE ZONES WHICH WAS USED IN A SENSITIVITY ANAL-         CARD    2
C YSIS OF THE PATHWAYS MODEL. DEFINITION AND/OR DERIVATION OF THE PARA-         CARD    3
C METERS WHICH FOLLOW ARE CONTAINED IN CHAPTER 2 OF HELTON AND IMAN,            CARD    4
C RISK METHODOLOGY FOR GEOLOGIC DISPOSAL OF RADIOACTIVE WASTE: SENSI-           CARD    5
C TIVITY ANALYSIS OF THE ENVIRONMENTAL TRANSPORT MODEL (DECEMBER, 1980).        CARD    6
         1                                                                      CARD    7
         1                                                                      CARD    8
    1.4E12    9.4E12         0         0    2.2E12         0                    CARD    9
         0         0         0         0                                        CARD   10
    2.0E10    1.1E11    9.8E10         0    4.0E10    1.1E08                    CARD   11
         0         0                                                            CARD   12
    2.2E10    3.5E06         0         0    4.0E10    1.1E08                    CARD   13
    2.7E08    2.3E09    1.9E13    3.0E09         0         0                    CARD   14
         2                                                                      CARD   15
    8.7E09    2.3E10         0         0    8.7E08    2.3E09                    CARD   16
         0         0                                                            CARD   17
C THE DATA READ BY SUBROUTINE DATA2 FOLLOWS. THIS DATA DESCRIBES RA226.         CARD   18
C CONCENTRATION RATIOS ARE FROM TABLE A-8, P. 1.109-31, AND TABLE C-5,          CARD   19
C P. 1.109-56, OF U. S. NRC REGULATIRY GUIDE 1.109 (MARCH, 1976).               CARD   20
         1                                                                      CARD   21
         1                                                                      CARD   22
     RA226   2.26E02   1.60E03         1                                        CARD   23
         2   1.00E00                                                            CARD   24
         1                                                                      CARD   25
    5.0E02    5.0E02    5.0E02    5.0E02                                        CARD   26
    1.0E00    5.0E01    2.5E02   3.1E-04   8.0E-03   3.4E-02                    CARD   27
         1                                                                      CARD   28
         0         0   2.67E18         0                                        CARD   29
C THE DATA READ BY SUBROUTINE DATA3 FOLLOWS. THIS DATA CONTROLS THE             CARD   30
C OPERATION OF THE DIFFERENTIAL EQUATION SOLVER USED FOR THE RADIONU-           CARD   31
C CLIDE TRANSPORT EQUATIONS.                                                    CARD   32
         1                                                                      CARD   33
   1.0E-10                                                                      CARD   34
   1.0E-20   1.0E-08        21         1                                        CARD   35
C THE DATA READ BY SUBROUTINE DATAM FOLLOWS. THIS DATA IS USED BY SUB-          CARD   36
C ROUTINE MANAGE TO CONTROL THE OPERATION OF THE PATHWAYS MODEL.                CARD   37
         1                                                                      CARD   38
         1                                                                      CARD   39
         1         0    7.5E02         2                                        CARD   40
         1         1         1         1        -1                              CARD   41
         1         1         1         1         0                              CARD   42
C THE DATA READ BY SUBROUTINE DATA4 FOLLOWS. THIS DATA IS USED BY SUB-          CARD   43
C ROUTINE INGEST IN THE CALCULATION OF RADIONUCLIDE INGESTION. INGESTION        CARD   44
C RATES ARE THE ADULT RATES FROM TABLE E-4, P. 1.109-39, OF U. S. NRC           CARD   45
C REGULATORY GUIDE 1.109 (OCTOBER, 1977).                                       CARD   46
         1                                                                      CARD   47
C THE DEFAULT VALUES FOR AGRICULTURAL PARAMETERS ARE USED.                      CARD   48
         0                                                                      CARD   49
C TWO DIETARY PATTERNS ARE CONSIDERED. THE PATTERNS DIFFER IN THAT THE          CARD   50
C FIRST INCLUDES IRRIGATION WHILE THE SECOND DOES NOT.                          CARD   51
         2                                                                      CARD   52
   3.70E02   6.90E00         0   1.90E02   1.10E02   9.50E01                    CARD   53
         3         4   3.00E02                                                  CARD   54
   3.70E02   6.90E00         0   1.90E02   1.10E02   9.50E01                    CARD   55
         3         4         0                                                  CARD   56
```

Table 3-1 (Continued)

```
C THE DATA READ BY SUBROUTINE DATA5 FOLLOWS. THIS DATA IS USED BY SUB-        CARD    57
C ROUTINE INHALE IN THE CALCULATION OF RADIONUCLIDE INHALATION. INHALA-        CARD    58
C TION RATE IS THE ADULT RATE FROM TABLE E-4, P. 1.109-39, OF U. S. NRC        CARD    59
C REGULATORY GUIDE 1.109 (OCTOBER, 1977). CONCENTRATION OF SUSPENDED           CARD    60
C MATERIAL IS SELECTED TO BE REPRESENTATIVE OF CONCENTRATIONS LISTED IN        CARD    61
C TABLE 1.4-5, P. 66, OF THE HANDBOOK OF ENVIRONMENTAL CONTROL, VOLUME         CARD    62
C 1.                                                                           CARD    63
         1                                                                     CARD    64
C TWO INHALATION PATTERNS ARE CONSIDERED. IN THE FIRST PATTERN, SUSPEND-       CARD    65
C ED MATERIAL IS DERIVED FROM THE SOIL SUBZONE. IN THE SECOND PATTERN,         CARD    66
C SUSPENDED MATERIAL IS DERIVED FROM THE SEDIMENT SUBZONE.                     CARD    67
         2                                                                     CARD    68
         2  3.50E-09   8.00E03   1.00E00                                       CARD    69
         4  3.50E-09   8.00E03  3.85E-02                                       CARD    70
C THE DATA READ BY SUBROUTINE ALTER FOLLOWS. THIS DATA IS USED TO DEFINE       CARD    71
C AND IMPLEMENT ALTERATIONS TO THE COEFFICIENTS IN THE RADIONUCLIDE            CARD    72
C TRANSPORT EQUATIONS.                                                         CARD    73
         0                                                                     CARD    74
C THE DATA READ BY SUBROUTINE ADD FOLLOWS. THIS DATA IS USED TO DEFINE         CARD    75
C AND IMPLEMENT ADDITIONAL COEFFICIENTS IN THE RADIONUCLIDE TRANSPORT          CARD    76
C EQUATIONS.                                                                   CARD    77
         0                                                                     CARD    78
C THE DATA READ BY SUBROUTINE REDUCE FOLLOWS. THIS DATA IS USED TO DE-         CARD    79
C FINE AND IMPLEMENT A REDUCTION IN THE NUMBER OF RADIONUCLIDE TRANSPORT       CARD    80
C EQUATIONS.                                                                   CARD    81
         0                                                                     CARD    82
C THE DATA READ BY SUBROUTINE INITIAL FOLLOWS. THIS DATA IS USED TO SET        CARD    83
C THE INITIAL VALUE CONDITIONS FOR THE RADIONUCLIDE TRANSPORT EQUATIONS.       CARD    84
         1                                                                     CARD    85
```

Table 3-2

Discussion of Input Data for Example 2[a]

Cards[b]	Discussion	Sections[c]
36-37	Comments for DATAM	4.5.1.1
38	Option for DATAM	4.5.1.2
39	Option for MANAGE	4.5.2.1
40	Solution of transport equations	4.5.2.2
41	Subroutine selection for SOL, CONC, INGEST, INHALE, and EXT	4.5.2.3
42	Subroutine options	4.5.2.4
43-46	Comments for DATA4	4.6.1.1
47	Option for DATA4	4.6.1.2
48	Comments for agricultural parameters	4.6.3.1
49	Option for agricultural parameters	4.6.3.2
50-51	Comments for ingestion patterns	4.6.3.5
52	Number of ingestion patterns	4.6.3.6
53-56	Description of ingestion patterns	4.6.3.7
57-63	Comments for DATA5	4.7.1.1
64	Option for DATA5	4.7.1.2
65-67	Comments for inhalation patterns	4.7.3.1
68	Number of inhalation patterns	4.7.3.2
69-70	Description of inhalation patterns	4.7.3.3

---

[a] Only cards 36 through 70 are discussed. Cards 1 through 35 and cards 71 through 85 are the same as cards 1 through 35 and cards 51 through 65, respectively, discussed in Table 2-2.

[b] Data card number in Table 3-1.

[c] Location of additional discussion in user manual (He81b).

CHAPTER 4

Example 3

This chapter presents an example involving three zones and two radionuclides. Further, ingestion and inhalation calculations are performed for all zones. The first zone consists of a 40-km stretch of river, the stationary sediments beneath the river, a 2-km-wide strip of floodplain on each side of the river, and the portions of a shallow aquifer which lie beneath the preceding strips of floodplain. The second zone begins immediately below the first zone and consists of a lake 40 km in length, a layer of stationary sediments beneath the lake, a 2-km-wide strip of land on each side of the lake, and the portions of the shallow aquifer which lie beneath the preceding strips of land. The third zone begins immediately below the second zone and consists of a 40-km stretch of river, the stationary sediments beneath the river, a 2-km-wide strip of floodplain on each side of the river, and the portions of the shallow aquifer which lie beneath the preceding strips of floodplain. The site used in this example was defined for a sensitivity analysis of the Pathways Model (Hel80). The derivation of the parameters which define this site is presented in Appendix A. The radionuclides are Cm245 and Pu241. They are assumed to enter the surface-water subzone of the first zone at the rates of 1.0 mg/yr for Cm245 and 1.77 x 10^{-3} mg/yr for Pu241. The rate for Pu241 was selected for equilibrium with the parent Cm245.

The general nature of example 3 is indicated in Figure 4-1. Then, the input data to PATH1 associated with this example are listed in Table 4-1, and the location in the user manual (Hel81b) of additional discussion of the card deck presented in Table 4-1 is indicated in Table 4-2. Finally, the model output corresponding to the input in Table 4-1 is listed on microfiche attached at the end of the report.

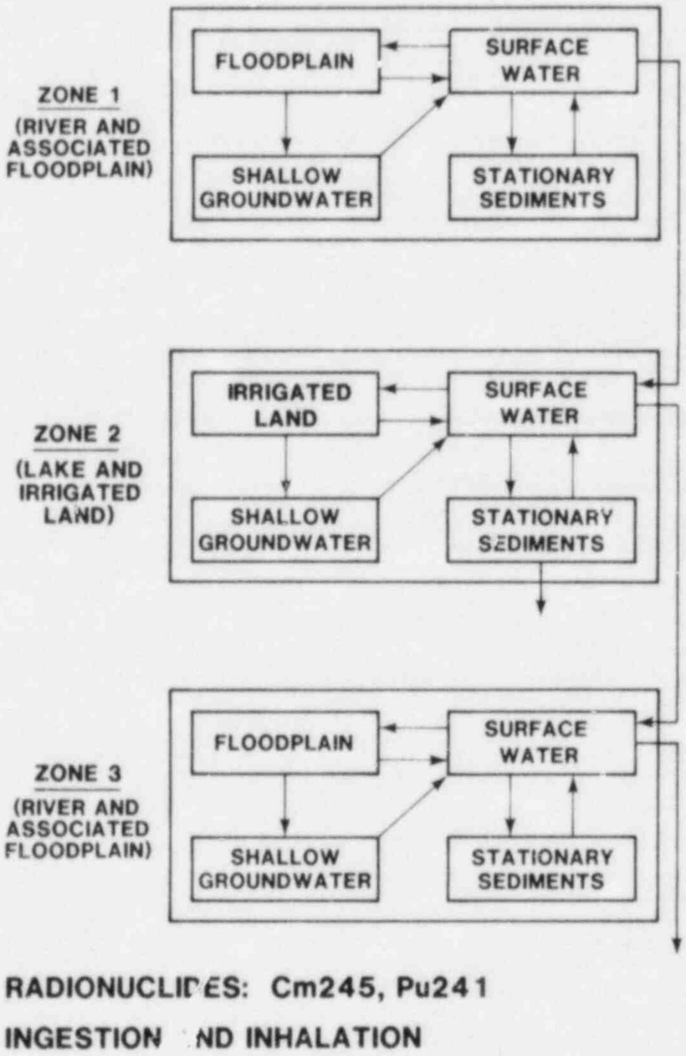


Figure 4-1. Example 3.

Table 4-1

Input Data for Example 3

```
C THE DATA READ BY SUBROUTINE DATA1 FOLLOWS. THIS DATA DESCRIBES A SITE          CARD     1
C INVOLVING THREE ZONES WHICH WAS USED IN A SENSITIVITY ANALYSIS OF THE          CARD     2
C PATHWAYS MODEL. DEFINITION AND/OR DERIVATION OF THE PARAMETERS WHICH           CARD     3
C FOLLOW ARE CONTAINED IN CHAPTER 2 OF J. HELTON ET AL, RISK METHODOL-           CARD     4
C OGY FOR GEOLOGIC DISPOSAL OF RADIOACTIVE WASTE: SENSITIVITY ANALYSIS           CARD     5
C OF THE ENVIRONMENTAL TRANSPORT MODEL, SAND79-1393 (DECEMBER, 1980).            CARD     6
         1                                                                       CARD     7
         3                                                                       CARD     8
    1.4E12    9.4E12         0         0    2.2E12         0                     CARD     9
         0         0         0         0                                         CARD    10
    1.4E12    9.4E12         0         0    2.2E12         0                     CARD    11
         0         0         0         0                                         CARD    12
    1.4E12    9.4E12         0         0    2.2E12         0                     CARD    13
         0         0         0         0                                         CARD    14
    2.0E10    1.1E11    9.8E10         0    4.0E10    1.1E08                     CARD    15
         0         0                                                             CARD    16
    2.0E10    1.1E11    9.8E10         0    4.8E10    1.9E06                     CARD    17
         0         0                                                             CARD    18
    2.0E10    1.1E11    9.8E10         0    4.0E10    1.1E08                     CARD    19
         0         0                                                             CARD    20
    2.2E10    3.5E06         0         0    4.0E10    1.1E08                     CARD    21
    8.7E08    2.3E09    1.9E13    3.0E09         0         0                     CARD    22
         2                                                                       CARD    23
    1.9E13    7.6E08         0         0    4.8E10    1.9E06                     CARD    24
    3.0E09    7.9E09    2.3E13    9.2E08         0         0                     CARD    25
         3                                                                       CARD    26
    3.2E10    1.9E06         0         0    4.0E10    1.1E08                     CARD    27
    1.3E09    3.4E09    2.7E13    1.6E09         0         0                     CARD    28
         4                                                                       CARD    29
    8.7E09    2.3E10         0         0    8.7E08    2.3E09                     CARD    30
         0         0                                                             CARD    31
    2.0E10    5.2E10         0         0    2.0E09    5.2E09                     CARD    32
    1.0E09    2.7E09                                                             CARD    33
    1.3E10    3.4E10         0         0    1.3E09    3.4E09                     CARD    34
         0         0                                                             CARD    35
C THE DATA READ BY SUBROUTINE DATA2 FOLLOWS. THIS DATA DESCRIBES A DECAY         CARD    36
C CHAIN SEGMENT CONSISTING OF CM245, PU241. CONCENTRATION RATIOS ARE             CARD    37
C FROM TABLE A-8, P. 1.109-31, AND TABLE C-5, P.1.109-56, OF U. S. NRC           CARD    38
C REGULATORY GUIDE 1.109 (MARCH, 1976).                                          CARD    39
         1                                                                       CARD    40
         2                                                                       CARD    41
     CM245   2.45E02   8.26E03         1                                         CARD    42
     PU241   2.41E02   1.46E01         1                                         CARD    43
         2   1.00E00                                                             CARD    44
         3   1.00E00                                                             CARD    45
         1                                                                       CARD    46
    1.0E03    1.0E03    1.0E03    1.0E03                                         CARD    47
    1.0E03    1.0E03    1.0E03    1.0E03                                         CARD    48
    1.0E00    2.5E01    1.0E03   2.5E-03   5.0E-06   2.0E-04                     CARD    49
    1.0E00    3.5E00    1.0E02   2.5E-04   2.0E-06   1.4E-05                     CARD    50
         1                                                                       CARD    51
         0         0    2.5E18         0         0                               CARD    52
         0         0    4.4E15         0         0                               CARD    53
C THE DATA READ BY SUBROUTINE DATA3 FOLLOWS. THIS DATA CONTROLS THE              CARD    54
C OPERATION OF THE DIFFERENTIAL EQUATION SOLVER USED FOR THE RADIONU-            CARD    55
C CLIDE TRANSPORT EQUATIONS.                                                     CARD    56
         1                                                                       CARD    57
   1.0E-25                                                                       CARD    58
   1.0E-23   1.0E-05        22         1                                         CARD    59
```

Table 4-1 (Continued)

```
C THE DATA READ BY SUBROUTINE DATAM FOLLOWS. THIS DATA IS USED BY SUB-           CARD   60
C ROUTINE MANAGE TO CONTROL THE OPERATION OF THE PATHWAYS MODEL.                 CARD   61
         1                                                                      CARD   62
         1                                                                      CARD   63
         1         0    5.0E+02         2                                       CARD   64
         1         1         1          1         -1                            CARD   65
         1         1         1          1          0                            CARD   66
C THE DATA READ BY SUBROUTINE DATA4 FOLLOWS. THIS DATA IS USED BY SUB-           CARD   67
C ROUTINE INGEST IN THE CALCULATION OF RADIONUCLIDE INGESTION. INGESTION         CARD   68
C RATES ARE THE ADULT RATES FROM TABLE E-4, P. 1.109-39, OF U. S. NRC            CARD   69
C REGULATORY GUIDE 1.109 (OCTOBER, 1977).                                        CARD   70
         1                                                                      CARD   71
C THE DEFAULT VALUES FOR AGRICULTURAL PARAMETERS ARE USED.                       CARD   72
         0                                                                      CARD   73
C THE TWO DIETARY PATTERNS FOR ZONE 1 FOLLOW.                                    CARD   74
         2                                                                      CARD   75
   3.70E02   6.90E00         0    1.90E02   1.10E02   9.50E01                   CARD   76
         3         4         0                                                  CARD   77
   3.70E02   6.90E00         0    1.90E02   1.10E02   9.50E01                   CARD   78
         3         4   3.00E02                                                  CARD   79
C THE TWO DIETARY PATTERNS FOR ZONE 2 FOLLOW.                                    CARD   80
         2                                                                      CARD   81
   3.70E02   6.90E00         0    1.90E02   1.10E02   9.50E01                   CARD   82
         3         4         0                                                  CARD   83
   3.70E02   6.90E00         0    1.90E02   1.10E02   9.50E01                   CARD   84
         3         4   3.00E02                                                  CARD   85
C THE TWO DIETARY PATTERNS FOR ZONE 3 FOLLOW.                                    CARD   86
         2                                                                      CARD   87
   3.70E02   6.90E00         0    1.90E02   1.10E02   9.50E01                   CARD   88
         3         4         0                                                  CARD   89
   3.70E02   6.90E00         0    1.90E02   1.10E02   9.50E01                   CARD   90
         3         4   3.00E02                                                  CARD   91
C THE DATA READ BY SUBROUTINE DATA5 FOLLOWS. THIS DATA IS USED BY SUB-           CARD   92
C ROUTINE INHALE IN THE CALCULATION OF RADIONUCLIDE INHALATION. INHALA-          CARD   93
C TION RATE IS THE ADULT RATE FROM TABLE E-4, P. 1.109-39, OF U. S. NRC          CARD   94
C REGULATORY GUIDE 1.109 (OCTOBER, 1977). CONCENTRATION OF SUSPENDED             CARD   95
C MATERIAL IS SELECTED TO BE REPRESENTATIVE OF CONCENTRATIONS LISTED IN          CARD   96
C TABLE 1.4-5, P. 66, OF THE HANDBOOK OF ENVIRONMENTAL CONTROL, VOL-             CARD   97
C UME 1.                                                                         CARD   98
         1                                                                      CARD   99
C THE INHALATION PATTERN FOR ZONE 1 FOLLOWS.                                     CARD  100
         1                                                                      CARD  101
         2  3.50E-09   8.00E03   1.00E00                                        CARD  102
C THE INHALATION PATTERN FOR ZONE 2 FOLLOWS.                                     CARD  103
         1                                                                      CARD  104
         2  3.50E-09   8.00E03   1.00E00                                        CARD  105
C THE INHALATION PATTERN FOR ZONE 3 FOLLOWS.                                     CARD  106
         1                                                                      CARD  107
         2  3.50E-09   8.00E03   1.00E00                                        CARD  108
C THE DATA READ BY SUBROUTINE ALTER FOLLOWS. THIS DATA IS USED TO DEFINE         CARD  109
C AND IMPLEMENT ALTERATIONS TO THE COEFFICIENTS IN THE RADIONUCLIDE              CARD  110
C TRANSPORT EQUATIONS.                                                           CARD  111
         0                                                                      CARD  112
C THE DATA READ BY SUBROUTINE ADD FOLLOWS. THIS DATA IS USED TO DEFINE           CARD  113
C AND IMPLEMENT ADDITIONAL COEFFICIENTS IN THE RADIONUCLIDE TRANSPORT            CARD  114
C EQUATIONS.                                                                     CARD  115
         0                                                                      CARD  116
C THE DATA READ BY SUBROUTINE REDUCE FOLLOWS. THIS DATA IS USED TO DE-           CARD  117
C FINE AND IMPLEMENT A REDUCTION IN THE NUMBER OF RADIONUCLIDE TRANSPORT         CARD  118
C EQUATIONS.                                                                     CARD  119
         0                                                                      CARD  120
C THE DATA READ BY SUBROUTINE INITIAL FOLLOWS. THIS DATA IS USED TO SET          CARD  121
C THE INITIAL VALUE CONDITIONS FOR THE RADIONUCLIDE TRANSPORT EQUATIONS.         CARD  122
         1                                                                      CARD  123
```

Table 4-2

Discussion of Input Data for Example 3

Cards[a]	Discussion	Sections[b]
1-6	Comments for DATA1	4.2.1.1
7	Option for DATA1	4.2.1.2
8	Number of zones	4.2.2.1
9-14	Description of groundwater subzones	4.2.2.2
15-20	Description of soil subzones	4.2.2.3
21-29	Description of surface-water subzones	4.2.2.4
30-35	Description of sediment subzones	4.2.2.5
36-39	Comments for DATA2	4.3.1.1
40	Option for DATA2	4.3.1.2
41	Number of radionuclides	4.3.2.1
42-43	Description of decay chain	4.3.2.2
44-45	Description of decay pattern	4.3.2.3
46-48	Description of distribution coefficients	4.3.2.4
49-50	Description of concentration ratios	4.3.2.5
51-53	Description of radionuclide input rates	4.3.2.6
54-56	Comments for DATA3	4.4.1.1
57	Option for DATA3	4.4.1.2
58	Minimum coefficient size	4.4.2.1
59	Parameters for GEARB	4.4.2.2
60-61	Comments for DATAM	4.5.1.1
62	Option for DATAM	4.5.1.2
63	Option for MANAGE	4.5.2.1
64	Solution of transport equations	4.5.2.2
65	Subroutine selection for SOL, CONC, INGEST, INHALE, and EXT	4.5.2.3
66	Subroutine options	4.5.2.4
67-70	Comments for DATA4	4.6.1.1
71	Option for DATA4	4.6.1.2
72	Comments for agricultural parameters	4.6.3.1
73	Option for agricultural parameters	4.6.3.2

---

[a] Data card number in Table 4-1.

[b] Location of additional discussion in user manual (Hel81b).

Table 4-2 (Continued)

Cards[a]	Discussion	Sections[b]
74	Comments for ingestion patterns in zone 1	4.6.3.5
75	Number of ingestion patterns in zone 1	4.6.3.6
76-79	Description of ingestion patterns in zone 1	4.6.3.7
80-91	Comments for, numbers of and descriptions of ingestion patterns in zones 2 and 3. Similar to cards 74 through 79.	
92-98	Comments for DATA5	4.7.1.1
99	Option for DATA5	4.7.1.2
100	Comments for inhalation patterns in zone 1	4.7.3.1
101	Number of inhalation patterns in zone 1	4.7.3.2
102	Description of inhalation patterns in zone 1	4.7.3.3
103-108	Comments for, numbers of and descriptions of inhalation patterns in zones 2 and 3. Similar to cards 100 through 104.	
109-111	Comments for ALTER	4.9.1.1
112	Option for ALTER	4.9.1.2
113-115	Comments for ADD	4.10.1.1
116	Option for ADD	4.10.1.2
117-119	Comments for REDUCE	4.11.1.1
120	Option for REDUCE	4.11.1.2
121-122	Comments for INITIAL	4.12.1.1
123	Option for INITIAL	4.12.1.2

---

[a] Data card number in Table 4-1.

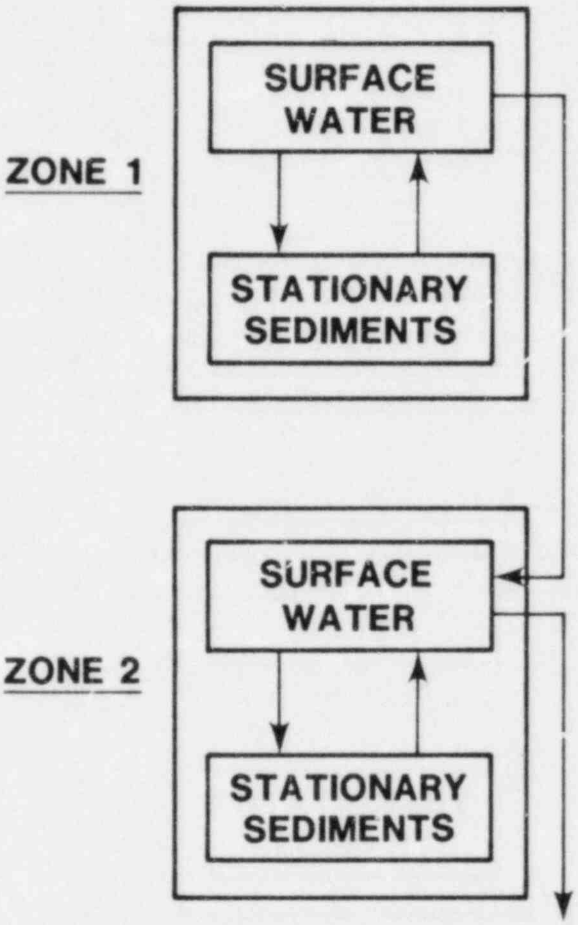
[b] Location of additional discussion in user manual (Hel81b).

CHAPTER 5

Example 4

This chapter presents an example which involves two zones. Each zone corresponds to a stretch of river and the stationary sediments beneath that stretch. For each zone, subroutine REDUCE is used to eliminate the groundwater and soil subzones. The groundwater and soil subzones are assigned nominal water volumes and solid masses of 1.0; this prevents the possibility of division by zero. A decay chain involving Cm246, Pu242, U238, Pu238 and U234 is considered. Each radionuclide enters the surface-water subzone of the first zone at the rate of 1.0 mg/yr and also the sediment subzone of the first zone at the rate of 1.0 mg/yr. No ingestion or inhalation calculations are performed. To reduce the amount of output, the print flags in subroutines COEF and MATPRT have been set to zero; this eliminates the printing of the coefficients for movement out of the individual compartments and the coefficient matrix for the radionuclide transport equations.

The general nature of example 4 is indicated in Figure 5-1. Then, the input data to PATH1 associated with this example are listed in Table 5-1, and the location in the user manual (Hel81b) of additional discussion of the card deck presented in Table 5-1 is indicated in Table 5-2. Finally, the model output corresponding to the input in Table 5-1 is listed on microfiche attached at the end of the report.



RADIONUCLIDES: Cm246, Pu242, U238,
Pu238, U234
NO INGESTION OR INHALATION

Figure 5-1. Example 4.

Table 5-1

Input Data for Example 4

```
C THE DATA READ BY SUBROUTINE DATA1 FOLLOWS. THIS DATA DESCRIBES A SITE     CARD     1
C INVOLVING TWO ZONES. ONLY THE SURFACE WATER AND SEDIMENT SUBZONES ARE     CARD     2
C USED. THE DATA IS SIMILAR TO WHAT MIGHT BE USED FOR THE COLUMBIA RIVER    CARD     3
C NEAR HANFORD. EACH ZONE IS A 30 MILE LENGTH OF RIVER.                     CARD     4
         1                                                                  CARD     5
         2                                                                  CARD     6
       1.0       1.0         0         0         0         0                CARD     7
         0         0         0         0                                    CARD     8
       1.0       1.0         0         0         0         0                CARD     9
         0         0         0         0                                    CARD    10
       1.0       1.0         0         0         0         0                CARD    11
         0         0                                                        CARD    12
       1.0       1.0         0         0         0         0                CARD    13
         0         0                                                        CARD    14
    8.6E09    7.9E05         0         0         0         0                CARD    15
         0    5.2E08    1.0E13    9.5E08         0         0                CARD    16
         2                                                                  CARD    17
    1.8E10    2.2E06         0         0         0         0                CARD    18
         0    2.2E05    1.5E13    1.8E09         0         0                CARD    19
         3                                                                  CARD    20
    1.3E09    5.2E09         0         0         0    5.2E08                CARD    21
         0         0                                                        CARD    22
    7.3E09    2.9E10         0         0         0    2.9E09                CARD    23
         0         0                                                        CARD    24
C THE DATA READ BY SUBROUTINE DATA2 FOLLOWS. THIS DATA DESCRIBES A DECAY    CARD    25
C SEGMENT INVOLVING CM246, PU242, U238, PU238 AND U234. BOTH U238 AND       CARD    26
C PU238 DECAY TO U234. EACH RADIONUCLIDE ENTERS THE SURFACE WATER           CARD    27
C SUBZONE OF ZONE 1 AT THE RATE OF 1.0 MG/YR AND THE SEDIMENT SUBZONE       CARD    28
C OF ZONE 1 AT THE RATE OF 1.0 MG/YR. CONCENTRATION RATIOS ARE FROM         CARD    29
C TABLE A-8, P. 1.109-31, AND TABLE C-5, P. 1.109-56, OF U. S. NRC REGU-    CARD    30
C LATORY GUIDE 1.109 (MARCH, 1976).                                         CARD    31
         1                                                                  CARD    32
         5                                                                  CARD    33
     CM246   2.46E02   4.71E03         1                                    CARD    34
     PU242   2.42E02   3.79E05         1                                    CARD    35
      U238   2.38E02   4.51E09         1                                    CARD    36
     PU238   2.38E02   8.90E01         1                                    CARD    37
      U234   2.34E02   2.47E05         1                                    CARD    38
         2    1.0E00                                                        CARD    39
         3    1.0E00                                                        CARD    40
         5    1.0E00                                                        CARD    41
         5    1.0E00                                                        CARD    42
         6    1.0E00                                                        CARD    43
         1                                                                  CARD    44
    1.5E03    1.5E03    1.5E03    1.5E03                                    CARD    45
    1.0E03    1.0E03    1.0E03    1.0E03                                    CARD    46
    5.0E02    5.0E02    5.0E02    5.0E02                                    CARD    47
    1.0E03    1.0E03    1.0E03    1.0E03                                    CARD    48
    5.0E02    5.0E02    5.0E02    5.0E02                                    CARD    49
    1.0E00    2.5E01    1.0E03   2.5E-03   5.0E-06   2.0E-04                CARD    50
    1.0E00    3.5E00    1.0E02   2.5E-04   2.0E-06   1.4E-05                CARD    51
    1.0E00    2.0E00    6.0E01   2.5E-03   5.0E-04   3.4E-04                CARD    52
    1.0E00    3.5E00    1.0E02   2.5E-04   2.0E-06   1.4E-05                CARD    53
    1.0E00    2.0E00    6.0E01   2.5E-03   5.0E-04   3.4E-04                CARD    54
         1                                                                  CARD    55
         0         0    2.4E18    2.4E18                                    CARD    56
         0         0    2.5E18    2.5E18                                    CARD    57
         0         0    2.5E18    2.5E18                                    CARD    58
         0         0    2.5E18    2.5E18                                    CARD    59
         0         0    2.6E18    2.6E18                                    CARD    60
```

Table 5-1 (Continued)

```
C THE DATA READ BY SUBROUTINE DATA3 FOLLOWS. THIS DATA CONTROLS THE         CARD    61
C OPERATION OF THE DIFFERENTIAL EQUATION SOLVER USED FOR THE RADIONU-       CARD    62
C CLIDE TRANSPORT EQUATIONS.                                                CARD    63
         1                                                                  CARD    64
   1.0E-10                                                                  CARD    65
   1.0E-20   1.0E-09        11         1                                    CARD    66
C THE DATA READ BY SUBROUTINE DATAM FOLLOWS. THIS DATA IS USED BY SUB-      CARD    67
C ROUTINE MANAGE TO CONTROL THE OPERATION OF THE PATHWAYS MODEL.            CARD    68
         1                                                                  CARD    69
         1                                                                  CARD    70
         1         0       1.0         2                                    CARD    71
         1         1        -1        -1        -1                          CARD    72
         1         1         0         0         0                          CARD    73
C THE DATA READ BY SUBROUTINE DATA4 FOLLOWS. THIS DATA IS USED BY SUB-      CARD    74
C ROUTINE INGEST TO PERFORM INGESTION CALCULATIONS.                         CARD    75
C NO INGESTION DATA IS READ IN THIS EXAMPLE.                                CARD    76
         0                                                                  CARD    77
C THE DATA READ BY SUBROUTINE DATA5 FOLLOWS. THIS DATA IS USED BY SUB-      CARD    78
C ROUTINE INHALE TO PERFORM INHALATION CALCULATIONS.                        CARD    79
C NO INHALATION DATA IS READ IN THIS EXAMPLE.                               CARD    80
         0                                                                  CARD    81
C THE DATA READ BY SUBROUTINE ALTER FOLLOWS. THIS DATA IS USED TO DEFINE    CARD    82
C AND IMPLEMENT ALTERATIONS TO THE COEFFICIENTS IN THE RADIONUCLIDE         CARD    83
C TRANSPORT EQUATIONS.                                                      CARD    84
         0                                                                  CARD    85
C THE DATA READ BY SUBROUTINE ADD FOLLOWS. THIS DATA IS USED TO DEFINE      CARD    86
C AND IMPLEMENT ADDITIONAL COEFFICIENTS IN THE RADIONUCLIDE TRANSPORT       CARD    87
C EQUATIONS.                                                                CARD    88
         0                                                                  CARD    89
C THE DATA READ BY SUBROUTINE REDUCE FOLLOWS. THIS DATA IS USED TO DE-      CARD    90
C FINE AND IMPLEMENT A REDUCTION IN THE NUMBER OF RADIONUCLIDE TRANSPORT    CARD    91
C EQUATIONS.                                                                CARD    92
         2                                                                  CARD    93
         1                                                                  CARD    94
         0         0         1         1                                    CARD    95
C THE DATA READ BY SUBROUTINE INITIAL FOLLOWS. THIS DATA IS USED TO SET     CARD    96
C THE INITIAL VALUE CONDITIONS FOR THE RADIONUCLIDE TRANSPORT EQUATIONS.    CARD    97
         1                                                                  CARD    98
```

Table 5-2

Discussion of Input Data for Example 4

Cards[a]	Discussion	Sections[b]
1-4	Comments for DATA1	4.2.1.1
5	Option for DATA1	4.2.1.2
6	Number of zones	4.2.2.1
7-10	Description of groundwater subzone	4.2.2.2
11-14	Description of soil subzone	4.2.2.3
15-20	Description of surface-water subzone	4.2.2.4
21-24	Description of sediment subzone	4.2.2.5
25-31	Comments for DATA2	4.3.1.1
32	Option for DATA2	4.3.1.2
33	Number of radionuclides	4.3.2.1
34-38	Description of decay chain	4.3.2.2
39-43	Description of decay pattern	4.3.2.3
44-49	Description of distribution coefficients	4.3.2.4
50-54	Description of concentration ratios	4.3.2.5
55-60	Description of radionuclide input rates	4.3.2.6
61-63	Comments for DATA3	4.4.1.1
64	Option for DATA3	4.4.1.2
65	Minimum coefficient size	4.4.2.1
66	Parameters for GEARB	4.4.2.2
67-68	Comments for DATAM	4.5.1.1
69	Option for DATAM	4.5.1.2
70	Option for MANAGE	4.5.2.1
71	Solution of transport equations	4.5.2.2
72	Subroutine selection for SOL, CONC, INGEST, INHALE, and EXT	4.5.2.3
73	Subroutine options	4.5.2.4
74-76	Comments for DATA4	4.6.1.1
77	Option for DATA4	4.6.1.2
78-80	Comments for DATA5	4.7.1.1
81	Option for DATA5	4.7.1.2
82-84	Comments for ALTER	4.9.1.1
85	Option for ALTER	4.9.1.2
86-88	Comments for ADD	4.10.1.1
89	Option for ADD	4.10.1.2

---

[a] Data card number in Table 5-1.

[b] Location of additional discussion in user manual (Hel81b).

Table 5-2 (Continued)

Cards[a]	Discussion	Sections[b]
90-92	Comments for REDUCE	4.11.1.1
93	Option for REDUCE	4.11.1.2
94	Pattern for equations to be zeroed	4.11.4.1
95	Subzones to be considered	4.11.4.2
96-97	Comments for INITIAL	4.12.1.1
98	Option for INITIAL	4.12.1.2

---

[a] Data card number in Table 5-1.

[b] Location of additional discussion in user manual (Hel81b).

CHAPTER 6

Example 5

This chapter illustrates several options which exist within PATH1. A site involving five subzones is considered. The first three zones involve stretches of river. The fourth zone is a bay or estuary; unlike the first three zones, it does not have soil or groundwater subzones. The fifth zone is introduced to record the total amount of radionuclide which has discharged from the fourth zone. Specifically, the surface-water subzone of the fifth zone is used to keep track of the radionuclides which have discharged from the surface-water subzone of the fourth zone, and the sediment subzone of the fifth zone is used to keep track of the radionuclides which have been trapped in the sediment subzone of the fourth zone. The radionuclides considered are Cs137 and Sr90.

Subroutine REDUCE is used to eliminate the unused subzones in the fourth and fifth zones. Subroutine ALTER is used to alter the definition of flows for the soil subzone of the first zone and the destination of the flows for the sediment subzone of the fourth zone. In the latter case, the flows are changed "from the sediment subzone of the fourth zone to a sink" to "from the sediment subzone of the fourth zone to the sediment subzone of the fifth zone." Subroutine INITIAL is used to set the initial values of the radionuclide transport equations to one curie for each radionuclide in the soil subzone of the first zone and to zero everywhere else. Further, the rate of input to the system is taken to be zero. To reduce the amount of output, the print flags in subroutines COEF and MATPRT have been set to zero; this eliminates the printing of the coefficients for movement out of the individual compartments and the coefficient matrix for the radionuclide transport equations.

The general nature of example 5 is indicated in Figure 6-1. Then, the input data to PATH1 associated with this example are listed in Table 6-1, and the location in the user manual (Hel81b) of additional discussion of the card deck presented in Table 6-1 is indicated in Table 6-2. Finally, the model output corresponding to the input in Table 6-1 is listed on microfiche attached at the end of the report.

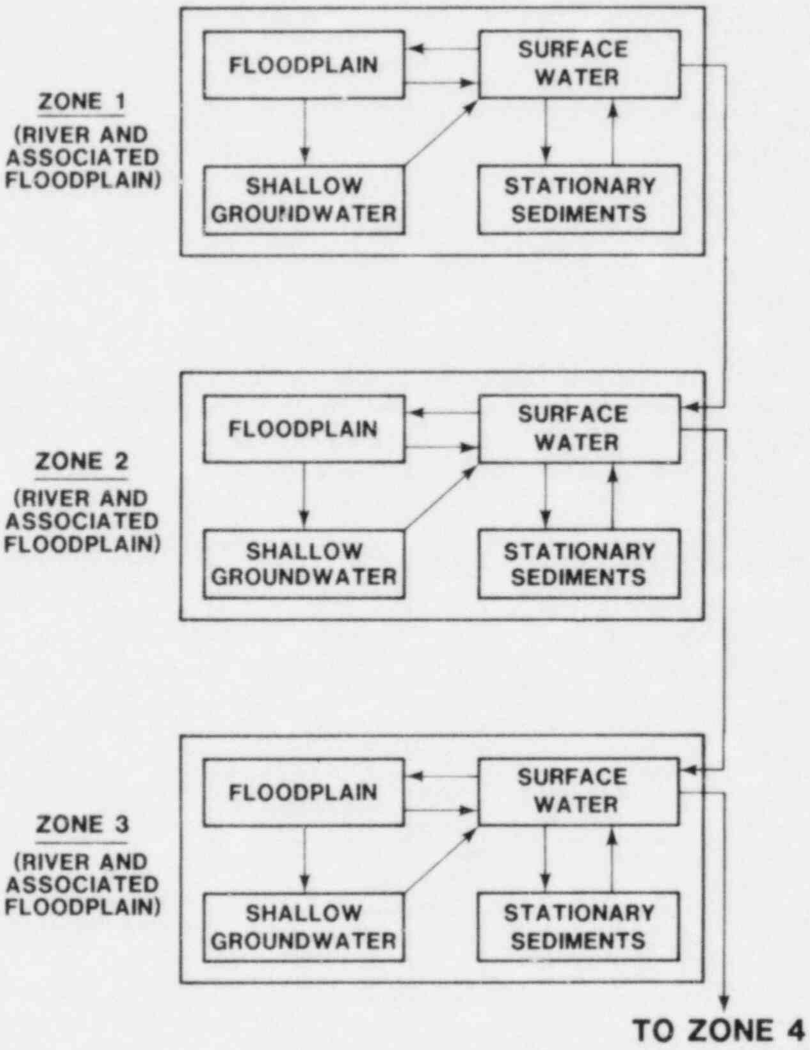
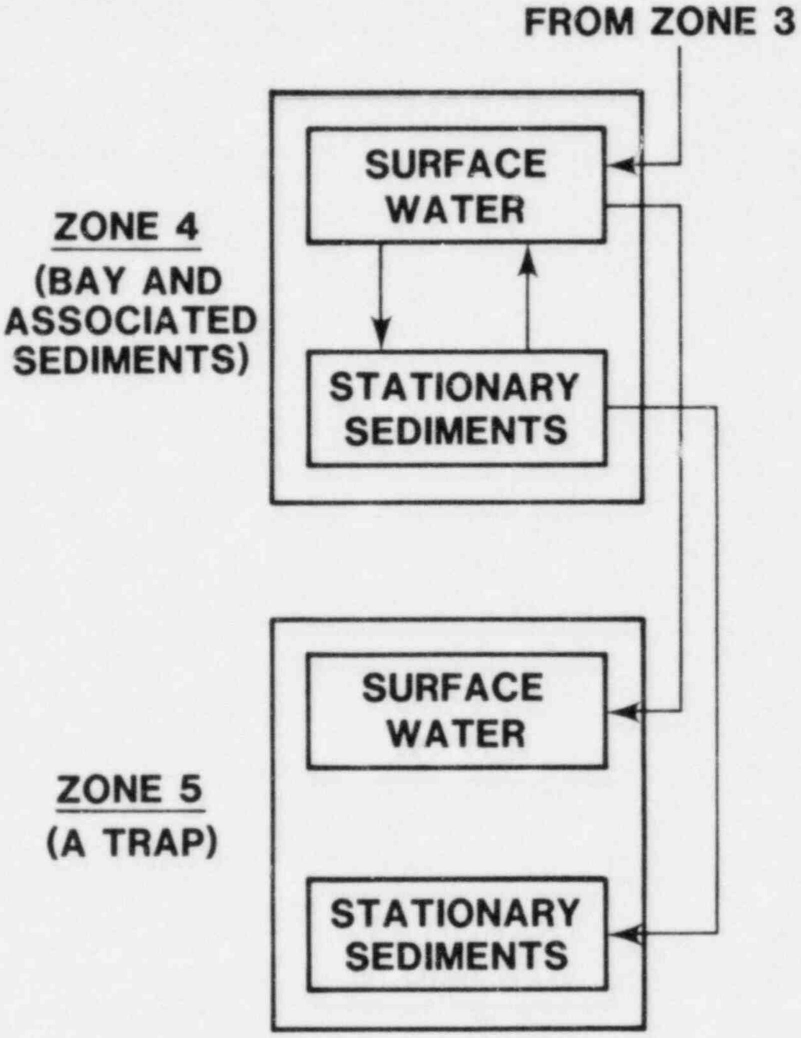


Figure 6-1. Example 5.



RADIONUCLIDES: Cs137, Sr90
NO INGESTION OR INHALATION

Figure 6-1. (Continued).

Table 6-1

Input Data for Example 5

```
C THE DATA READ BY SUBROUTINE DATA1 FOLLOWS. THIS DATA DESCRIBES A SITE     CARD   1
C INVOLVING 5 ZONES. THE FIRST THREE ZONES ARE OBTAINED BY SCALING ZONE     CARD   2
C 1 USED IN A SENSITIVITY ANALYSIS OF THE PATHWAYS MODEL. DEFINITION        CARD   3
C AND/OR DERIVATION OF THE PARAMETERS WHICH DEFINE THIS ZONE ARE CON-       CARD   4
C TAINED IN CHAPTER 2 OF HELTON AND IMAN, RISK METHODOLOGY FOR GEOLOGIC     CARD   5
C DISPOSAL OF RADIOACTIVE WASTE: SENSITIVITY ANALYSIS OF THE ENVIRONMEN-    CARD   6
C TAL TRANSPORT MODEL (DECEMBER, 1980). THE SCALE FACTORS FOR THE FIRST     CARD   7
C THREE ZONES ARE 0.25, 1.0 AND 15.0, RESPECTIVELY. ZONE 4 CORRESPONDS      CARD   8
C TO AN ESTUARY OR BAY. ZONE 5 IS USED TO CALCULATE THE QUANTITY OF UN-     CARD   9
C DECAYED RADIONUCLIDES WHICH HAVE DISCHARED FROM THE SYSTEM.               CARD  10
         1                                                                  CARD  11
         5                                                                  CARD  12
    3.5E11    2.4E12         0         0    5.5E11         0                CARD  13
         0         0         0         0                                    CARD  14
    1.4E12    9.4E12         0         0    2.2E12         0                CARD  15
         0         0         0         0                                    CARD  16
    2.1E13    1.4E14         0         0    3.3E13         0                CARD  17
         0         0         0         0                                    CARD  18
    1.0E00    1.0E00         0         0         0         0                CARD  19
         0         0         0         0                                    CARD  20
    1.0E00    1.0E00         0         0         0         0                CARD  21
         0         0                                                        CARD  22
    5.0E09    2.8E10    2.4E10         0    1.0E10    2.8E07                CARD  23
         0         0                                                        CARD  24
    2.0E10    1.1E11    9.8E10         0    4.0E10    1.1E08                CARD  25
         0         0                                                        CARD  26
    3.0E11    1.6E12    1.5E12         0    6.0E11    1.6E09                CARD  27
         0         0                                                        CARD  28
    1.0E00    1.0E00         0         0         0         0                CARD  29
         0         0                                                        CARD  30
    1.0E00    1.0E00         0         0         0         0                CARD  31
         0         0                                                        CARD  32
    5.5E09    8.5E05         0         0         0         0                CARD  33
    2.2E08    5.8E08    1.5E13    2.3E09         0         0                CARD  34
         2                                                                  CARD  35
    2.2E10    3.5E06         0         0    4.0E10    1.1E08                CARD  36
    2.7E08    2.3E08    1.9E13    3.0E09         0         0                CARD  37
         3                                                                  CARD  38
    3.3E11    5.3E07         0         0    6.0E11    1.6E09                CARD  39
    1.3E10    3.4E10    7.9E13    2.0E10         0         0                CARD  40
         4                                                                  CARD  41
    9.0E12    4.5E08         0         0         0         0                CARD  42
    1.5E11    4.0E11    2.4E14    9.8E09         0         0                CARD  43
         5                                                                  CARD  44
    1.0E00    1.0E00         0         0         0         0                CARD  45
         0         0         0         0         0         0                CARD  46
         6                                                                  CARD  47
    2.2E09    5.8E09         0         0    2.2E08    5.8E08                CARD  48
         0         0                                                        CARD  49
    8.7E09    2.3E10         0         0    8.7E08    2.3E09                CARD  50
         0         0                                                        CARD  51
    1.3E11    3.4E11         0         0    1.3E10    3.4E10                CARD  52
         0         0                                                        CARD  53
    3.0E11    7.8E11         0         0    1.5E11    3.9E11                CARD  54
    3.8E09    9.8E09                                                        CARD  55
    1.0E00    1.0E00         0         0         0         0                CARD  56
         0         0                                                        CARD  57
```

Table 6-1 (Continued)

```
C THE DATA READ BY SUBROUTINE DATA2 FOLLOWS. THIS DATA DESCRIBES                    CARD    58
C CS137 AND SR90. CONCENTRATION RATIOS ARE FROM TABLE A-8, P.1.109-                 CARD    59
C 31, AND TABLE C-5, P. 1.109-56, OF U. S. NRC REGULATORY GUIDE                     CARD    60
C 1.109 (MARCH, 1976).                                                              CARD    61
         1                                                                          CARD    62
         2                                                                          CARD    63
     CS137   1.37E02    3.0E01          1                                           CARD    64
      SR90    9.0E01    2.8E01          1                                           CARD    65
         3   1.00E00                                                                CARD    66
         3   1.00E00                                                                CARD    67
         5                                                                          CARD    68
    1.0E03    1.0E03    1.0E03    1.0E03                                            CARD    69
    1.5E02    1.5E02    1.5E02    1.5E02                                            CARD    70
    1.0E03    1.0E03    1.0E03    1.0E03                                            CARD    71
    1.5E02    1.5E02    1.5E02    1.5E02                                            CARD    72
    1.0E03    1.0E03    1.0E03    1.0E03                                            CARD    73
    1.5E02    1.5E02    1.5E02    1.5E02                                            CARD    74
    1.0E02    1.0E02    1.0E02    1.0E02                                            CARD    75
    1.5E01    1.5E01    1.5E01    1.5E01                                            CARD    76
         0         0         0         0                                            CARD    77
         0         0         0         0                                            CARD    78
    1.0E00    1.0E03    1.0E02   1.0E-02   1.2E-02   4.0E-03                        CARD    79
    1.0E00    3.0E01    1.0E02   1.7E-02   8.0E-04   6.0E-04                        CARD    80
         1                                                                          CARD    81
         0         0         0         0                                            CARD    82
         0         0         0         0                                            CARD    83
C THE DATA READ BY SUBROUTINE DATA3 FOLLOWS. THIS DATA CONTROLS THE OP-             CARD    84
C ERATION OF THE DIFFERENTIAL EQUATION SOLVER USED FOR THE RADIONUCLIDE             CARD    85
C TRANSPORT EQUATIONS.                                                              CARD    86
         1                                                                          CARD    87
   1.0E-10                                                                          CARD    88
   1.0E-20   1.0E-10        21         1                                            CARD    89
C THE DATA READ BY SUBROUTINE DATAM FOLLOWS. THIS DATA IS USED BY SUB-              CARD    90
C ROUTINE MANAGE TO CONTROL THE OPERATION OF THE PATHWAYS MODEL.                    CARD    91
         1                                                                          CARD    92
         1                                                                          CARD    93
         2         0    1.0E01         2                                            CARD    94
         1         1        -1        -1        -1                                  CARD    95
         1         1         0         0         0                                  CARD    96
C THE DATA READ BY SUBROUTINE DATA4 FOLLOWS. THIS DATA IS USED BY SUB-              CARD    97
C ROUTINE INGEST TO PERFORM INGESTION CALCULATIONS.                                 CARD    98
C NO INGESTION DATA IS READ IN THIS EXAMPLE.                                        CARD    99
         0                                                                          CARD   100
C THE DATA READ BY SUBROUTINE DATA5 FOLLOWS. THIS DATA IS USED BY SUB-              CARD   101
C ROUTINE INHALE TO PERFORM INHALATION CALCULATIONS.                                CARD   102
C NO INHALATION DATA IS READ IN THIS EXAMPLE.                                       CARD   103
         0                                                                          CARD   104
C THE DATA READ BY SUBROUTINE ALTER FOLLOWS. THIS DATA IS USED TO DEFINE            CARD   105
C AND IMPLEMENT ALTERATIONS TO THE COEFFICIENTS IN THE RADIONUCLIDE                 CARD   106
C TRANSPORT EQUATIONS.                                                              CARD   107
         1                                                                          CARD   108
         4                                                                          CARD   109
         2         2       .10         3                                            CARD   110
         6         2       .10         7                                            CARD   111
        28         3   1.3E-02        36                                            CARD   112
        32         3   1.3E-02        40                                            CARD   113
C THE DATA READ BY SUBROUTINE ADD FOLLOWS. THIS DATA IS USED TO DEFINE              CARD   114
C AND IMPLEMENT ADDITIONAL COEFFICIENTS IN THE RADIONUCLIDE TRANSPORT               CARD   115
C EQUATIONS.                                                                        CARD   116
         0                                                                          CARD   117
```

Table 6-1 (Continued)

```
C THE DATA READ BY SUBROUTINE REDUCE FOLLOWS. THIS DATA IS USED TO DE-         CARD  118
C FINE AND IMPLEMENT A REDUCTION IN THE NUMBER OF RADIONUCLIDE TRANSPORT        CARD  119
C EQUATIONS.                                                                    CARD  120
        2                                                                       CARD  121
        5                                                                       CARD  122
        1         1         1         1                                         CARD  123
        1         1         1         1                                         CARD  124
        1         1         1         1                                         CARD  125
        0         0         1         1                                         CARD  126
        0         0         1         1                                         CARD  127
C THE DATA READ BY SUBROUTINE INITIAL FOLLOWS. THIS DATA IS USED TO SET          CARD  128
C THE INITIAL VALUE CONDITIONS FOR THE RADIONUCLIDE TRANSPORT EQUATIONS.        CARD  129
        2                                                                       CARD  130
        0    5.2E19         0         0                                         CARD  131
        0    4.8E19         0         0                                         CARD  132
        0         0         0         0                                         CARD  133
        0         0         0         0                                         CARD  134
        0         0         0         0                                         CARD  135
        0         0         0         0                                         CARD  136
        0         0         0         0                                         CARD  137
        0         0         0         0                                         CARD  138
        0         0         0         0                                         CARD  139
        0         0         0         0                                         CARD  140
```

Table 6-2

Discussion of Input Data for Example 5

Cards[a]	Discussion	Sections[b]
1-10	Comments for DATA1	4.2.1.1
11	Option for DATA1	4.2.1.2
12	Number of zones	4.2.2.1
13-22	Description of groundwater subzone	4.2.2.2
23-32	Description of soil subzone	4.2.2.3
33-47	Description of surface-water subzone	4.2.2.4
48-57	Description of sediment subzone	4.2.2.5
58-61	Comments for DATA2	4.3.1.1
62	Option for DATA2	4.3.1.2
63	Number of radionuclides	4.3.2.1
64-65	Description of decay chain	4.3.2.2
66-67	Description of decay pattern	4.3.2.3
68-78	Description of distribution coefficients	4.3.2.4
79-80	Description of concentration ratios	4.3.2.5
81-83	Description of radionuclide input rates	4.3.2.6
84-86	Comments for DATA3	4.4.1.1
87	Option for DATA3	4.4.1.2
88	Minimum coefficient size	4.4.2.1
89	Parameters for GEARB	4.4.2.2
90-91	Comments for DATAM	4.5.1.1
92	Option for DATAM	4.5.1.2
93	Option for MANAGE	4.5.2.1
94	Solution of transport equations	4.5.2.2
95	Subroutine selection for SOL, CONC, INGEST, INHALE and EXT	4.5.2.3
96	Subroutine options	4.5.2.4
97-99	Comments for DATA4	4.6.1.1
100	Option for DATA4	4.6.1.2
101-103	Comments for DATA5	4.7.1.1
104	Option for DATA5	4.7.1.2
105-107	Comments for ALTER	4.9.1.1
108	Option for ALTER	4.9.1.2
109	Number of alterations	4.9.3.1
110-113	Description of alterations	4.9.3.2

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[a] Data card number in Table 6-1.

[b] Location of additional discussion in user manual (Fel81b).

Table 6-2 (Continued)

Cards[a]	Discussion	Sections[b]
114-116	Comments for ADD	4.10.1.1
117	Option for ADD	4.10.1.2
118-120	Comments for REDUCE	4.11.1.1
121	Option for REDUCE	4.11.1.2
122	Pattern for equations to be zeroed	4.11.4.1
123-127	Subzones to be considered	4.11.4.2
128-129	Comments for INITIAL	4.12.1.1
130	Option for INITIAL	4.12.1.2
131-140	Description of initial values	4.12.3

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[a] Data card number in Table 6-1.

[b] Location of additional discussion in user manual (Hel81b).

APPENDIX A

This appendix is a reprint of Chapter 2 and the reference list of (Hel80).

CHAPTER 2

REFERENCE SITE

2.1 INTRODUCTION

This chapter describes a site which is later modified to produce the sites used for the sensitivity analyses described in Chapters 3 and 5. Care is taken to describe the assumptions used to produce this site and the reasons for their adoption. From these assumptions, the input variables for the Environmental Transport Model are derived. In similar manner, the input variables for the Environmental Transport Model for sensitivity analysis A and sensitivity analysis B are derived in Chapters 3 and 5, respectively. Derivation of all model inputs is documented to permit examination of the assumptions underlying the sensitivity analysis results presented in Chapters 4 and 6. In the following discussions, it is assumed that the reader is familiar with the Environmental Transport Model; descriptions of the model are contained in this project's interim report (Ca78, Chapter 4) and in the model's user manual (He81b).

Section 2.2 contains a general description of the reference site. This site involves three zones and is defined to be consistent with the reference site described in the project's interim report (Ca78). The properties of the groundwater, soil, surface-water and sediment subzones are derived in Sections 2.3, 2.4, 2.5 and 2.6, respectively.

2.2 GENERAL DESCRIPTION

The hypothetical site described in this section is consistent with the reference site defined in Campbell et al (Ca78). The site is located in a symmetrical, upland valley which is drained by the river L. The upper end of the valley is elliptical with major and minor axes of length 350 km and 180 km, respectively; a waste repository is located on the minor axis 43 km from the river. Below the repository, the valley is assumed to have a constant width of 180 km. The preceding assumption is a slight deviation from the reference site given in Campbell et al (Ca78), where the valley is described as parabolic. This modification is made to permit the same aquifer discharge rates into river L to be used both at the repository and downstream from the repository. Figures 2-1 and 2-2 provide general representations of the site. Further, Table 2-1 contains a synopsis of important site characteristics.

Three zones are defined for this site, as shown in Figure 2-3. The first zone consists of a 40-km stretch of river, the stationary sediments beneath the river, a 2-km-wide strip of flood plain on each side of the river, and the portions of the upper sand and gravel aquifer which lie beneath the preceding strips of flood plain. This zone extends downstream from the point on river L opposite the repository. The second zone begins immediately below the first zone and consists of a lake 40 km in length, a layer of stationary sediments beneath the lake, a 2-km-

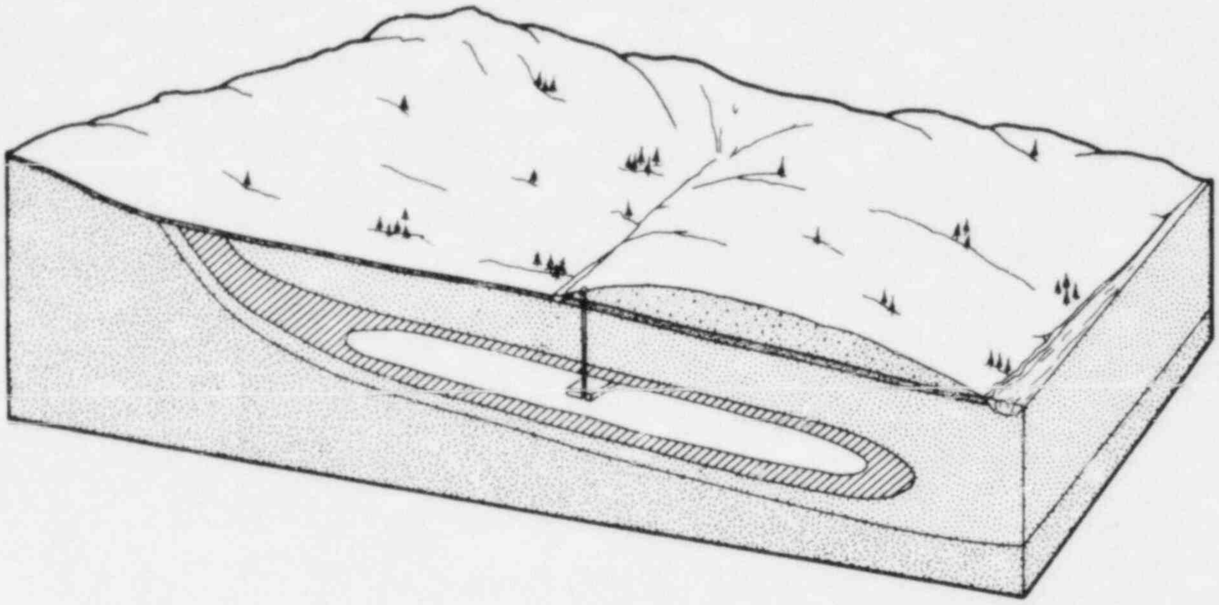

Figure 2-1. Physiographic Setting for Reference Site. One side of the symmetric basin is shown. The upper end of the valley is elliptic with the repository located on the minor axis; the sides of the valley are parallel below the repository.

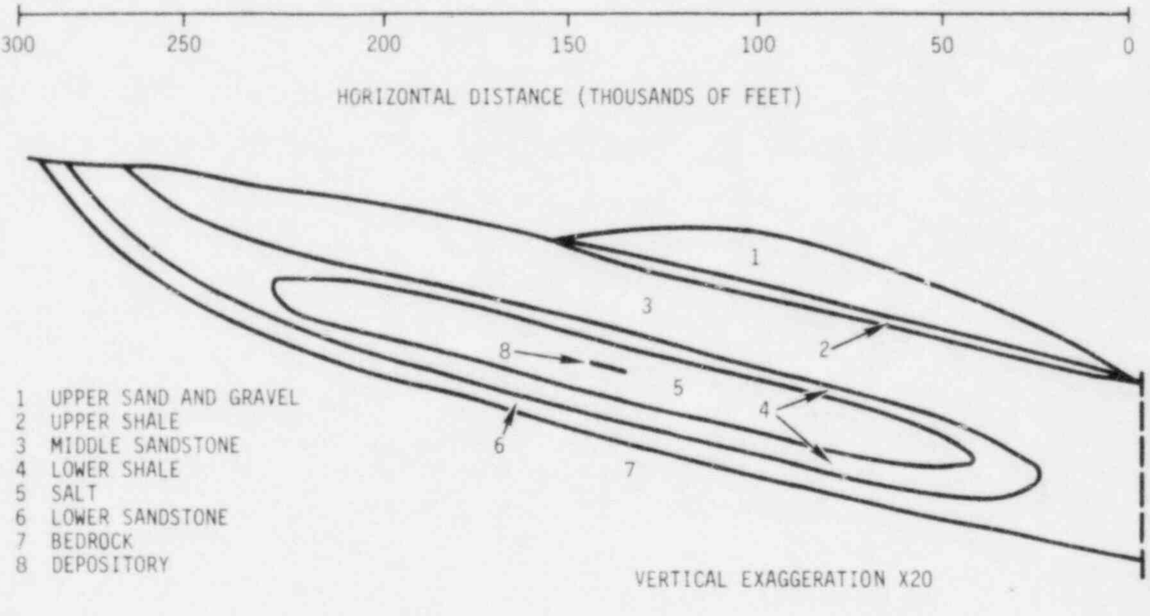

Figure 2-2. Geologic Cross Section at Reference Site. This figure is an adaptation of Figure 1.2.2 in Campbell et al (Ca78).

Table 2-1

Properties of the Reference Site*

Property	English Units	Metric Units
Rainfall	4.0×10^{1} in/yr	1.0×10^{0} m/yr
Water loss due to evapo-transpiration	1.6×10^{1} in/yr	4.1×10^{-1} m/yr
Recharge to groundwater system	2.4×10^{1} in/yr	6.1×10^{1} m/yr
Width of valley at and below repository	6.0×10^{5} ft	1.8×10^{5} m
Area of valley above repository	2.7×10^{11} ft^{2}	2.5×10^{10} m^{2}
Discharge of river L at repository	1.5×10^{9} ft^{3}/day	1.5×10^{13} L/yr
Discharge of upper sand and gravel aquifer (both sides of river)	1.6×10^{3} ft^{3}/day/ft	5.4×10^{7} L/yr/m
Discharge of middle sandstone aquifer (both sides of river)	1.5×10^{3} ft^{3}/day/ft	5.1×10^{7} L/yr/m
Total discharge to river (both sides of river)	3.1×10^{3} ft^{3}/day/ft	1.0×10^{8} L/yr/m

*These properties are obtained in Campbell et al (Ca78) where the aquifer discharge rates are given for one side of the river; the values in this table are for the discharges from both sides of the river and were obtained by doubling the discharge rates for one side of the river.

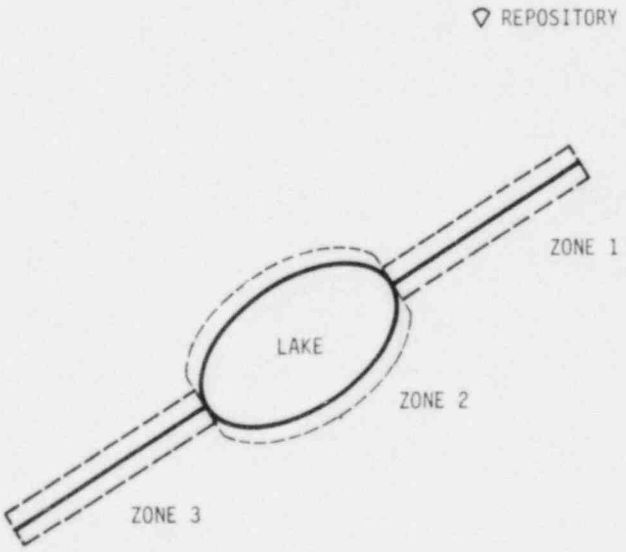

Figure 2-3. Zone Selection. Three zones are selected. Zones 1 and 3 contain portions of river L, and zone 2 contains a lake on river L. Each zone consists of a water body 40 km long, a layer of stationary sediments, a 2-km-wide strip of land on each side of the water body, and the portions of the upper sand and gravel aquifer which lie beneath the preceding strips of land.

wide strip of land on each side of the lake, and the portions of the upper sand and gravel aquifer which lie beneath the preceding strips of land. Further, the lake is assumed to be elliptical with major and minor axes of length 40 km and 6.4 km, respectively, and to contain a water volume equal to 1 year's flow of the river L at the head of the lake. The preceding assumptions result in the lake having a perimeter of 90 km and an area of 200 km^2. The third zone begins immediately below the second zone and consists of a 40-km stretch of river, the stationary sediments beneath the river, a 2-km-wide strip of flood plain on each side of the river, and the portions of the upper sand and gravel aquifer which lie beneath the preceding strips of flood plain. The zones are partitioned in a manner which results in the previously described strips of land in each zone having the same area. In subsequent sections, additional assumptions about zone properties are made, subzones are defined, and input variables for the Environmental Transport Model are derived.

2.3 GROUNDWATER SUBZONES

For each zone, the groundwater subzone is taken to be the portion of the upper sand and gravel aquifer extending from the bottom of the soil subzone to the top of the upper shale layer, which is assumed to be impermeable. The layer comprising the groundwater subzones is assumed to have an average thickness of 30 metres, a porosity of 30%, a saturation of 100% and a mean particle density of 2.8 g/cm^3. The porosity and density assumptions are consistent with representative values contained in Tables 2-2 and 2-3, respectively. Water is assumed to move directly from the groundwater subzones to the surface-water subzones; that is, there is no discharge from the groundwater subzones to soil or sediment subzones. This discharge is assumed to equal the discharge of the upper sand and gravel aquifer, which is 5.4×10^7 L/yr/m, and to involve only dissolved materials; specifically, there is no movement of solid material out of the groundwater subzones. However, if it was assumed that the river was eroding the groundwater subzones, then one might wish to include such a movement. The inclusion of groundwater subzones is not felt to be important and is done primarily for illustration. These subzones could also be used as second soil or sediment layers or omitted entirely.

The groundwater subzone properties which are supplied as input to the Environmental Transport Model are now derived. As required in Section 2.2, the zones are partitioned in a manner which results in the groundwater subzones having the same areas and volumes. In particular,

$$\begin{aligned} A(I) &= 2(2.0 \times 10^3 \text{ m})(4.0 \times 10^4 \text{ m}) \quad \text{for } I = 1, 2, 3 \\ &= 1.6 \times 10^8 \text{ m}^2 \end{aligned} \qquad (2.1)$$

and

$$\begin{aligned} V(I) &= (30 \text{ m})(1.6 \times 10^8 \text{ m}^2) \qquad \text{for } I = 1, 2, 3 \\ &= 4.8 \times 10^9 \text{ m}^3, \end{aligned} \qquad (2.2)$$

where A(I) and V(I) denote the area and volume, respectively, of the groundwater subzone of zone I. The amounts of water and solid material in the subzones are given by Equations (2.3) and (2.4).

Table 2-2

Porosity of Selected Sediments and Rocks*

Material	Porosity (Percent of Total Volume)
Sand (stream)	48
Sand and silt (glacial outwash)	36
Sand and gravel with large pebbles (glacial outwash)	25
Glacial clay (till), sandy and gravelly	21
Clays, assorted	45 (avg)
Silt (lake)	36
Silt and clay (Mississippi River delta)	80-90
Sandstone (gas bearing, Bartlesville, Okla.)	23 (avg)
Sandstone	16 (avg)
Limestone, marble, dolomite	5 (avg)
Granite, schist, gneiss, quartzite	<1

*From Dapples (Da59), p 313 (Table 9.4).

Table 2-3

Approximate Specific Gravities*

Substance	Specific Gravity
Andesite	2.66
Basalt, dense	2.90
Basalt, scoriaceous	2.15
Clay	2.20
Diabase	2.94
Diorite	2.86
Dolomite	2.80
Gabbro	2.98
Gneiss	2.65 - 2.80
Granite	2.65
Gravel, dry	1.55
Gravel, wet	2.00
Limestone	2.60
Marble	2.78
Quartz, porphyry	2.63
Rhyolite	2.50
Sand, dry	1.69
Sand, wet	2.25
Sandstone	2.60
Shale	2.70
Schist	2.69
Slate	2.75
Syenite	2.74
Trachyte	2.58

*From Cummins and Given (Cu73), p 34-31 (Table 34-20).

$$Z(1,1,I) = (4.8 \times 10^9\ \mathrm{m}^3)(0.30)(1.0 \times 10^3\ \mathrm{L/m}^3) \quad \text{for } I = 1,\ 2,\ 3$$

$$= 1.4 \times 10^{12}\ \mathrm{L} \tag{2.3}$$

and

$$Z(2,1,I) = (4.8 \times 10^9\ \mathrm{m}^3)(0.70)(2.8 \times 10^3\ \mathrm{kg/m}^3) \quad \text{for } I = 1,\ 2,\ 3$$

$$= 9.4 \times 10^{12}\ \mathrm{kg}, \tag{2.4}$$

respectively. Further, water movement from groundwater subzones to surface-water subzones is given by

$$Z(5,1,I) = (5.4 \times 10^7\ \mathrm{L/yr/m})(4.0 \times 10^4\ \mathrm{m}) \quad \text{for } I = 1,\ 2,\ 3$$

$$= 2.2 \times 10^{12}\ \mathrm{L/yr}. \tag{2.5}$$

All other inputs which can be supplied to the Environmental Transport Model for groundwater subzones are taken to be zero. The groundwater subzone properties obtained in this section are summarized in Table 2-4.

2.4 SOIL SUBZONES

For zones 1 and 3, the soil subzone is assumed to be a 2-km-wide strip on each side of the river. These strips are assumed to have a depth of 0.5 metre, a porosity of 50%, a saturation of 50%, and a mean particle density of 2.8 g/cm^3. The porosity and density assumptions are consistent with representative values contained in Table 2-5. Water flow through the soil to the groundwater below is 0.60 m/yr. Movement of water and solid material between these two soil subzones ard their associated surface-water subzones is assumed to be due to overbank flooding. Rates for such movements are both site specific and difficult to obtain. The following values are selected for use:

1. Annual water flow from a soil subzone to the corresponding surface-water subzone is the water volume required to fill the pore space of the soil subzone (see Equation (2.11)).
2. Annual solid flow from a soil subzone to the corresponding surface-water subzone is 10^{-3} of the mass of solids contained in the soil subzone (see Equation (2.12)).

In subsequent sensitivity analyses, the two preceding rates will be varied over a range of values to determine their impact on predictions made by the Environmental Transport Model. To maintain equilibrium, it is assumed that movement from the surface-water subzones to the soil subzones is equal to movement from the soil subzones to the surface-water subzones.

For zone 2, the soil subzone is assumed to be a 2-km-wide strip on each side of the lake. Soil subzone properties for zone 2 are taken to be the same as the soil subzone properties for zones 1 and 3 with the exception that water and solid material movements between the subzone and the corresponding surface-water subzone are defined differently. For this zone, such movements are assumed to result from an irrigation rate of 0.30 m/yr. The water is withdrawn from the lake and contains

Table 2-4

Groundwater Subzone Properties for Reference Site

Property	Zone 1	Zone 2	Zone 3
Z(1,1,I)	1.4×10^{12}	1.4×10^{12}	1.4×10^{12}
Z(2,1,I)	9.4×10^{12}	9.4×10^{12}	9.4×10^{12}
Z(3,1,I)	0	0	0
Z(4,1,I)	0	0	0
Z(5,1,I)	2.2×10^{12}	2.2×10^{12}	2.2×10^{12}
Z(6,1,I)	0	0	0
Z(7,1,I)	0	0	0
Z(8,1,I)	0	0	0
Z(9,1,I)	0	0	0
Z(10,1,I)	0	0	0

Z(1,1,I) = volume of water in subzone (in litres).

Z(2,1,I) = mass of solids in subzone (in kg).

Z(3,1,I) = rate of water outflow (in L/yr) from subzone to soil subzone.

Z(4,1,I) = rate of solid outflow (in kg/yr) from subzone to soil subzone.

Z(5,1,I) = rate of water outflow (in L/yr) from subzone to surface-water subzone.

Z(6,1,I) = rate of solid outflow (in kg/yr) from subzone to surface-water subzone.

Z(7,1,I) = rate of water outflow (in L/yr) from subzone to sediment subzone.

Z(8,1,I) = rate of solid outflow (in kg/yr) from subzone to sediment subzone.

Z(9,1,I) = rate of water outflow (in L/yr) from subzone to a sink.

Z(10,1,I) = rate of solid outflow (in kg/yr) from subzone to a sink.

Table 2-5

Porosity of Soils in Natural State[a]

Description	Porosity,[b] %	Void ratio[c]	Water content, %	Mass Per Unit Volume			
				g/cm^3		lb/ft^3	
				Dry	Sat	Dry	Sat
Uniform sand, loose	46	0.85	32	1.43	1.89	90	118
Uniform sand, dense	34	0.51	19	1.75	2.09	109	131
Mixed-grained sand, loose	40	0.67	25	1.59	1.99	99	124
Mixed-grained sand, dense	30	0.43	16	1.86	2.16	116	135
Glacial till, very mixed-grained	20	0.25	9	2.12	2.32	132	145
Soft glacial clay	55	1.2	45	--	1.77	--	111
Stiff glacial clay	37	0.6	22	--	2.07	--	129
Soft slightly organic clay	66	1.9	70	--	1.58	--	99
Soft very organic clay	75	3.0	110	--	1.43	--	89
Soft bentonite	84	5.2	194	--	1.27	--	79

[a] From *Soil Mechanics in Engineering Practice*, 2nd ed, K. Terzaghi and R. B. Peck (New York: John Wiley and Sons, 1967), p 28, Table 6.3.

[b] Porosity is the percentage ratio of volume of voids to total volume.

[c] Void ratio is the ratio of volume of voids to moist solids.

the same concentration of suspended solids as the lake. This defines a movement of water and solid material from the lake (i.e., the surface-water subzone) to the soil subzone. To maintain equilibrium, it is assumed that movement from the soil subzone to the surface-water subzone is equal to movement from the surface-water subzone to the soil subzone. Here, the tacit assumption is that runoff and erosional materials pass through the soil subzones without significant mixing with the materials that actually constitute the subzones. Such might be the case if runoff and erosional materials from the entire valley were primarily transported through the soil subzones to the surface-water subzones in stream channels. If this assumption was felt to be unreasonable for a given situation, the parameter definitions would have to modified in some appropriate manner. Such modifications are considered in analysis B.

The soil subzone properties which are supplied as input to the Environmental Transport Model are now derived. As required in Section 2.2., the zones are partitioned in a manner which results in the soil subzones having the same areas and volumes. In particular,

$$A(I) = 2(2.0 \times 10^3 \text{ m})(4.0 \times 10^4 \text{ m}) \quad \text{for } I = 1, 2, 3$$

$$= 1.6 \times 10^8 \text{ m}^2 \qquad (2.6)$$

and

$$V(I) = (0.50\ \mathrm{m})(1.6 \times 10^8\ \mathrm{m}^2) \quad \text{for } I = 1, 2, 3$$

$$= 8.0 \times 10^7\ \mathrm{m}^3, \tag{2.7}$$

where A(I) and V(I) denote the area and volume, respectively, of the soil subzone of zone I. The amounts of water and solid material in the subzones are given by

$$Z(1,2,I) = (8.0 \times 10^7\ \mathrm{m}^3)(0.50)(0.50)(1.0 \times 10^3\ \mathrm{L/m}^3) \quad \text{for } I = 1, 2, 3$$

$$= 2.0 \times 10^{10}\ \mathrm{L} \tag{2.8}$$

and

$$Z(2,2,I) = (8.0 \times 10^7\ \mathrm{m}^3)(0.50)(2.8 \times 10^3\ \mathrm{kg/m}^3) \quad \text{for } I = 1, 2, 3$$

$$= 1.1 \times 10^{11}\ \mathrm{kg}, \tag{2.9}$$

respectively. Further, water movement from the soil subzones to the groundwater subzones is given by

$$Z(3,2,I) = (0.60\ \mathrm{m/yr})(1.6 \times 10^8\ \mathrm{m}^2)(1.0 \times 10^3\ \mathrm{L/m}^3) \quad \text{for } I = 1, 2, 3$$

$$= 9.8 \times 10^{10}\ \mathrm{L/yr}. \tag{2.10}$$

Water and solid movements from the soil subzone to the surface-water subzones are now determined. For zones 1 and 3, these rates are given by

$$Z(5,2,I) = (0.50)(8.0 \times 10^7\ \mathrm{m}^3)(1.0 \times 10^3\ \mathrm{L/m}^3)(1.0/\mathrm{yr}) \quad \text{for } I = 1 \text{ and } 3$$

$$= 4.0 \times 10^{10}\ \mathrm{L/yr} \tag{2.11}$$

and

$$Z(6,2,I) = (1.1 \times 10^{11}\ \mathrm{kg})(1.0 \times 10^{-3}/\mathrm{yr}) \quad \text{for } I = 1 \text{ and } 3$$

$$= 1.1 \times 10^8\ \mathrm{kg/yr}, \tag{2.12}$$

respectively. It follows from (2.34) that the suspended solid concentration in the lake is 4.0×10^{-5} kg/L. Thus, the water and solid movements from the soil subzone to the surface-water subzone for zone 2 are given by

$$Z(5,2,2) = (1.6 \times 10^8\ \mathrm{m}^2)(0.30\ \mathrm{m/yr})(1.0 \times 10^3\ \mathrm{L/m}^3)$$

$$= 4.8 \times 10^{10}\ \mathrm{L/yr} \tag{2.13}$$

and

$$Z(6,2,2) = (4.8 \times 10^{10}\ \mathrm{L/yr})(4.0 \times 10^{-5}\ \mathrm{kg/L})$$

$$= 1.9 \times 10^6\ \mathrm{kg/yr}, \tag{2.14}$$

respectively.

All other inputs which can be supplied to the Environmental Transport Model for soil subzones are taken to be zero. The soil subzone properties obtained in this section are summarized in Table 2-6.

Table 2-6

Soil Subzone Properties for Reference Site

Property	Zone 1	Zone 2	Zone 3
Z(1,2,I)	2.0×10^{10}	2.0×10^{10}	2.0×10^{10}
Z(2 2,I)	1.1×10^{11}	1.1×10^{11}	1.1×10^{11}
Z(3,2,I)	9.8×10^{10}	9.8×10^{10}	9.8×10^{10}
Z(4,2,I)	0	0	0
Z(5,2,I)	4.0×10^{10}	4.8×10^{10}	4.0×10^{10}
Z(6,2,I)	1.1×10^{8}	1.9×10^{6}	1.1×10^{8}
Z(7,2,I)	0	0	0
Z(8,2,I)	0	0	0

Z(1,2,I) = volume of water in subzone (in litres).

Z(2,2,I) = mass of solids in subzone (in kg).

Z(3,2,I) = rate of water outflow (in L/yr) from subzone to groundwater subzone.

Z(4,2,I) = rate of solid outflow (in kg/yr) from subzone to groundwater subzone.

Z(5,2,I) = rate of water outflow (in L/yr) from subzone to surface-water subzone.

Z(6,2,I) = rate of solid outflow (in kg/yr) from subzone to surface-water subzone.

Z(7,2,I) = rate of water outflow from subzone (in L/yr) to a sink.

Z(8,2,I) = rate of solid outflow (in kg/yr) from subzone to a sink.

2.5 SURFACE-WATER SUBZONES

The surface-water subzones for zones 1 and 3 are 40-km-long stretches of river L for each zone. For zone 2, the surface-water subzone is an elliptical lake with major and minor axes of length 40 km and 6.4 km, respectively. The river is assumed to have a velocity of 1.0 m/s in zones 1 and 3. This is shown to be a reasonable assumption in the next paragraph. Further, the lake in zone 2 is assumed to hold a water volume equal to 1 year's discharge of river L at the head of the lake. The amount of sediment carried in the river is derived from assumptions about erosion in the river's watershed. In particular, it is assumed that (1) the watershed is eroding at the rate of 5.0 cm/1000 years (see Tables 2-7, 2-8 and 2-9), (2) the material being eroded has a bulk density of 2.8 g/cm^3 (see Table 2-3) and (3) 33% of the eroded material is carried in solution (see Tables 2-10 and 2-11). The figures referred to in the previous sentence indicate the selected values are consistent with values that have been observed. The study by Judson and Ritter (Ju64) also indicates that this selection is reasonable.

Relations describing the annual flow of river L are now derived. As indicated in Table 2-1, the discharge of river L at the repository is 1.5×10^{13} L/yr, and this discharge increases downstream at the constant rate of 1.0×10^{8} L/yr/m.

Table 2-7

Past and Present Rates of Denudation[a]

Region	2 Area Denuded (10^6 km^2)	3 Time (10^6 yr)	4 Volume Deposits (10^6 km^3)	5 Denudation (km)	6 Past Rate (cm/10^3 yr)	7 Present Rate[b] (cm/10^3 yr)	8 Ratio: 6/7
Appalachian	1.0	125	7.8	7.8	6.2	0.8	7.8
Mississippi	3.2 (1.6)[c]	150	11.1	6.9	4.6	4.2	1.1
Himalaya	1.0	40	8.5	8.5	21	100	0.2
Rocky Mountain, Lower Cretaceous	0.8	25	0.6	0.7	3	--	--
Rocky Mountain, Upper Cretaceous	<0.4	40	2.2	>4.8	12 - 20	--	--

[a] Reprinted from Menard (Me61), p 155 (Table I) by permission of the University of Chicago Press.

[b] Suspended load of rivers.

[c] Area denuded in past.

Table 2-8

Relative Rates of Denudation in Uplands and Lowlands and in Different Climates*

Physiographic Environment	Estimated Rate of Denudation (cm/1000 yr)
LOWLANDS: Slope < 0.001	
Climate with cold winter	2.9
Intermediate maritime climate (Lower Rhine, Seine)	2.7
Hot-dry climate (Mediterranean, New Mexico)	1.2
Hot-moist climate with dry season	3.2
Equatorial climate (dense rain forest)	2.2
MOUNTAINS: Slope ≥ 0.01	
Semihumid periglacial climate	60
Extreme nival climate (Southeastern Alaska)	80
Climate of Mediterranean high mountain chains	45
Hot-dry climate (Southwestern United States, Tunisia)	18
Hot-moist climate (Usumacinta)	92

*From Leopold et al (Le64), p 29, (Figure 3.2); Copyright © 1964. Figures are not of uniform quality due to limited sample and variable estimates of contribution of suspended load, bed load, and dissolved load of rivers.

Table 2-9

Denudation Rates of Drainage Basins Within the United States*

Effective Precipitation (inches)	Mean Sediment Yield (tons/mi^2)	Mean Denudation (ft/1000 yr)	Mean Denudation (yr/ft)
		Gaging-Station Data	
10	670	0.29	3400
10-15	780	0.34	2900
15-20	550	0.24	4200
20-30	550	0.24	4200
30-40	400	0.17	5900
40-60	220	0.10	10000
		Reservoir Data	
8-9	1400	0.61	1600
10	1180	0.51	2000
11	1500	0.65	1500
14-25	1130	0.49	2000
25-30	1430	0.62	1600
30-38	790	0.34	2900
38-40	560	0.24	4200
40-55	470	0.21	4800
55-100	440	0.19	5300

*From Schumm (Sc63), p H2 (Table 1).

Table 2-10

Dissolved and Suspended Load in Selected Rivers in Different Climatic Regions of the United States[a]

River and Location	Elevation (ft)	Drainage Area (mi^2)	Average Discharge (ft^3/s)	Discharge ÷ Drainage Area (ft^3/s/mi^2)	Years of Record in Sample[b]	Average Suspended Load	Average Dissolved Load	Total Avg. Susp. and Dis. Load	Total Avg. Load ÷ Drain. Area (t/mi^2·yr)	Dissolved Load as % of Total Load (%)
						(10^6 tons/year)				
Little Colorado at Woodruff, Arizona	5125	8,160	63.3	0.0078	6	1.6	0.02	1.62	199	1.2
Canadian River near Amarillo, Texas	2989	19,445	621	0.032	1	6.41	0.124	6.53	336	1.9
Colorado River near San Saba, Texas	1096	30,600	1449	0.047	5	3.02	0.208	3.23	105	6.4
Bighorn River at Kane, Wyoming	3609	15,900	2391	0.150	1	1.60	0.207	1.80	114	12
Green River at Green River, Utah	4040	40,600	6737	0.166	26 - 20	19	2.5	21.5	530	12
Colorado River near Cisco, Utah	4090	24,100	8457	0.351	25 - 20	15	4.4	19.4	808	23
Iowa River at Iowa City, Iowa	627	3,271	1517	0.464	3	1.164	0.485	1.67	510	29
Mississippi River at Red River Landing, La.	--	1,144,500	569,500[c]	0.497	3	284	101.8	385.8	337	26
Sacramento River at Sacramento, Calif.	0	27,000[d]	25,000	0.926	3	2.85	2.29	5.14	190	44
Flint River near Montezuma, Georgia	256	2,900	3528	1.22	1	0.400	0.132	0.53	183	25
Juniata River near New Port, Penna.	364	3,354	4329	1.29	7	0.322	0.566	0.89	265	64
Delaware River at Trenton, New Jersey	8	6,780	11,370	1.73	9 - 4	1.003	0.830	1.83	270	45

[a] From Leopold et al (Le64), p 76 (Figure 3.10); Copyright © 1964.

[b] Computation of load, dissolved or suspended, depends on discharge for same period. Years of record pertain to number of years used for related values of discharge and of suspended and dissolved load. Where two figures are shown, the first is for suspended load and the second is for dissolved load.

[c] From USGS records for Vicksburg, Mississippi, station.

[d] Estimated.

Table 2-11

Suspended and Dissolved Loads Carried by North American Rivers*

Basin	Area, mi^2	Estimated total load, tons/mi^2·yr	Dissolved load, %	Suspended load, %
North Atlantic	159,400	169	77	23
South Atlantic	123,900	270	35	65
East Gulf	142,100	261	45	55
West Gulf	315,700	108	33	67
Mississippi River	1,265,000	477	23	77
Laurentian	175,000	117	99	1
Colorado River	230,000	438	12	88
South Pacific	72,700	252	70	30
North Pacific	270,000	120	83	17
Great Basin	223,000	140	64	36
Hudson Bay	62,000	49	57	43

*From Morisawa (Mo68), p 42 (Figure 4.1; Copyright © 1968. Used with the permission of McGraw-Hill Book Company.

Thus, the annual discharge D(x) at a point on the river x metres below the repository is

$$D(x) = 1.5 \times 10^{13} \text{ L/yr} + (x \text{ m})(1.0 \times 10^{8} \text{ L/yr/m}). \qquad (2.15)$$

The preceding relation is used to determine water flows out of the surface-water subzones. For comparison with values in Figure 2-4, D(x) must be expressed in ft^3/s rather than L/yr. This yields

$$\begin{aligned} D(x) &= [1.5 \times 10^{13} \text{ L/yr} + (x \text{ m})(1.0 \times 10^{8} \text{ L/yr/m})] \\ &\quad \cdot[(3.15 \times 10^{7} \text{ s/yr})^{-1} (2.83 \times 10^{1} \text{ L/ft}^3)^{-1}] \\ &= 1.7 \times X0^{4} \text{ ft}^3\text{/s} + (x \text{ m})(1.1 \times 10^{-1} \text{ ft}^3\text{/s/m}). \qquad (2.16) \end{aligned}$$

Thus, the river discharge ranges from 1.7×10^4 ft^3/s at the upper end of zone 1 to 3.0×10^4 ft^3/s at the lower end of zone 3. Hence, as indicated in Figure 2-4, an assumed river velocity of 1.0 m/s is reasonable for this discharge range.

The water volumes for the surface-water subzones of zones 1 and 3 are now determined. It is assumed that the water volume for these subzones is given by

$$V = L(A_1 + A_2)/2, \qquad (2.17)$$

where

L = length of surface-water subzone (in metres)

A_1 = cross-sectional area at upper end of surface-water subzone (in m^2)

A_2 = cross-sectional area at lower end of surface-water subzone (in m^2).

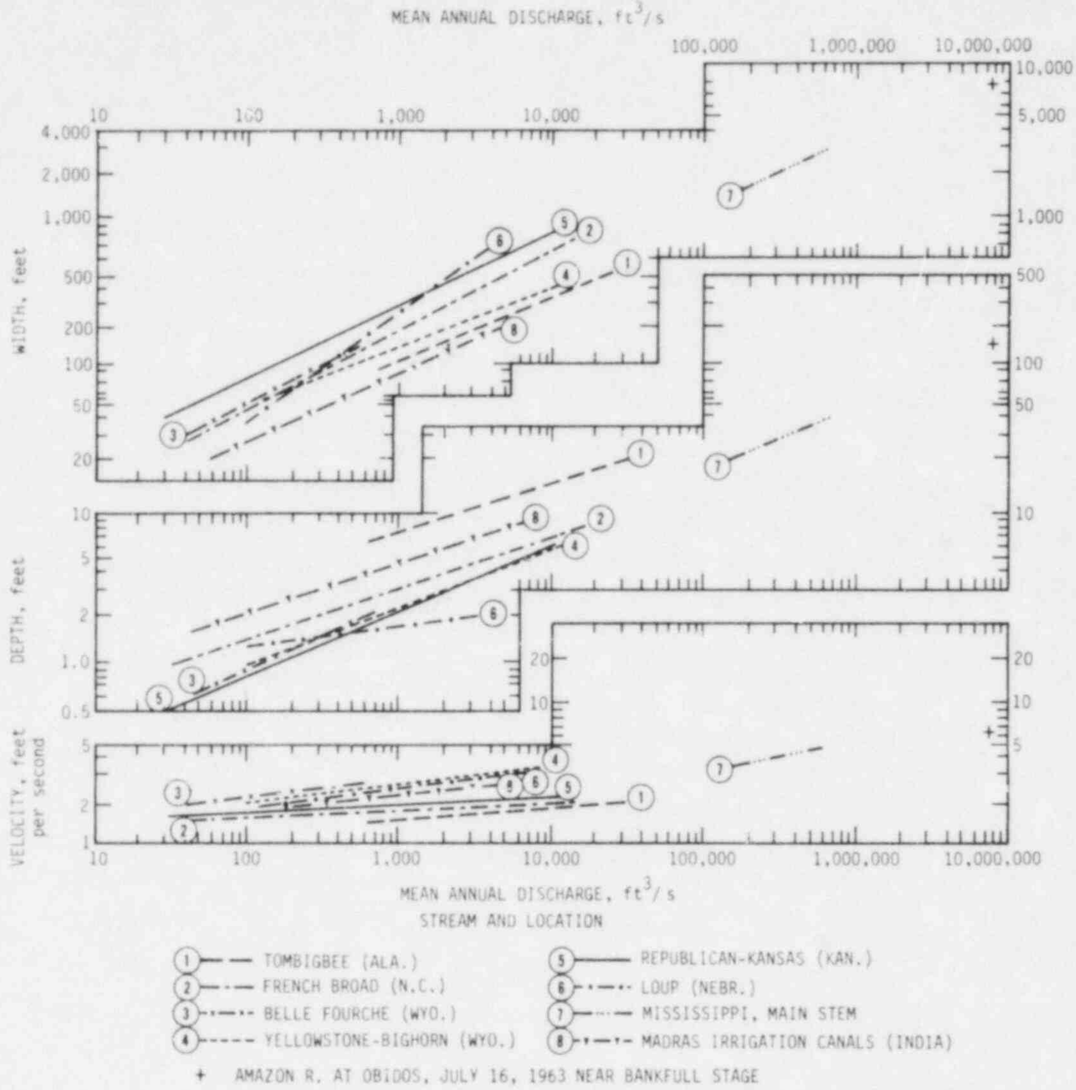

Figure 2-4. Width, Depth, and Velocity in Relation to Mean Annual Discharge as Discharge Increases Downstream in Various River Systems. From Leopold et al (Le64), p 242 (Figure 7.21); Copyright © 1964.

Further, for a given point x on the river, the cross sectional area A(x) at x is given by

$$A(x) = D(x)/v(x), \qquad (2.18)$$

where

$D(x)$ = river discharge at x (in m^3/s)

$v(x)$ = river velocity at x (in m/s).

Selected cross-sectional areas and discharges are compiled in Table 2-12. From Equation (2.17) and values in Table 2-12, it follows that

$$Z(1,3,1) = (4.0 \times 10^4 \text{ m})(4.8 \times 10^2 \text{ m}^2 + 6.0 \times 10^2 \text{ m}^2)(1.0 \times 10^3 \text{ L/m}^3)/2$$

$$= 2.2 \times 10^{10} \text{ L} \qquad (2.19)$$

and

$$Z(1,3,3) = (4.0 \times 10^4\ \mathrm{m})(7.3 \times 10^2\ \mathrm{m}^2 + 8.6 \times 10^2\ \mathrm{m}^2)(1.0 \times 10^3\ \mathrm{L/m}^3)/2$$

$$= 3.2 \times 10^{10}\ \mathrm{L}\ . \qquad (2.20)$$

Further, it is assumed that the lake which constitutes the surface-water subzone of zone 2 contains a volume equal to 1 year's flow of river L at the head of the lake. Thus, from Table 2-12, it follows that

$$Z(1,3,2) = 1.9 \times 10^{13}\ \mathrm{L}. \qquad (2.21)$$

The amount of suspended sediments in each surface-water subzone is now determined; however, several intermediate calculations will be necessary. If the valley containing the river L is eroding at the rate E cm/1000 yr, the material being eroded has a bulk density of D $\mathrm{g/cm}^3$ and a fraction F of the eroded material is carried in solution, then the annual suspended sediment yield, Y $\mathrm{kg/m}^2$, is given by

$$Y = (E\ \mathrm{cm/1000\ yr})(D\ \mathrm{g/cm}^3)(1.0 - F)$$

$$= (E)(D)(1.0 - F)(1.0 \times 10^{-3}\ \mathrm{g/cm}^2/\mathrm{yr})$$

$$= (E)(D)(1.0 - F)(1.0 \times 10^{-2}\ \mathrm{kg/m}^2/\mathrm{yr}). \qquad (2.22)$$

Further, if the lake in zone 2 traps a fraction T of the suspended sediments entering it, then the annual suspended sediment mass S(I) moving downstream from zone I is given by

$$S(1) = [(1.8 \times 10^5\ \mathrm{m})(4.0 \times 10^4\ \mathrm{m}) + 2.5 \times 10^{10}\ \mathrm{m}^2][Y\ \mathrm{kg/m}^2/\mathrm{yr}]$$

$$= 3.2 \times 10^{10}\ Y\ \mathrm{kg/yr}, \qquad (2.23)$$

Table 2-12

Selected Discharges and Cross-Sectional Areas for River L*

	Distance Below Repository (in Metres)			
	0	4.0×10^4	8.0×10^4	1.2×10^5
River Discharge (in L/yr)	1.5×10^{13}	1.9×10^{13}	2.3×10^{13}	2.7×10^{13}
River Discharge (in m^3/s)	4.8×10^{12}	6.0×10^2	7.3×10^2	8.6×10^2
River Discharge (in ft^3/s)	1.7×10^4	2.1×10^4	2.6×10^4	3.1×10^4
River Cross-Sectional Area (in m^2)	4.8×10^2	6.0×10^2	7.3×10^2	8.6×10^2

*Values in this table are derived from Equations (2.15) and (2.18).

$$S(2) = [1.0 - T][(1.8 \times 10^5 \text{ m})(8.0 \times 10^4 \text{ m}) + 2.5 \times 10^{10} \text{ m}^2] \cdot [Y \text{ kg/m}^2\text{/yr}]$$

$$= 3.9 \times 10^{10}(1.0 - T)\ Y \text{ kg/yr} \qquad (2.24)$$

and

$$S(3) = S(2) + (1.8 \times 10^5 \text{ m})(4.0 \times 10^4 \text{ m})(Y \text{ kg/m}^2\text{/yr})$$

$$= 3.9 \times 10^{10}\ (1.0 - T)\ Y \text{ kg/yr} + 7.2 \times 10^9\ Y \text{ kg/yr}$$

$$= [3.9 \times 10^{10}\ (1.0 - T) + 7.2 \times 10^9]\ Y \text{ kg/yr}, \qquad (2.25)$$

where 1.8×10^5 m and 2.5×10^{10} m^2 are the width of the valley below the repository and the area of the valley above the repository, respectively (as given in Table 2-1) and 40 km is the length of each zone. The preceding three equations are derived with the assumptions that (1) the surface-water subzones in zones 1 and 2 receive all suspended sediments produced in the valley above the lower end of each zone, (2) the surface-water subzone in zone 3 receives all suspended sediment flowing downstream from zone 2 plus all suspended sediment produced in the valley between the upper and lower ends of the zone, and (3) the surface-water subzones in zones 1 and 3 are in equilibrium in the sense that the amount of suspended sediment flowing out of each subzone is equal to the amount flowing in. No attempt is made to incorporate an increased sediment load in zone 3 which might result from increased scouring as the river attempts to increase its sediment load in compensation for sediments trapped in the lake.

It is assumed that the valley is eroding at an average rate of 5.0 cm/1000 yr, that the eroded material has a bulk density of 2.8 g/cm^3 and that 33% of the eroded material is carried in solution. Thus, from Equation (2.22), the suspended sediment yield is

$$Y = (5.0)(2.8)(1.0 - 0.33)(1.0 \times 10^{-2} \text{ kg/m}^2\text{/yr})$$

$$= 9.4 \times 10^{-2} \text{ kg/m}^2\text{/yr}. \qquad (2.26)$$

The lake in zone 2 is assumed to have a trap efficiency of 75%. There is wide variation in observed trap efficiencies; additional information on lake sedimentation is given by Brune (Br53), Colby (Col63), Borland (Bor71) and Dendy (De74). With 75% trap efficiency, it follows from Equations (2.23), (2.24) and (2.25) that the amounts of sediment moving downstream from the surface-water subzones are given by

$$Z(10,3,1) = S(1)$$

$$= (3.2 \times 10^{10})(9.4 \times 10^{-2}) \text{ kg/yr}$$

$$= 3.0 \times 10^9 \text{ kg/yr}, \qquad (2.27)$$

$$Z(10,3,2) = S(2)$$

$$= (3.9 \times 10^{10})(1.0 - 0.75)(9.4 \times 10^{-2}) \text{ kg/yr}$$

$$= 9.2 \times 10^{8} \text{ kg/yr} \qquad (2.28)$$

and

$$Z(10,3,3) = S(3)$$

$$= [3.9 \times 10^{10} (1.0 - 0.75) + 7.2 \times 10^{9}][9.4 \times 10^{-2}] \text{ kg/yr}$$

$$= 1.6 \times 10^{9} \text{ kg/yr}. \qquad (2.29)$$

Further, as indicated in Table 2-12, the volumes of water moving downstream from the surface-water subzones are given by

$$Z(9,3,1) = 1.9 \times 10^{13} \text{ L/yr} \qquad (2.30)$$

$$Z(9,3,2) = 2.3 \times 10^{13} \text{ L/yr} \qquad (2.31)$$

$$Z(9,3,3) = 2.7 \times 10^{13} \text{ L/yr}. \qquad (2.32)$$

The amount of suspended sediment in each surface-water subzone is now determined. The concentration C(I) of suspended sediment in zone I is given by

$$C(1) = Z(10,3,1,)/Z(9,3,1)$$

$$= (3.0 \times 10^{9} \text{ kg/yr})/(1.9 \times 10^{13} \text{ L/yr})$$

$$= 1.6 \times 10^{-4} \text{ kg/L}, \qquad (2.33)$$

$$C(2) = Z(10,3,2)/Z(9,3,2)$$

$$= (9.2 \times 10^{8} \text{ kg/yr})/(2.3 \times 10^{13} \text{ L/yr})$$

$$= 4.0 \times 10^{-5} \text{ kg/L} \qquad (2.34)$$

and

$$C(3) = Z(10,3,3)/Z(9,3,3)$$

$$= (1.6 \times 10^{9} \text{ kg/yr})/(2.7 \times 10^{13} \text{ L/yr})$$

$$= 5.9 \times 10^{-5} \text{ kg/L}. \qquad (2.35)$$

Thus, the mass of supended sediment in each surface-water subzone is given by

$$Z(2,3,1) = C(1)\ Z(1,3,1)$$

$$= (1.6 \times 10^{-4} \text{ kg/L})(2.2 \times 10^{10} \text{ L})$$

$$= 3.5 \times 10^{6} \text{ kg}, \qquad (2.36)$$

$$Z(2,3,2) = C(2)\ Z(1,3,2)$$

$$= (4.0 \times 10^{-5}\ \mathrm{kg/L})(1.9 \times 10^{13}\ \mathrm{L})$$

$$= 7.6 \times 10^{8}\ \mathrm{kg} \qquad (2.37)$$

and

$$Z(2,3,3) = C(3)\ Z(1,3,3)$$

$$= (5.9 \times 10^{-5}\ \mathrm{kg/L})(3.2 \times 10^{10}\ \mathrm{L})$$

$$= 1.9 \times 10^{6}\ \mathrm{kg}. \qquad (2.38)$$

For each zone, the soil and surface-water subzones are assumed to be in equilibrium in the sense that the rates of water and solid movement from the soil subzone to the surface-water subzone are equal to the rates of water and solid movement from the surface-water subzone to the soil subzone. Values for these rates are derived in Equations (2.11) through (2.14) of Section 2.4. In particular,

$$Z(5,3,I) = Z(5,2,I) = 4.0 \times 10^{10}\ \mathrm{L/yr} \quad \text{for } I = 1 \text{ and } 3 \qquad (2.39)$$

$$Z(5,3,2) = Z(5,2,2) = 4.8 \times 10^{10}\ \mathrm{L/yr} \qquad (2.40)$$

$$Z(6,3,I) = Z(6,2,I) = 1.1 \times 10^{8}\ \mathrm{kg/yr} \quad \text{for } I = 1 \text{ and } 3 \qquad (2.41)$$

$$Z(6,3,2) = Z(6,2,2) = 1.9 \times 10^{6}\ \mathrm{kg/yr}. \qquad (2.42)$$

For zones 1 and 3, the surface-water and sediment subzones are assumed to be in equilibrium in the sense that the rates of water and solid movement from the surface-water subzone to the sediment subzone are equal to the rates of water and solid movement from the sediment subzone to the surface-water subzone. Values for these rates are derived in Equations (2.71), (2.73), (2.74) and (2.76). In particular,

$$Z(7,3,1) = Z(5,4,1) = 8.7 \times 10^{8}\ \mathrm{L/yr} \qquad (2.43)$$

$$Z(7,3,3) = Z(5,4,3) = 1.3 \times 10^{9}\ \mathrm{L/yr} \qquad (2.44)$$

$$Z(8,3,1) = Z(6,4,1) = 2.3 \times 10^{9}\ \mathrm{kg/yr} \qquad (2.45)$$

$$Z(8,3,3) = Z(6,4,3) = 2.4 \times 10^{9}\ \mathrm{kg/yr}. \qquad (2.46)$$

The movements of water and solid material from the surface-water subzone of zone 2 to the sediment subzone are now determined. If T denotes the fraction of incoming sediments trapped by the lake and Y is defined as in (2.22), then the annual amount of solid material trapped in the lake is given by

$$S = 3.9 \times 10^{10}\ T\ Y\ \mathrm{kg/yr}, \qquad (2.47)$$

which is obtained by replacing the factor 1.0 - T in Equation (2.24) with T. As derived in (2.61), the amount of water associated with solids moving between the surface-water and sediment subzones is taken to be 3.8×10^{-1} L/kg. Thus, the annual amount W of water trapped in lake sediments is given by

$$
\begin{aligned}
W &= (3.9 \times 10^{10}\ T\ Y\ \text{kg/yr})(\text{[illegible]} \times 10^{-1}\ \text{L/kg}) \\
&= 1.5 \times 10^{10}\ T\ Y\ \text{L/yr}. \qquad (2.48)
\end{aligned}
$$

Specifically, with $Y = 9.4 \times 10^{-2}$ kg/m^2/yr as calculated in (2.26) and $T = 0.75$, the preceding expressions for S and W become

$$
\begin{aligned}
S &= (3.9 \times 10^{10})(0.75)(9.4 \times 10^{-2})\ \text{kg/yr} \\
&= 2.7 \times 10^{9}\ \text{kg/yr} \qquad (2.49)
\end{aligned}
$$

and

$$
\begin{aligned}
W &= (2.7 \times 10^{9}\ \text{kg/yr})(3.8 \times 10^{-1}\ \text{L/kg}) \\
&= \text{[illegible]}.0 \times 10^{9}\ \text{L/yr}, \qquad (2.50)
\end{aligned}
$$

respectively.

The symbols Z(5,4,2) and Z(6,4,2) denote the rates of water and solid movement, respectively, from the sediment subzone of zone 2 to the surface-water subzone. Hence, by using the values for S and W given in (2.47) and (2.48), it follows that the corresponding movements Z(7,3,2) and Z(8,3,2) of water and solid material, respectively, from the surface-water subzone of zone 2 to the sediment subzone are given by

$$
Z(7,3,2) = Z(5,4,2) + 1.5 \times 10^{10}\ T\ Y\ \text{L/yr} \qquad (2.51)
$$

and

$$
Z(8,3,2) = Z(6,4,2) + 3.9 \times 10^{10}\ T\ Y\ \text{kg/yr}. \qquad (2.52)
$$

In particular, with the values for S and W given in (2.49) and (2.50) and the values for Z(5,4,2) and Z(6,4,2) given in (2.72) and (2.75), it follows that

$$
\begin{aligned}
Z(7,3,2) &= 2.0 \times 10^{9}\ \text{L/yr} + 1.0 \times 10^{9}\ \text{L/yr} \\
&= 3.0 \times 10^{9}\ \text{L/yr} \qquad (2.53)
\end{aligned}
$$

and

$$
\begin{aligned}
Z(8,3,2) &= 5.2 \times 10^{9}\ \text{kg/yr} + 2.7 \times 10^{9}\ \text{kg/yr} \\
&= 7.9 \times 10^{9}\ \text{kg/yr}. \qquad (2.54)
\end{aligned}
$$

All other inputs which can be supplied to the Environmental Transport Model for surface-water subzones are taken to be zero. Although annual water movement rates from surface-water to sediment are defined, these rates could have been taken to be zero with very little effect on model predictions. The surface-water subzone properties obtained in this section are summarized in Table 2-13.

Table 2-13

Surface-Water Subzone Properties for Reference Site

Property	Zone 1	Zone 2	Zone 3
Z(1,3,I)	2.2×10^{10}	1.9×10^{13}	3.2×10^{10}
Z(2,3,I)	3.5×10^{6}	7.6×10^{8}	1.9×10^{6}
Z(3,3,I)	0	0	0
Z(4,3,I)	0	0	0
Z(5,3,I)	4.0×10^{10}	4.8×10^{10}	4.0×10^{10}
Z(6,3,I)	1.1×10^{8}	1.9×10^{6}	1.1×10^{8}
Z(7,3,I)	8.7×10^{8}	3.0×10^{9}	1.3×10^{9}
Z(8,3,I)	2.3×10^{9}	7.9×10^{9}	3.4×10^{9}
Z(9,3,I)	1.9×10^{13}	2.3×10^{13}	2.7×10^{13}
Z(10,3,I)	3.0×10^{9}	9.2×10^{8}	1.6×10^{9}
Z(11,3,I)	0	0	0
Z(12,3,I)	0	0	0
INTZ(I)	2	3	4

Z(1,3,I) = volume of water in subzone (in litres).

Z(2,3,I) = mass of solids in subzone (in kg).

Z(3,3,I) = rate of water outflow (in L/yr) from subzone to groundwater subzone.

Z(4,3,I) = rate of solid outflow (in kg/yr) from subzone to groundwater subzone.

Z(5,3,I) = rate of water outflow (in L/yr) from subzone to soil subzone.

Z(6,3,I) = rate of solid outflow (in kg/yr) from subzone to soil subzone.

Z(7,3,I) = rate of water outflow (in L/yr) from subzone to sediment subzone.

Z(8,3,I) = rate of solid outflow (in kg/yr) from subzone to sediment subzone.

Z(9,3,I) = rate of water outflow (in L/yr) from subzone to surface-water subzone in zone INTZ(I).

Z(10,3,I) = rate of solid outflow (in kg/yr) from subzone to surface-water subzone in zone INTZ(I).

Z(11,3,I) = rate of water outflow (in L/yr) from subzone to a sink.

Z(12,3,I) = rate of solid outflow (in kg/yr) from subzone to a sink.

INTZ(I) = number of zone into which the surface water of zone I discharges.

2.6 SEDIMENT SUBZONES

For zones 1 and 3, the sediment subzones are assumed to have a depth of 2.0 metres, a porosity of 50% and a mean particle density of 2.6 g/cm^3. The porosity and density assumptions are consistent with values indicated in Tables 2-2 and 2-3. The depth assumption of 2.0 metres is rather arbitrary. Table 2-14 contains some examples of scour depth. Over long periods of time, the maximum scour depth essentially defines the depth of the sediment subzone. Further, it is assumed that 10% of the sediment is resuspended each year. Again, the selection of this resuspension rate is arbitrary. The effects of sediment depth and resuspension rates are considered in the chapters on sensitivity analysis. Further, the sediment subzone in zone 2 is assumed to have a depth of 20 cm, a porosity of 50%, a mean particle density of 2.6 g/cm^3 and a 10% annual resuspension rate.

Table 2-14

Selected Data on Amounts of Scour Observed in Various Rivers*

Maximum Depth of Scour Below Normal Bed Elevation (ft)	Particle Size in River Bed, or Material Encountered	Flow Depth (ft)	Location and Source of Data
10 to 15	Silt, gravel	20	Pacolet River
22	Sand, gravel	24 stage	Colorado River, U.S. Bureau of Reclamation, 1950
75	Sand, gravel, cobbles	50 stage	Black Canyon, Colorado River (freq. = 1/50 yrs)
126	Sand to gravel (cobbles)	35	Black Canyon
55	2- by 6-in. plank embedded in sand, gravel, in gorge 100 - 150 ft wide		Black Canyon
32	Cobbles moved, boulders smoothed to bedrock	? 12 to 20	Canadian River at Eufaula Dam
40	Bank pilings in sand		Rio Grande
60	Bridge pier in silt, sand		Lane and Borland (1954)
12 to 15	Scoured to bedrock		Yellow River $w \approx 600$ ft annual flood
0	Fine sand	10 to 12	Colorado River, cable at Imperial Dam
20	Very fine sand	10	Colorado River, Yuma, Lane and Borland (1954)
1.75 to 2 x regime depth	Sand, silt	"Regime" depth	Lacey in Blench (1957, p. 103)
$0.5\ y_1$	Width constricted to 1/2 that upstream	y_1 = upstream depth	Bridge piers, Laursen (1960)

---

*From Leopold et al (Le64), p 229 (Figure 7.3); Copyright © 1964

Sediment subzone properties are now derived. Figure 2-4 indicates that a 2.5-metre depth is reasonable for river L in zones 1 and 3. With respect to Figure 2-4, river L has a discharge rate of $1.7 \times 10^4\ \text{ft}^3/\text{s}$ at the top of zone 1 and a discharge rate of $3.1 \times 10^4\ \text{ft}^3/\text{s}$ at the bottom of zone 3 (See Table 2-12). Therefore, 2.5 metres is assumed to be the mean depth of river L in zones 1 and 3. Further, it follows from the cross-sectional areas contained in Table 2-12 that the mean cross-sectional areas C(1) and C(3) of river L in zones 1 and 3 are given by

$$C(1) = [4.8 \times 10^2\ \text{m}^2 + 6.0 \times 10^2\ \text{m}^2]/2 = 5.4 \times 10^2\ \text{m}^2 \qquad (2.55)$$

and

$$C(3) = [7.3 \times 10^2\ \text{m}^2 + 8.6 \times 10^2\ \text{m}^2]/2 = 8.0 \times 10^2\ \text{m}^2, \qquad (2.56)$$

respectively. Thus, the average widths W(1) and W(3) of river L in zones 1 and 3 are given by

$$W(1) = (5.4 \times 10^{2}\ \mathrm{m}^{2})/(2.5\ \mathrm{m}) = 2.2 \times 10^{2}\ \mathrm{m} \tag{2.57}$$

and

$$W(3) = (8.0 \times 10^{2}\ \mathrm{m}^{2})/(2.5\ \mathrm{m}) = 3.2 \times 10^{2}\ \mathrm{m}, \tag{2.58}$$

respectively. The preceding widths match relatively well with those illustrated in Figure 2-4.

If A(I) denotes the surface area of the sediment subzone in zone I and D(I) denotes its depth, then the water volume V(I) and the solid mass M(I) contained in the subzone are given by

$$V(I) = (0.50)\ A(I)\ D(I) \tag{2.59}$$

and

$$M(I) = (0.50)(2.6 \times 10^{3}\ \mathrm{kg/m^{3}})\ A(I)\ D(I), \tag{2.60}$$

repectively. Thus, the ratio R of water volume to sediment mass is

$$R = V(I)/M(I) = 3.8 \times 10^{-4}\ \mathrm{m^{3}/kg} = 3.8 \times 10^{-1}\ \mathrm{L/kg}. \tag{2.61}$$

Further,

$$A(1) = (4.0 \times 10^{4}\ \mathrm{m})(2.2 \times 10^{2}\ \mathrm{m}) = 8.8 \times 10^{6}\ \mathrm{m}^{2} \tag{2.62}$$

$$A(2) = \pi(2.0 \times 10^{4}\ \mathrm{m})(3.2 \times 10^{3}\ \mathrm{m}) = 2.0 \times 10^{8}\ \mathrm{m}^{2} \tag{2.63}$$

and

$$A(3) = (4.0 \times 10^{4}\ \mathrm{m})(3.2 \times 10^{2}\ \mathrm{m}) = 1.3 \times 10^{7}\ \mathrm{m}^{2}, \tag{2.64}$$

where A(2) is the area of an ellipse with major and minor axes of length 40 km and 6.4 km, respectively.

The solid mass in each sediment subzone is now determined. Then, the water volumes are determined by using (2.61). In particular,

$$\begin{aligned} Z(2,4,1) &= (0.50)(2.6 \times 10^{3}\ \mathrm{kg/m^{3}})(8.8 \times 10^{6}\ \mathrm{m}^{2})(2.0\ \mathrm{m}) \\ &= 2.3 \times 10^{10}\ \mathrm{kg}, \end{aligned} \tag{2.65}$$

$$\begin{aligned} Z(2,4,2) &= (0.50)(2.6 \times 10^{3}\ \mathrm{kg/m^{3}})(2.0 \times 10^{8}\ \mathrm{m}^{2})(0.20\ \mathrm{m}) \\ &= 5.2 \times 10^{10}\ \mathrm{kg} \end{aligned} \tag{2.66}$$

and

$$\begin{aligned} Z(2,4,3) &= (0.50)(2.6 \times 10^{3}\ \mathrm{kg/m^{3}})(1.3 \times 10^{7}\ \mathrm{m}^{2})(2.0\ \mathrm{m}) \\ &= 3.4 \times 10^{10}\ \mathrm{kg}. \end{aligned} \tag{2.67}$$

Further,

$$Z(1,4,1) = (3.8 \times 10^{-1}\ \mathrm{L/kg})(2.3 \times 10^{10}\ \mathrm{kg}) = 8.7 \times 10^{9}\ \mathrm{L} \tag{2.68}$$

$$Z(1,4,2) = (3.8 \times 10^{-1}\ \mathrm{L/kg})(5.2 \times 10^{10}\ \mathrm{kg}) = 2.0 \times 10^{10}\ \mathrm{L} \quad (2.69)$$

$$Z(1,4,3) = (3.8 \times 10^{-1}\ \mathrm{L/kg})(3.4 \times 10^{10}\ \mathrm{kg}) = 1.3 \times 10^{10}\ \mathrm{L}. \quad (2.70)$$

For each zone, it is assumed that 10% of the sediments are resuspended each year. Thus, the rates of water and solid movement from sediment subzones to surface-water subzones are given by

$$Z(5,4,1) = (0.10/\mathrm{yr})\ Z(1,4,1) = 8.7 \times 10^{8}\ \mathrm{L/yr} \quad (2.71)$$

$$Z(5,4,2) = (0.10/\mathrm{yr})\ Z(1,4,2) = 2.0 \times 10^{9}\ \mathrm{L/yr} \quad (2.72)$$

$$Z(5,4,3) = (0.10/\mathrm{yr})\ Z(1,4,3) = 1.3 \times 10^{9}\ \mathrm{L/yr} \quad (2.73)$$

$$Z(6,4,1) = (0.10/\mathrm{yr})\ Z(2,4,1) = 2.3 \times 10^{9}\ \mathrm{kg/yr} \quad (2.74)$$

$$Z(6,4,2) = (0.10/\mathrm{yr})\ Z(2,4,2) = 5.2 \times 10^{9}\ \mathrm{kg/yr} \quad (2.75)$$

$$Z(6,4,3) = (0.10/\mathrm{yr})\ Z(2,4,3) = 3.4 \times 10^{9}\ \mathrm{kg/yr}. \quad (2.76)$$

The sediment subzone in zone 2 is assumed to be 20 cm thick. However, the lake is assumed to trap 75% of the sediment entering it. Thus, there must be a movement from this sediment subzone to a sink, that is, to a deeper sediment layer which is not subject to resuspension. It is assumed that no compaction occurs in this lower layer and that the water-solid ratio remains as represented in (2.61). Specifically, by using (2.49) and (2.61), it follows that the movements of water and solid material from the sediment subzone of zone 2 to a sink are given by

$$\begin{aligned} Z(7,4,2) &= (2.7 \times 10^{9}\ \mathrm{kg/yr})(3.8 \times 10^{-1}\ \mathrm{L/kg}) \\ &= 1.0 \times 10^{9}\ \mathrm{L/yr} \end{aligned} \quad (2.77)$$

and

$$Z(8,4,2) = 2.7 \times 10^{9}\ \mathrm{kg/yr}, \quad (2.78)$$

respectively.

All other inputs which can be supplied to the Environmental Transport Model for sediment subzones are taken to be zero. As already noted in the preceding section, annual rates for water movement between sediment subzones and surface-water subzones (or sinks) will have little effect on model predictions in the present context and could have been taken to be zero. The sediment subzone properties obtained in this section are summarized in Table 2-15.

In zone 2, the surface-water subzone is a lake. In modeling radionuclide discharges from waste repositories, careful consideration must be given as to whether or not lakes in the repository vicinity should be considered. In particular, lakes are transient geologic features. For the time scales that must be represented in such modeling, a given lake may not exist for a sufficiently long period to justify its inclusion in the modeling effort. For this reason, the life expectancy of the lake in zone 2 is now examined.

Table 2-15

Sediment Subzone Properties for Reference Site

Property	Zone 1	Zone 2	Zone 3
Z(1,4,I)	8.7×10^{9}	2.0×10^{10}	1.3×10^{10}
Z(2,4,I)	2.3×10^{10}	5.2×10^{10}	3.4×10^{10}
Z(3,4,I)	0	0	0
Z(4,4,I)	0	0	0
Z(5,4,I)	8.7×10^{8}	2.0×10^{9}	1.3×10^{9}
Z(6,4,I)	2.3×10^{9}	5.2×10^{9}	3.4×10^{9}
Z(7,4,I)	0	1.0×10^{9}	0
Z(8,4,I)	0	2.7×10^{9}	0

Z(1,4,I) = volume of water in subzone (in litres).
Z(2,4,I) = mass of solids in subzone (in kg).
Z(3,4,I) = rate of water outflow (in L/yr) from subzone to groundwater subzone.
Z(4,4,I) = rate of solid outflow (in kg/yr) from subzone to groundwater subzone.
Z(5,4,I) = rate of water outflow (in L/yr) from subzone to surface-water subzone.
Z(6,4,I) = rate of solid outflow (in kg/yr) from subzone to surface-water subzone.
Z(7,4,I) = rate of water outflow (in L/yr) from subzone to a sink.
Z(8,4,I) = rate of solid outflow (in kg/yr) from subzone to a sink.

The lake is assumed to trap 75% of the sediments entering it. As derived in (2.78), this amounts to 2.7×10^{9} kg/yr. With the assumption that the sediment has a density of 2.6 g/cm^3 and a constant porosity of 50% (i.e., no compaction), it follows that the lake is being reduced by an annual volume V given by

$$\begin{aligned} V &= (2.7 \times 10^{9}\ \mathrm{kg/yr})/(2.6 \times 10^{3}\ \mathrm{kg/m^3})(0.50) \\ &= 2.1 \times 10^{6}\ \mathrm{m^3/yr}. \end{aligned} \tag{2.79}$$

The sediment surface area is given in (2.63) as 2.0×10^{8} m^2. Thus, the annual rise R in sediment level is given by

$$R = (2.1 \times 10^{6}\ \mathrm{m^3/yr})/(2.0 \times 10^{8}\ \mathrm{m^2}) = 1.0 \times 10^{-2}\ \mathrm{m/yr}. \tag{2.80}$$

The lake is assumed to initially hold a volume of water equal to 1 year's discharge of river L at the head of the lake; as indicated in Table 2-12, this volume is 1.9×10^{10} m^3. Thus, the average depth D of the lake is given by

$$D = (1.9 \times 10^{10}\ \mathrm{m^3})/(2.0 \times 10^{8}\ \mathrm{m^2}) = 9.5 \times 10^{1}\ \mathrm{m}. \tag{2.81}$$

Thus, with the annual sediment rise obtained in (2.80), the time T required for the lake to completely fill in is given by

$$T = (9.5 \times 10^{1}\ \mathrm{m})/(1.0 \times 10^{-2}\ \mathrm{m/yr}) = 9.5 \times 10^{3}\ \mathrm{yr}. \tag{2.82}$$

Hence, with no major change in the valley's erosion rate, it seems reasonable to assume that the lake lasts for at least several thousand years. Further, it is assumed the volume remains at 1.9 x 10^{10} m^3 during this time. It can be shown that, although changing the volume of the lake affects the amount of radionuclides that it contains, it does not have a large effect on the radionuclide concentration.

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APPENDIX B

Examples of Mixed-Cell Models

B-1. Introduction

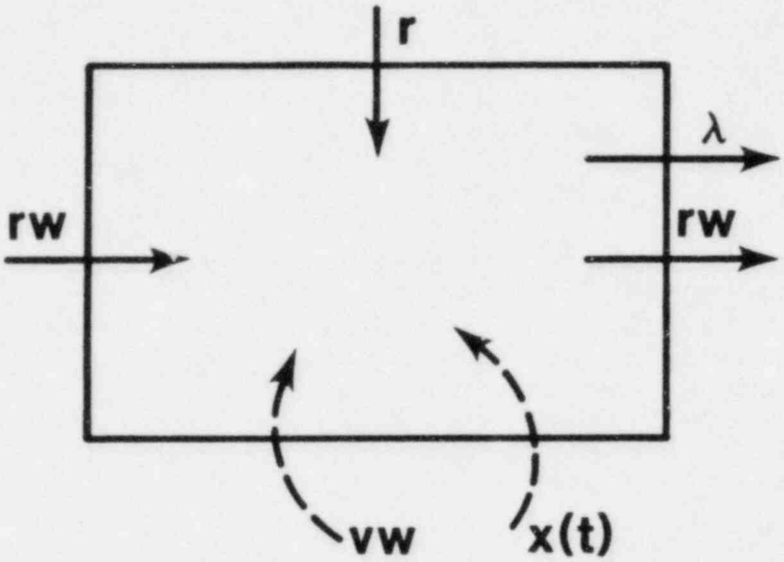
The purpose of this appendix is to present a sequence of examples which motivate and illustrate the mathematical model which underlies the Pathways Model. The intent is to give the reader a feeling for the use of mixed-cell (i.e., compartment) models to represent the movement of radionuclides. The presentation is elementary and is intended for individuals who are not familiar with such models.

In Section B-2, the differential equation for a single radionuclide in a single uniformly-mixed cell is developed. Next, in Section B-3, this example is expanded to include radionuclide partitioning between liquid and solid phases in the cell. An example of additional complexity is considered in Section B-4. This example involves a single radionuclide which moves between two uniformly-mixed cells and is partitioned between the liquid and solid phase of each cell. Finally, in Section B-5, the preceding example is expanded to include a decay segment involving two radionuclides.

B-2. One Cell Without Partitioning

The differential equation for a single uniformly-mixed cell without radionuclide partitioning between a liquid and a solid phase is presented in this section. The situation under consideration is indicated in Figure B-1. The cell is assumed to have a constant volume vw (units: L). Further, it is assumed that water enters and leaves the cell at a rate rw (units: L/yr) and that a radionuclide with decay constant λ (units: yr^{-1}) enters the cell at a rate r (units: atoms/yr). It is desired to determine the amount x(t) (units: atoms) of the radionuclide present in the cell at time t (units: yrs). The basic assumption used in deriving x(t) is that the cell is uniformly-mixed; mathematically, this means that the radionuclide concentration c(t) (units: atoms/L) at any time t is given by

$$c(t) = x(t)/vw. \qquad (B\text{-}1)$$



r: rate at which radionuclide enters cell (units: atoms/yr)

rw: rate at which water enters and leaves cell (units: L/yr)

λ: decay constant for radionuclide (units: yr^{-1})

vw: volume of water in cell (units: L)

$x(t)$: amount of radionuclide in cell at time t (units: atoms)

Figure B-1. Flows Associated With a Single Uniformly-Mixed Cell With no Radionuclide Partitioning Between a Liquid and a Solid Phase.

A differential equation representing the rate of change of x(t) is now derived. Then, x(t) can be obtained by solving this equation. The derivative dx(t)/dt (units: atoms/yr) is defined by the limit

$$\lim_{t \to 0} \frac{x(t + \Delta t) - x(t)}{\Delta t} \qquad \text{(B-2)}$$

and represents the rate at which x(t) is changing. In turn, this rate is equal to the difference between the rate r_1 (units: atoms/yr) at which the radionuclide is entering the cell and the rate r_2 (units: atoms/yr) at which the radionuclide is leaving the cell. The rate r_1 is given by r. The rate r_2 is the sum of two components: a rate due to physical flow out of the cell and a rate due to radioactive decay. The rate due to physical flow is equal to the product of the radionuclide concentration x(t)/vw in the cell and the rate of water flow rw out of the cell; the rate due to decay is equal to the product of the decay constant λ and the amount x(t) of radionuclide present. Thus,

$$r_1 = r \text{ and } r_2 = [(rw/vw) + \lambda]\ x(t), \qquad \text{(B-3)}$$

and hence, the desired equation is given by

$$\begin{aligned} dx(t)/dt &= r_1 - r_2 \\ &= r - [(rw/vw) + \lambda]\ x(t). \qquad \text{(B-4)} \end{aligned}$$

Also associated with the preceding equation is an initial value condition $x(0) = x_0$, which represents the amount of radionuclide present at time t = 0.

Thus, determination of x(t) reduces to the solution of an initial value problem of the form

$$dx(t)/dt = r - ax(t),\ x(0) = x_0, \qquad \text{(B-5)}$$

where

$$a = (rw/vw) + \lambda. \qquad \text{(B-6)}$$

Such problems are relatively easy to solve and applicable solution techniques include separation of variables, introduction of integration factors, and application of Laplace transforms. The preceding techniques are discussed in introductory texts on differential equations (e.g., Si72, Bra78, Ros74) and lead to the following unique solution for the initial value problem in (B-5):

$$x(t) = e^{-at}\, x_0 + (r/a)(1 - e^{-at}). \qquad \text{(B-7)}$$

If the initial value condition is x(0) = 0, then the preceding solution becomes

$$x(t) = (r/a)(1 - e^{-at}). \qquad \text{(B-8)}$$

Further, regardless of the initial value condition, the steady state or asymptotic solution sx to which any solution of (B-5) converges is given by

$$\begin{aligned} sx &= \lim_{t\to\infty} x(t) \\ &= \lim_{t\to\infty} [e^{-at}\, x_0 + (r/a)(1 - e^{-at})] \\ &= x_0 \lim_{t\to\infty} e^{-at} + (r/a)\left(1 - \lim_{t\to\infty} e^{-at}\right) \\ &= x_0(0) + (r/a)(1 - 0) \\ &= r/a \qquad \text{(B-9)} \end{aligned}$$

since a > 0.

An example is now presented. This example is adapted from the description of a site used in a sensitivity analysis of the Environmental Transport Model (Hel80). Specifically, the surface-water subzone of Zone 1 with the radionuclide Cm245 is considered. For this example,

$$r = 1.0 \text{ mg/yr} = 2.5 \times 10^{18} \text{ atoms/yr},$$

$$rw = 1.9 \times 10^{13} \text{ L/yr},$$

$$\lambda = 8.4 \times 10^{-5} \text{ yr}^{-1},$$

$$vw = 2.2 \times 10^{10} \text{ L},$$

and so

$$\begin{aligned} a &= (rw/vw) + \lambda \\ &= [(1.9 \times 10^{13} \text{ L/yr})/(2.2 \times 10^{10} \text{ L})] + 8.4 \times 10^{-5} \text{ yr}^{-1} \\ &= 8.6 \times 10^{2} \text{ yr}^{-1}. \end{aligned} \qquad \text{(B-10)}$$

Thus, the resultant differential equation is given by

$$\begin{aligned} dx(t)/dt &= r - ax(t) \\ &= 2.5 \times 10^{18} - (8.6 \times 10^{2})x(t). \end{aligned} \qquad \text{(B-11)}$$

As indicated in (B-8), the solution to (B-11) with the initial value condition $x(0) = 0$ is given by

$$\begin{aligned} x(t) &= [(2.5 \times 10^{18})/(8.6 \times 10^{2})][1 - \exp-(8.6 \times 10^{2})t] \\ &= 2.9 \times 10^{15} [1 - \exp(-860t)] \text{ atoms}. \end{aligned} \qquad \text{(B-12)}$$

Further, as indicated in (B-9), the asymptotic solution sx to (B-11) is given by

$$sx = (2.5 \times 10^{18})/(8.6 \times 10^{2}) = 2.9 \times 10^{15} \text{ atoms.} \tag{B-13}$$

Since exp(-860t) approaches zero very rapidly as t increases, the asymptotic solution is approached very rapidly.

In the preceding, x(t) is used to represent the amount of radionuclide present at time t in the cell. As indicated in (B-1), the concentration at time t is given by the quotient x(t)/vw. Also, x(t) is expressed in atoms; this simplifies the treatment of decay chains. However, the units can be changed to grams or curies by use of appropriate conversion factors. Specifically, the factor

$$c_{ag} = a_{wt}/6.024 \times 10^{23} \tag{B-14}$$

can be used to convert from atoms to grams, where a_{wt} (units: gm/gm-mole) denotes the atomic weight of the radionuclide under consideration and 6.024×10^{23} is Avogadro's number (units: molecules/gm-mole) and the factor

$$\begin{aligned} c_{ac} &= \frac{\ln(2.0)/(hl)(3.16 \times 10^{7})}{3.70 \times 10^{10}} \\ &= \lambda/(3.16 \times 10^{7})(3.70 \times 10^{10}) \\ &= \lambda/(1.17 \times 10^{18}) \end{aligned} \tag{B-15}$$

can be used to convert from atoms to curies, where ln(2.0) denotes the natural logarithm of 2.0, hl denotes the half-life (units: yrs) of the radionuclide under consideration, λ is the decay constant (units: yr^{-1}) for the radionulcide under consideration and is equal to ln(2.0)/hl, 3.16×10^{7} is the number of seconds per year and 3.70×10^{10} is the number of decays per second per curie.

For Cm245, the conversion factors c_{ag} and c_{ac} are given by

$$c_{ag} = 245/6.024 \times 10^{23} = 4.1 \times 10^{-22} \text{ gm/atom} \tag{B-16}$$

and

$$c_{ac} = 8.4 \times 10^{-5}/1.17 \times 10^{18} = 7.2 \times 10^{-23} \text{ ci/atom.} \tag{B-17}$$

Use of these conversion factors in conjunction with the solutions given in (B-12) and (B-13) yields

$$x(t) = \{2.9 \times 10^{15}[1 - \exp(-860t)] \text{ atoms}\}$$

$$\cdot\{4.1 \times 10^{-22} \text{ gm/atom}\}$$

$$= 1.2 \times 10^{-6}[1 - \exp(-860t)] \text{ gm} \tag{B-18}$$

$$x(t) = \{2.9 \times 10^{15}[1 - \exp(-860t)] \text{ atoms}\}$$

$$\cdot\{7.2 \times 10^{-23} \text{ ci/atom}\}$$

$$= 2.1 \times 10^{-7}[1 - \exp(-860t)] \text{ ci} \tag{B-19}$$

$$sx = (2.9 \times 10^{15} \text{ atoms}) (4.1 \times 10^{-22} \text{ gm/atoms})$$

$$= 1.2 \times 10^{-6} \text{ gm} \tag{B-20}$$

and

$$sx = (2.9 \times 10^{15} \text{ atoms}) (7.2 \times 10^{-23} \text{ ci/atom})$$

$$= 2.1 \times 10^{-7} \text{ ci.} \tag{B-21}$$

Further, as already discussed, the preceding values can be converted to concentrations through division by $vw = 2.2 \times 10^{10}$L.

The function appearing in (B-18) is graphed in Figure B-2. This is the solution to the differential equation appearing in (B-11) with initial value $x(0) = 0$ and units expressed in grams. As can be seen in this figure, $x(t)$ increases monotonically from the initial value to the asymptotic solution given in (B-20). This pattern of behavior will always be exhibited by solutions to initial value problems of the form indicated in (B-5) when $r > 0$, $a > 0$ and $r/a \geq x_0$. If $r > 0$, $a > 0$ and $r/a \leq x_0$, then $x(t)$ would decrease monotonically to the asymptotic solution r/a. The rate at which the asymptotic solution is approached depends only on the size of a; the larger a is, the more rapidly the asymptotic solution is approached. For the equation in (B-11), a is "large" and so the asymptotic solution is approached "rapidly".

B-3. One Cell With Partitioning

The differential equation for a single uniformly-mixed cell with radionuclide partitioning between a liquid and a solid phase is presented in this section. The situation under consideration is indicated in Figure B-3. The cell is assumed to have a constant volume vw (units: L) and to contain a constant mass ms of solid material (units: kg). Further, it is assumed that water enters and leaves the cell at a rate rw (units: L/yr), that solid material enters and leaves the cell at a rate rs (units: kg/yr), and that a radionuclide with decay constant λ (units: yr^{-1}) enters the cell at a rate r (units: atoms/yr). The partitioning of the radionuclide between the liquid and solid phases of the system is assumed to be described by the ratio

$$kd = \frac{\text{conc. of radionuclide sorbed to solids}}{\text{conc. of radionuclide dissolved in water}} = \frac{as/ms}{aw/vw} , \tag{B-22}$$

where as (units: atoms) is the amount of radionuclide in the system sorbed to solids and aw (units: atoms) is the amount of radionuclide in the system dissolved in water. The ratio in (B-22) is known as a kd-value

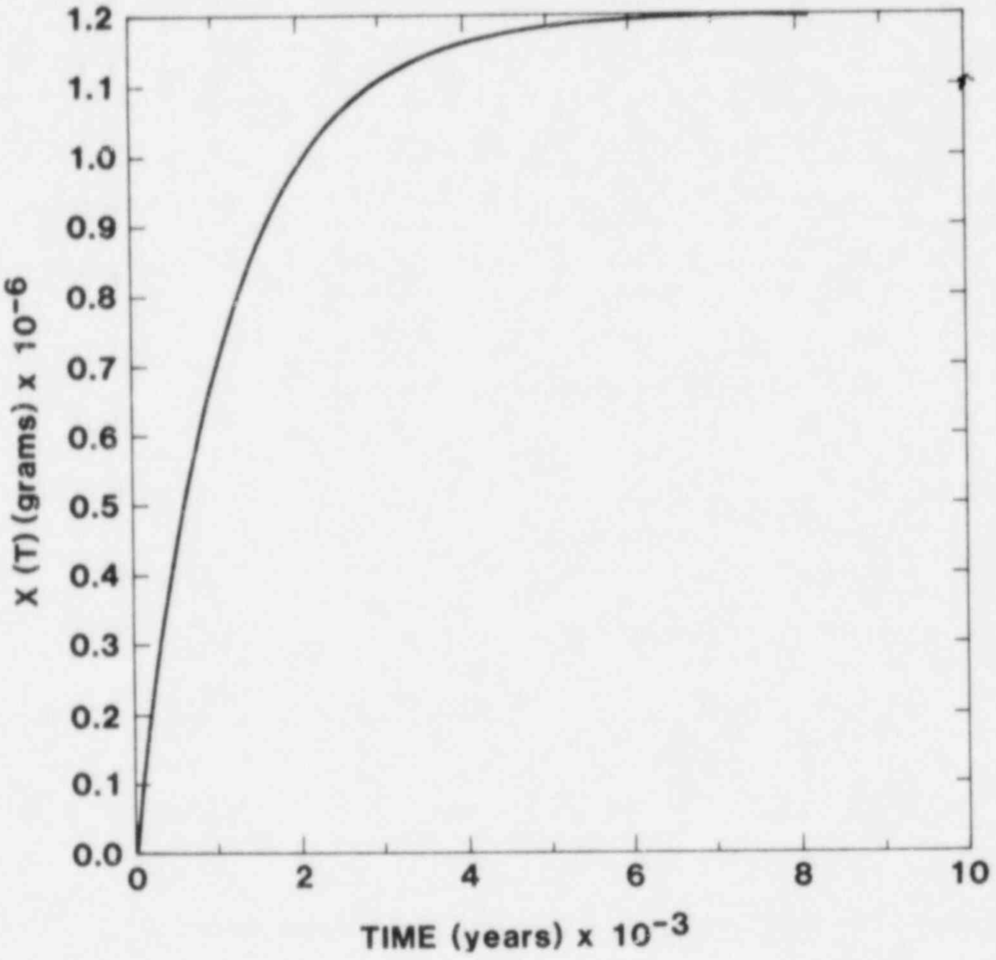
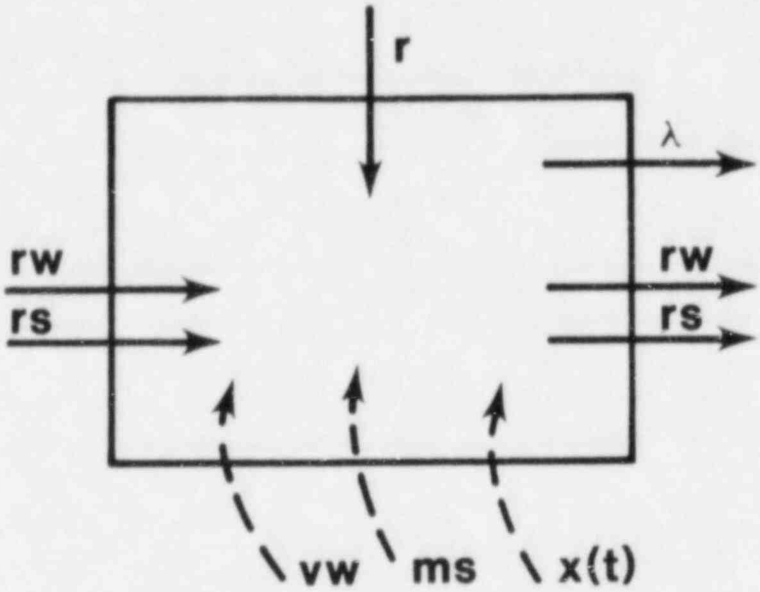


Figure B-2. Solution to Differential Equation Representing Amount of Radionuclide in Single Uniformly-Mixed Cell. This figure presents the graph of the function given in (B-18), which is the solution to the differential equation in (B-11) with initial value $x(0) = 0$ and units expressed in grams.



r: rate at which radionuclide enters cell (units: atoms/yr)

rw: rate at which water enters and leaves cell (units: L/yr)

rs: rate at which solid material enters and leaves cell (units: kg/yr)

λ: decay constant for radionuclide (units: yr^{-1})

vw: volume of water in cell (units: L)

ms: mass of solids in cell (units: kg)

x(t): amount of radionuclide in cell at time t (units: atoms)

Figure B-3. Flows Associated With a Single Uniformly-Mixed Cell With Radionuclide Partitioning Between a Liquid and a Solid Phase.

or a distribution coefficient; background on its use and derivation can be obtained in Appo et al. (Ap77), Baker et al. (Ba66) and Borg et al. (Bor76).

It is desired to determine the amount x(t) (units: atoms) of the radionuclide present in the cell at time t (units: yr). Three basic assumptions underlie the derivation of x(t). First, it is assumed that the radionuclide is uniformly distributed through the cell and is partitioned between the liquid and solid phases on the basis of its distribution coefficient. A derivation for this partitioning is presented in the next paragraph. Second, it is assumed that the flow of water and solid material out of the cell is the only mechanism involved in the physical transport of the radionuclide. Third, it is assumed that all radionuclides associated with a phase, liquid or solid, remain with that phase in movements out of the cell. In essence, the cell is treated as a uniformly mixed "vessel" in which the radionuclides are partitioned between the liquid and solid phases on the basis of the distribution coefficient and such that radionuclides can be carried out of this "vessel" and out of the system only by movements of water or solid material.

A derivation for the partitioning of a radionuclide between the liquid and solid phases of a system is now presented. The following notation is used in the derivation:

x = amount of radionuclide in system (in atoms),

xs = amount of radionuclide in system sorbed to solids (in atoms),

xw = amount of radionuclide in system dissolved in water (in atoms),

ms = mass of solid in system (in kilograms), and

vw = volume of water in system (in liters).

Assume x, ms, vw and kd are known for the system under consideration. Now, xs and xw are determined. Since

$$kd = (xs/ms)(xw/vw)^{-1} \text{ and } x = xs + xw, \qquad \text{(B-23)}$$

it follows that

$$(kd)(ms) = (xs)(vw)(xw)^{-1} \text{ and } xw = x - xs. \qquad (B\text{-}24)$$

Thus,

$$(kd)(ms) = (xs)(vw)(x - xs)^{-1}. \qquad (B\text{-}25)$$

Further, multiplication by (x - xs) gives

$$(kd)(ms)(x) - (kd)(ms)(xs) = (xs)(vw) \qquad (B\text{-}26)$$

or

$$(kd)(ms)(x) = [(kd)(ms) + vw]\ xs, \qquad (B\text{-}27)$$

and hence

$$xs = \left[\frac{(kd)(ms)}{(kd)(ms) + vw} \right] x. \qquad (B\text{-}28)$$

Further, since xw = x - xs,

$$xw = \left[1 - \frac{(kd)(ms)}{(kd)(ms) + vw} \right] x. \qquad (B\text{-}29)$$

The relations in (B-28) and (B-29) represent the desired partitioning.

A differential equation representing the rate of change of x(t) is now derived. Then, x(t) can be obtained by solving this equation. The following derivation is similar to that presented in Section B-2 for a uniformly-mixed cell without partitioning. As there, dx(t)/dt is equal to the difference between the rate r_1 at which the radionuclide is entering the cell and the rate r_2 at which the radionuclide is leaving the cell.

The rate r_1 is given by r. The rate r_2 is the sum of three components: a rate due to physical flow out of the cell with solid material, a rate due to physical flow out of the cell with water, and a rate due to radioactive decay. The two rates due to physical flow are equal to the products of the concentrations xs(t)/ms and xw(t)/vw with the flow rates rs and rw, where xs(t) represents the amount of radionuclide in the cell sorbed to solid material and xw(t) represents the amount of radionuclide in the cell dissolved in water. The functions xs(t) and xw(t) can be obtained from (B-28) and (B-29). The rate due to decay is equal to the product of the decay constant λ and the amount x(t) of radionuclide present. Thus,

$$r_1 = r \tag{B-30}$$

and

$$\begin{aligned} r_2 &= [xs(t)/ms][rs] + [xw(t)/vw]\,[rw] + \lambda x(t) \\ &= \left[\frac{(kd)(ms)}{(kd)(ms) + vw}\right]\left[x(t)\right]\left[\frac{rs}{ms}\right] \\ &\quad + \left[1 - \frac{(kd)(ms)}{(kd)(ms) + vw}\right]\left[x(t)\right]\left[\frac{rw}{vw}\right] + \lambda x(t) \end{aligned}$$

[From (B-28) and (B-29)]

$$= \left[\frac{s(rs)}{ms} + \frac{(1 - s)(rw)}{vw} + \lambda\right] x(t), \tag{B-31}$$

where

$$s = \frac{(kd)(ms)}{(kd)(ms) + vw}\,. \tag{B-32}$$

Hence, the desired equation is given by

$$dx(t)/dt = r_1 - r_2$$

$$= r - \left[\frac{s(rs)}{ms} + \frac{(1 - s)(rw)}{vw} + \lambda\right] x(t) \ . \quad \text{(B-33)}$$

Also associated with the preceding equation is an initial value condition $x(0) = x_0$.

Thus, as in Section B-2, determination of x(t) reduces to the solution of an initial value problem of the form

$$dx(t)/dt = r - ax(t),\ x(0) = x_0, \quad \text{(B-34)}$$

where

$$a = \frac{s(rs)}{ms} + \frac{(1 - s)(rw)}{vw} + \lambda \quad \text{(B-35)}$$

with s defined as in (B-32). Various forms of the solution to the preceding initial value problem are given in (B-7), (B-8) and (B-9).

An example is now presented. This example is adapted from the description of a site used in a sensitivity analysis of the Environmental Transport Model (Hel80). Specifically, the soil subzone of Zone 1 with the radionuclide Cm245 is considered. For this example,

$r = 1.0$ mg/yr $= 2.5 \times 10^{18}$ atoms/yr

$rs = 1.1 \times 10^8$ kg/yr

$rw = 1.4 \times 10^{11}$ L/yr

$\lambda = 8.4 \times 10^{-5}$ yr^{-1}

$ms = 1.1 \times 10^{11}$ kg

$vw = 2.0 \times 10^{10}$ L

$kd = 1.0 \times 10^3$ L/kg.

Thus,

$$s = \frac{(1.0 \times 10^3)(1.1 \times 10^{11})}{(1.0 \times 10^3)(1.1 \times 10^{11}) + 2.0 \times 10^{10}} = 1.0 \times 10^0 \qquad \text{(B-36)}$$

and

$$a = \frac{(1.0)(1.1 \times 10^8)}{1.1 \times 10^{11}} + \frac{(1.0 - 1.0)(1.4 \times 10^{11})}{2.0 \times 10^{10}} + 8.4 \times 10^{-5}$$

$$= 1.0 \times 10^{-3} \text{ yr}^{-1}. \qquad \text{(B-37)}$$

Hence, the resultant differential equation is given by

$$dx(t)/dt = r - a\,x(t)$$

$$= 2.5 \times 10^{18} - (1.0 \times 10^{-3})\,x(t). \qquad \text{(B-38)}$$

As indicated in (B-8), the solution to (B-38) with the initial value condition $x(0) = 0$ is given by

$$x(t) = [(2.5 \times 10^{18})/(1.0 \times 10^{-3})][1 - \exp-(1.0 \times 10^{-3})t]$$

$$= 2.5 \times 10^{21}\ [1 - \exp(-0.001t)] \text{ atoms.} \qquad \text{(B-39)}$$

Further, as indicated in (B-9), the asymptotic solution sx to (B-38) is given by

$$sx = (2.5 \times 10^{18})/(1.0 \times 10^{-3}) = 2.5 \times 10^{21} \text{ atoms.} \qquad \text{(B-40)}$$

Due to the smaller size of a, the asymptotic solution for (B-38) is not approached as rapidly as the asymptotic solution for (B-11). The conversion factors c_{ag} and c_{ac} for Cm245 to convert from atoms to grams and from atoms to curies are given in (B-16) and (B-17), respectively. When c_{aq} is used, the expressions in (B-39) and (B-40) become

$$x(t) = \{2.5 \times 10^{21} [1 - \exp(-0.001t)]\}\{4.1 \times 10^{-22} \text{ gm/atom}\}$$

$$= 1.0 - \exp(-0.001t) \text{ gm} \qquad \text{(B-41)}$$

and

$$sx = 1.0 \text{ gm}. \qquad \text{(B-42)}$$

The function appearing in (B-41) is graphed in Figure B-4.

The relations appearing in (B-28) and (B-29) can be used to express x(t) as the sum xs(t) + xw(t), where xs(t) is the amount of radionuclide in the compartment at time t sorbed to solids and xw(t) is the amount of radionuclide in the compartment at time t dissolved in water. Specifically,

$$xs(t) = (s)\ x(t) \qquad \text{(B-43)}$$

and

$$xw(t) = (1.0 - s)\ x(t), \qquad \text{(B-44)}$$

where s is defined in (B-32). In the example of this section with only two significant digits retained, s is calculated in (B-36) to be 1.0, and so xs(t) = x(t) and xw(t) = 0. However, if calculations are performed with four significant digits, then

$$s = \frac{(1.000 \times 10^{3})(1.100 \times 10^{11})}{(1.000 \times 10^{3})(1.100 \times 10^{11}) + 2.000 \times 10^{10}}$$

$$= 9.998 \times 10^{-1}. \qquad \text{(B-45)}$$

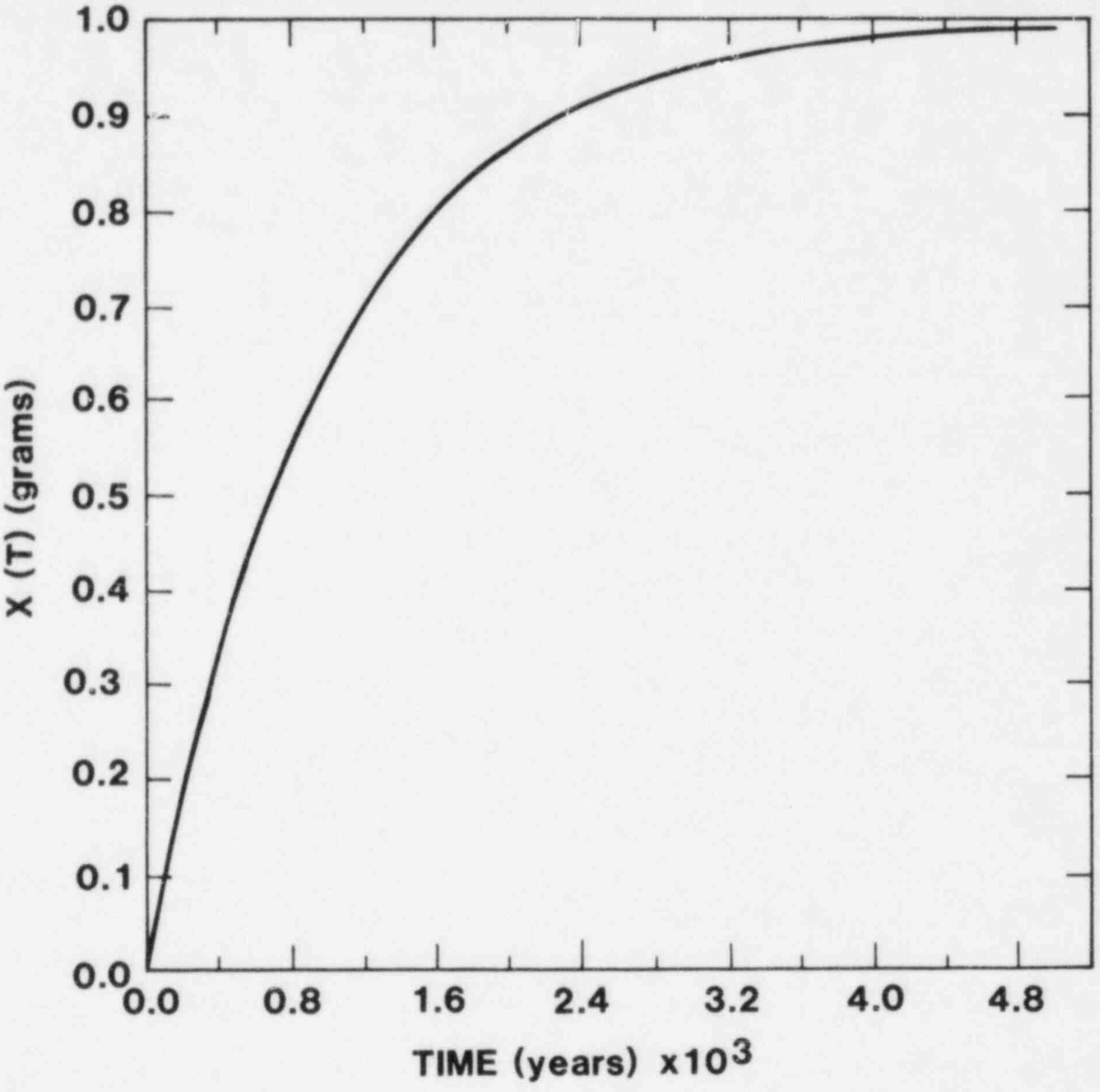


Figure B-4. Solution to Differential Equation Representing Amount of Radionuclide in Single Uniformly-Mixed Cell With Partitioning. This figure represents the graph of the function given in (B-41), which is the solution to the differential equation in (B-38) with initial value x(0) = 0 and units expressed in grams.

Clearly, most of the radionuclide will be associated with solid material in the system.

The example of the preceding paragraph indicates that the solid and liquid components of a compartment may be of unequal importance in influencing radionuclide movement. The cause of this is best seen by examining the definition of a in (B-35) and the definition of s in (B-32). The coefficient a is the sum of three terms:

$$\frac{s(rs)}{ms}, \quad \frac{(1 - s)(rw)}{vw}, \quad \lambda. \qquad (B\text{-}46)$$

If any one of these terms is much larger than the other two, then its value will dominate the behavior of the solution to (B-34). Further, the behavior of the first two terms is influenced by the relationship between vw and the product (kd)(ms) in the definition of s. If (kd)(ms) is much larger than vw, then s is close to 1 and so the second term in (B-46) may be of reduced importance; if (kd)(ms) is much smaller than vw, then s is close to 0 and so the first term in (B-46) may be of reduced importance. However, the relative size of the ratios rs/ms and rw/vw is also important. Therefore, as s is used as an intermediate quantity in the calculation of the rate constants in (B-46), care must be taken in its determination to avoid the introduction of errors by inappropriate rounding.

B-4. Two Cells With Partitioning

The system of differential equations for two uniformly-mixed cells with radionuclide partitioning between liquid and solid phases is presented in this section. The situation under consideration is indicated in Figure B-5. A single radionuclide is considered and the partitioning of this radionuclide between the liquid and solid phases of each cell is described with a distribution coefficient. It is desired to determine the amounts $x_1(t)$ and $x_2(t)$ (units: atoms) of the radionuclide present in each cell at time t (units: yr). Three basic assumptions underlie the derivation of a system of differential equations defining $x_1(t)$ and $x_2(t)$. First, it is assumed that the radionuclide is uniformly distributed through each cell and is partitioned between the liquid and solid phases on the basis

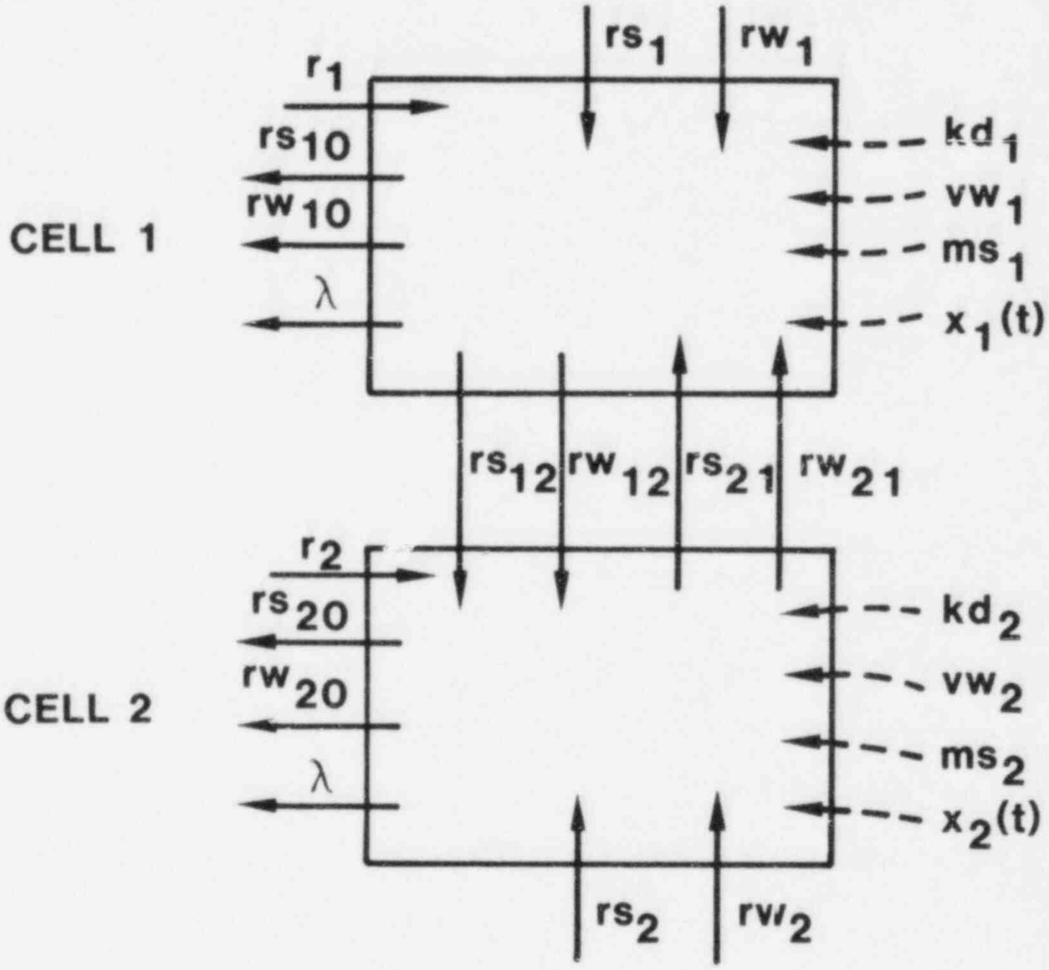


Figure B-5. Flows Associated With Two Uniformly-Mixed Cells With Radionuclide Partitioning Between a Liquid and a Solid Phase. Symbols are defined in Table B-1. With the assumption that ms_i and vw_i are constants, the following equalities must hold:

$$rs_1 + rs_{21} = rs_{10} + rs_{12},\ rs_2 + rs_{12} = rs_{20} + rs_{21},$$

$$rw_1 + rw_{21} = rw_{10} + rw_{12},\ rw_2 + rw_{12} = rw_{20} + rw_{21}.$$

Table B-1

Symbols Appearing in Figure B-5

r_i = rate at which radionuclide enters cell i (units: atoms/yr)

rs_i = rate at which solid material enters cell i from outside the system (units: kg/yr)

rw_i = rate at which water enters cell i from outside the system (units: L/yr)

rs_{ij} = rate at which solid material flows from cell i to cell j, where j = 0 is used to designate a movement out of the system (units: kg/yr)

rw_{ij} = rate at which water flows from cell i to cell j, where j = 0 is used to designate a movement out of the system (units: L/yr)

λ = decay constant for radionuclide (units: yr^{-1})

kd_i = distribution coefficient for radionuclide in cell i (units: L/kg)

ms_i = mass of solids in cell i (units: kg)

vw_i = volume of water in cell i (units: L)

$x_i(t)$ = amount of radionuclide in cell i (units: atoms) of its distribution coefficient for that cell. A derivation for this partitioning is presented in the previous section. Second, it is assumed that the flow of water and solid material between cells or out of the system is the only mechanism involved in the physical transport of radionuclides. Third, it is assumed that all radionuclides associated with a phase, liquid or solid, remain with that phase in movements between cells or out of the system. In essence, each cell is treated as a uniformly mixed "vessel" in which the radionuclides are partitioned between the liquid and solid phase on the basis of distribution coefficients and such that radionuclides can be carried between these "vessels" or out of a "vessel" and out of the system only by movements of water or solid material.

Differential equations representing the rate of change of $x_i(t)$, $i = 1, 2$, are now derived. Then, $x_1(t)$ and $x_2(t)$ can be obtained by solving the resultant vector differential equation. The derivation of the differential equation for each $x_i(t)$ is similar to that demonstrated in the preceding section for a single uniformly-mixed cell with partitioning. As there, $dx_i(t)/dt$ is equal to the difference between the rate r_{i1} at which the radionuclide is entering the ith cell and the rate r_{i2} at which the radionuclide is leaving the ith cell. In the following, it is convenient to use $xs_i(t)$ and $xw_i(t)$ (units: atoms), $i = 1, 2$, to represent the amount of radionuclide in the solid and liquid phases, respectively, of cell i.

The rate r_{11} is the sum of three components: the rate at which the radionuclide enters cell 1 from outside the system, the rate at which the radionuclide is carried from cell 2 to cell 1 by the movement of solid material, and the rate at which the radionuclide is carried from cell 2 to cell 1 by the movement of water. Thus,

$$r_{11} = r_1 + \left[\frac{xs_2(t)}{ms_2}\right]\left[rs_{21}\right] + \left[\frac{xw_2(t)}{vw_2}\right]\left[rw_{21}\right]$$

$$= r_1 + [s_2][x_2(t)][rs_{21}/ms_2] + [1-s_2][x_2(t)][rw_{21}/vw_2]$$

[From (B-28) and B-29)]

$$= r_1 + \left[\frac{(s_2)(rs_{21})}{ms_2} + \frac{(1 - s_2)(rw_{21})}{vw_2} \right] x_2(t), \quad \text{(B-47)}$$

where

$$s_2 = \frac{(kd_2)(ms_2)}{(kd_2)(ms_2) + vw_2} . \quad \text{(B-48)}$$

The rate r_{12} is also the sum of three components: the rate at which the radionuclide is carried out of cell 1 by the movement of solid material, the rate at which the radionuclide is carried out of cell 1 by the movement of water, and the rate at which the radionuclide is lost due to radioactive decay. Thus,

$$r_{12} = \left[\frac{xs_1(t)}{ms_1} \right] \left[rs_{10} + rs_{12} \right] + \left[\frac{xw_1(t)}{vw_1} \right] \left[rw_{10} + rw_{12} \right] + \lambda \left[x_1(t) \right]$$

$$= [s_1][x_1(t)] \left[\frac{rs_{10} + rs_{12}}{ms_1} \right] + [1 - s_1][x_1(t)] \left[\frac{rw_{10} + rw_{12}}{vw_1} \right]$$

$$+ \lambda [x_1(t)] \qquad \text{[From (B-28) and (B-29)]}$$

$$= \left[\frac{(s_1)(rs_{10} + rs_{12})}{ms_1} + \frac{(1 - s_1)(rw_{10} + rw_{12})}{vw_1} + \lambda \right] x_1(t), \quad \text{(B-49)}$$

where

$$s_1 = \frac{(kd_1)(ms_1)}{(kd_1)(ms_1) + vw_1} . \quad \text{(B-50)}$$

The rates r_{21} and r_{22} are derived similarly to r_{11} and r_{12} and are given by

$$r_{21} = r_2 + \left[\frac{(s_1)(rs_{12})}{ms_1} + \frac{(1 - s_1)(rw_{12})}{vw_1} \right] x_1(t) \qquad \text{(B-51)}$$

and

$$r_{22} = \left[\frac{(s_2)(rs_{20} + rs_{21})}{ms_2} + \frac{(1 - s_2)(rw_{20} + rw_{21})}{vw_2} + \lambda \right] x_2(t). \qquad \text{(B-52)}$$

The desired equations can now be stated. Specifically,

$$dx_1(t)/dt = r_{11} - r_{12} = r_1 + a_{12}x_2(t) - a_{11}\, x_1(t) \qquad \text{(B-53)}$$

$$dx_2(t)/dt = r_{21} - r_{22} = r_2 + a_{21}\, x_1(t) - a_{22}\, x_2(t),$$

where

$$a_{11} = \frac{(s_1)(rs_{10} + rs_{12})}{ms_1} + \frac{(1 - s_1)(rw_{10} + rw_{12})}{vw_1} + \lambda \qquad \text{(B-54)}$$

$$a_{12} = \frac{(s_2)(rs_{21})}{ms_2} + \frac{(1 - s_2)(rw_{21})}{vw_2} \qquad \text{(B-55)}$$

$$a_{21} = \frac{(s_1)(rs_{12})}{ms_1} + \frac{(1 - s_1)(rw_{12})}{vw_1} \qquad \text{(B-56)}$$

$$a_{22} = \frac{(s_2)(rs_{20} + rs_{21})}{ms_2} + \frac{(1 - s_2)(rw_{20} + rw_{21})}{vw_2} + \lambda . \qquad \text{(B-57)}$$

The representation used for the system in (B-53) was selected to facilitate its reformulation as the following vector differential equation:

$$\frac{d}{dt} x(t) = R + Ax(t), \qquad \text{(B-58)}$$

where,

$$x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}, \; R = \begin{bmatrix} r_1 \\ r_2 \end{bmatrix}, \text{ and } A = \begin{bmatrix} -a_{11} & a_{12} \\ a_{21} & -a_{22} \end{bmatrix}. \qquad \text{(B-59)}$$

Usually, such systems are easier to deal with when reformulated in this manner. Various methods exist to solve systems of the form appearing in (B-53) and (B-58). For example, differential operators, Laplace transforms or eigen-value techniques can be used when the system is relatively simple. Discussions of such techniques can be found in Boyce and DiPrima (Boy69) and other introductory texts on differential equations. However, in most situations it is necessary to use some type of numerical scheme to determine an approximate solution. Elementary discussions of such procedures can be found in Conti and de Boor (Co80) and other introductory texts on numerical analysis. Also, if A^{-1} exists, then there exists a unique vector sx to which every solution of (B-58) converges; the asymptotic solution sx is given by

$$sx = -A^{-1}R. \qquad \text{(B-60)}$$

Treatments of matrix algebra are provided in Noble and Daniel (No77), Rice (Ri81) and numerous other texts.

An example is now presented. This example is adapted from the description of a site used in a sensitivity analysis of the Environmental Transport Model (Hel80). Specifically, the soil and surface-water subzones of zone 1 with the radionuclide Cm245 are considered and assumed to correspond to cells 1 and 2, respectively. The values for the parameters indicated in Figure B-5 are given in Table B-2.

The vector differential equation appearing in (B-57) is now derived for the example. First, from (B-50) and (B-48),

$$s_1 = \frac{(1.0 \times 10^3)(1.1 \times 10^{11})}{(1.0 \times 10^3)(1.1 \times 10^{11}) + 2.0 \times 10^{10}} = 0.9998 \tag{B-61}$$

and

$$s_2 = \frac{(1.0 \times 10^3)(3.5 \times 10^6)}{(1.0 \times 10^3)(3.5 \times 10^6) + 2.2 \times 10^{10}} = 0.1373. \tag{B-62}$$

Now, from (B-54) through (B-57),

$$a_{11} = \frac{(0.9998)(0 + 1.1\text{x}10^8)}{1.1 \times 10^{11}}$$

$$+ \frac{(1 - 0.9998)(9.3\text{x}10^{10} + 4.0\text{x}10^{10})}{2.0 \times 10^{10}} + 8.4 \times 10^{-5}$$

$$= 1.0 \times 10^{-3} + 1.4 \times 10^{-3} + 8.4 \times 10^{-5}$$

$$= 2.5 \times 10^{-3}\ \text{yr}^{-1}, \tag{B-63}$$

$$a_{12} = \frac{(0.1373)(1.1 \times 10^8)}{3.5 \times 10^6} + \frac{(1 - 0.1373)(4.0 \times 10^{10})}{2.2 \times 10^{10}}$$

$$= 4.3 \times 10^0 + 1.6 \times 10^0$$

$$= 5.9\ \text{yr}^{-1}, \tag{B-64}$$

Table B-2

Parameter Values for an Example of a Two Cell System

	Cell 1 (Soil)	Cell 2 (Surface Water)
r_i	0	2.5×10^{18} atoms/yr
rs_i	0	3.0×10^{9} kg/yr
rw_i	9.8×10^{10} L/yr	1.9×10^{13} L/yr
rs_{i0}	0	3.0×10^{9} kg/yr
rs_{ij}, $j \neq 0$	1.1×10^{8} kg/yr	1.1×10^{8} kg/yr
rw_{i0}	9.8×10^{10} L/yr	1.9×10^{13} L/yr
rw_{ij}, $j \neq 0$	4.0×10^{10} L/yr	4.0×10^{10} L/yr
ms_i	1.1×10^{11} kg	3.5×10^{6} kg
vw_i	2.0×10^{10} L	2.2×10^{10} L
kd_i	1.0×10^{3} L/kg	1.0×10^{3} L/kg

$$\lambda = 8.4 \times 10^{-5} \text{ yr}^{-1}$$

$$a_{21} = \frac{(0.9998)(1.1 \times 10^8)}{1.1 \times 10^{11}} + \frac{(1 - 0.9998)(4.0 \times 10^{10})}{2.0 \times 10^{10}}$$

$$= 1.0 \times 10^{-3} + 4.0 \times 10^{-4}$$

$$= 1.4 \times 10^{-3} \text{ yr}^{-1} \qquad \text{(B-65)}$$

and

$$a_{22} = \frac{(0.1373)(3.0\times10^9 + 1.1\times10^8)}{3.5 \times 10^6}$$

$$+ \frac{(1 - 0.1373)(1.9\times10^{13} + 4.0\times10^{10})}{2.2 \times 10^{10}}$$

$$+ 8.4 \times 10^{-5}$$

$$= 1.2 \times 10^2 + 7.5 \times 10^2 + 8.4 \times 10^{-5}$$

$$= 8.7 \times 10^2 \text{ yr}^{-1} . \qquad \text{(B-66)}$$

Thus, the desired equation is

$$\frac{d}{dt} \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} 0 \\ 2.5 \times 10^{18} \end{bmatrix} + \begin{bmatrix} -2.5\times10^{-3} & 5.9\times10^0 \\ 1.4\times10^{-3} & -8.7\times10^2 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}. \qquad \text{(B-67)}$$

The preceding equation can be solved numerically to obtain $x_1(t)$ and $x_2(t)$. Further, the asymptotic solution $[sx_1 \ sx_2]^T$ can be obtained from the product

$$\begin{bmatrix} sx_1 \\ sx_2 \end{bmatrix} = - \begin{bmatrix} -2.5 \times 10^{-3} & 5.9 \times 10^0 \\ 1.4 \times 10^{-3} & -8.7 \times 10^2 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 2.5 \times 10^{18} \end{bmatrix}. \qquad \text{(B-68)}$$

The results of such calculations are shown in Figure B-6; units are converted to grams as discussed in Section B-2.

B-5. Two Cells With Two Radionuclides and Partitioning

The system of differential equations for two uniformly-mixed cells with two radionuclides and radionuclide partitioning between liquid and solid phases is presented in this section. Physically, the situation under consideration is the same as that indicated in Figure B-5 with the exception that there are now two radionuclides. This necessitates the introduction of the following additional variables:

r_{ij} = rate at which radionuclide j enters cell i from outside the system (units: atoms/yr)

λ_j = decay constant for radionuclide j (units: yr^{-1})

kd_{ij} = distribution coefficient for radionuclide j in cell i (units: L/kg)

$x_{ij}(t)$ = amount of radionuclide j in cell i (units: atoms).

All other notation is the same as indicated in Figure B-5. It is assumed that the first radionuclide decays to the second.

Differential equations representing the rate of change of $x_{ij}(t)$, i, j = 1, 2, are now obtained. The two equations representing the change of the first radionuclide are the same as the two equations derived in the preceding section. Thus, from (B-53) through (B-57),

$$dx_{11}(t)/dt = r_{11} - a_{11}\, x_{11}(t) + a_{13}\, x_{21}(t)$$
$$dx_{21}(t)/dt = r_{21} + a_{31}\, x_{11}(t) - a_{33}\, x_{21}(t) \; , \qquad (B-69)$$

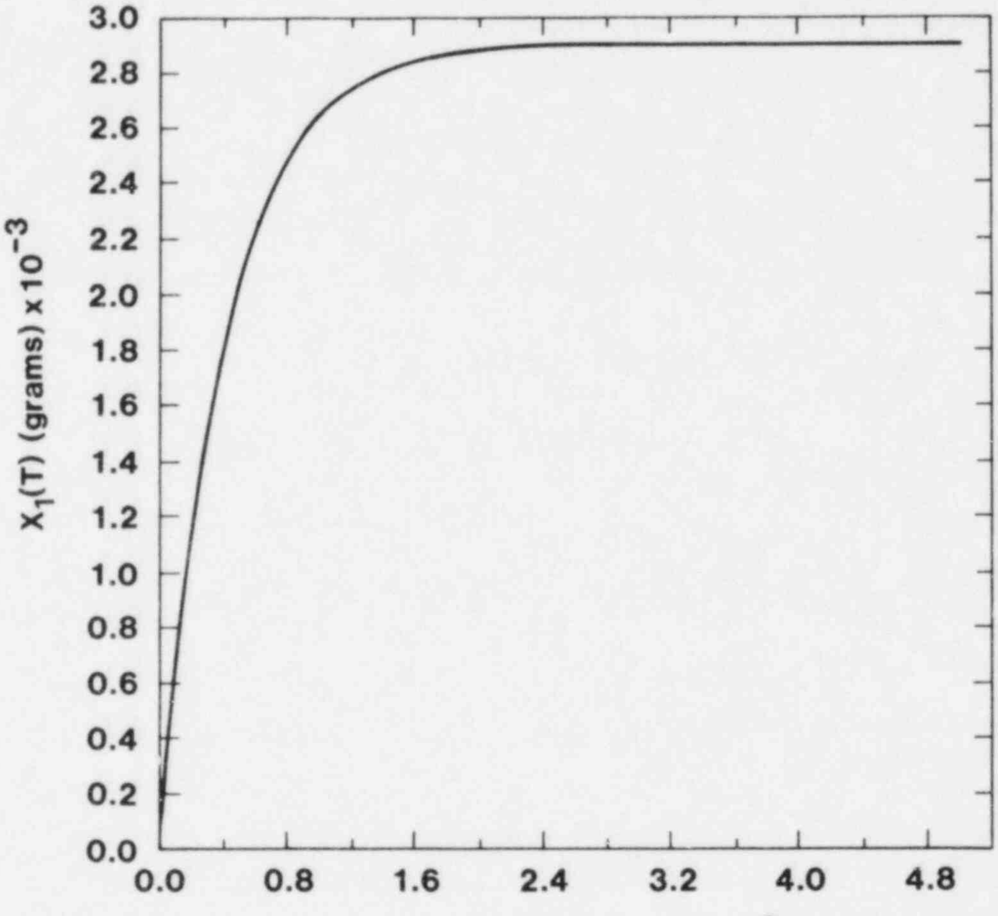


Figure B-6. Solutions to System of Differential Equations Representing Amount of Radionuclide in Two Uniformly-Mixed Cells. This figure represents the solution to the equation in (B-66) with initial value $x(0) = 0$ and units expressed in grams.

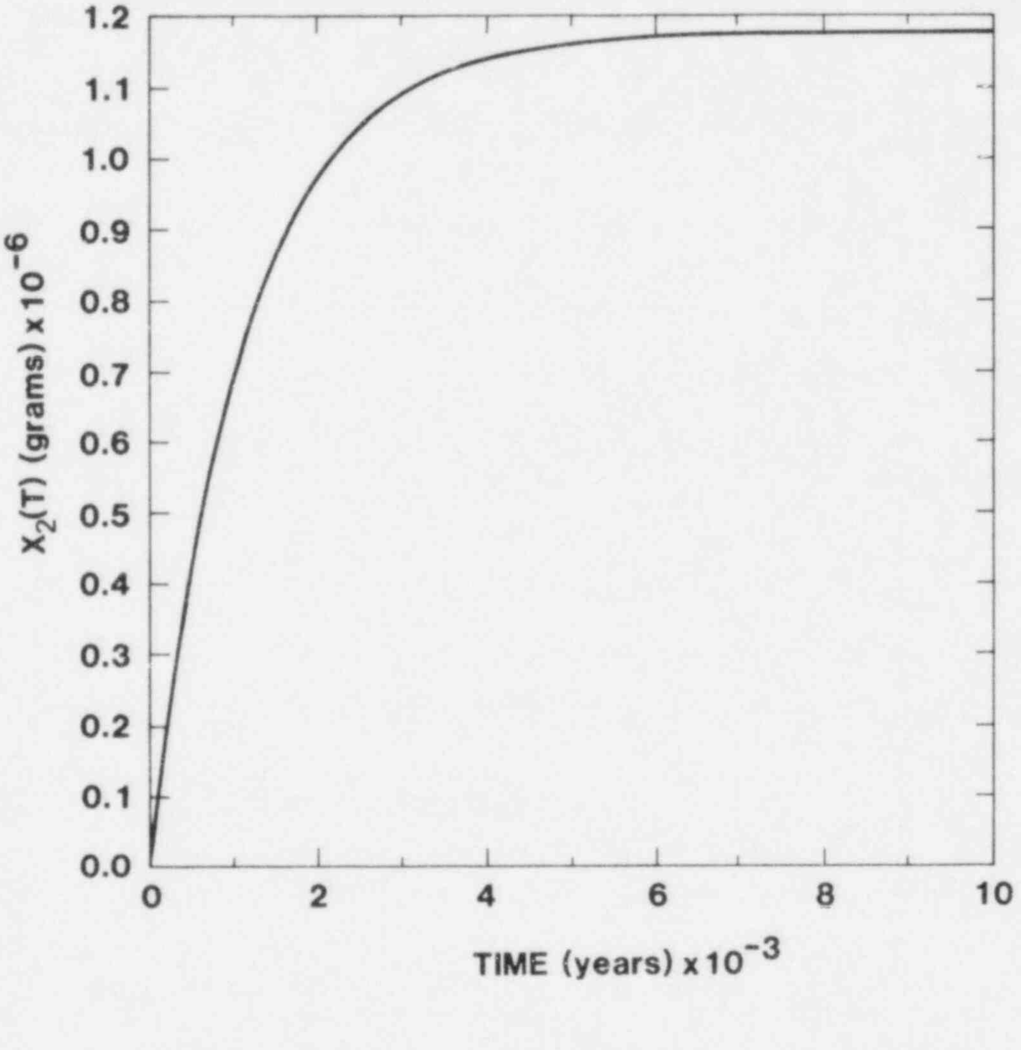


Figure B-6 (Continued)

where

$$a_{11} = \frac{(s_{11})(rs_{10} + rs_{12})}{ms_1} + \frac{(1 - s_{11})(rw_{10} + rw_{12})}{vw_1} + \lambda_1, \quad \text{(B-70)}$$

$$a_{13} = \frac{(s_{21})(rs_{21})}{ms_2} + \frac{(1 - s_{21})(rw_{21})}{vw_2}, \quad \text{(B-71)}$$

$$a_{31} = \frac{(s_{11})(rs_{12})}{ms_1} + \frac{(1 - s_{11})(rw_{12})}{vw_1}, \quad \text{(B-72)}$$

$$a_{33} = \frac{(s_{21})(rs_{20} + rs_{21})}{ms_2} + \frac{(1 - s_{21})(rw_{20} + rw_{21})}{vw_2} + \lambda_1, \quad \text{(B-73)}$$

with

$$s_{i1} = \frac{(kd_{i1})(ms_i)}{(kd_{i1})(ms_i) + vw_i} \quad \text{(B-74)}$$

for i = 1, 2. The preceding choice of subscripts for the a_{ij} is motivated by their use in a later matrix formulation of the problem.

The two equations representing the change of the second radionuclide are now given. These equations are very similar to the equations for the first radionuclide. The only difference is that it is necessary to include the increase in the second radionuclide due to the decay of the first radionuclide. Specifically,

$$dx_{12}/dt = r_{12} + a_{21}\, x_{11}(t) - a_{22}\, x_{12}(t) + a_{24}\, x_{22}(t) \quad \text{(B-75)}$$

$$dx_{22}/dt = r_{21} + a_{42}\, x_{12}(t) + a_{43}\, x_{21}(t) - a_{44}\, x_{22}(t) ,$$

where

$$a_{21} = a_{43} = \lambda_1 , \quad \text{(B-76)}$$

$$a_{22} = \frac{(s_{12})(rs_{10} + rs_{12})}{ms_1} + \frac{(1 - s_{12})(rw_{10} + rw_{12})}{vw_1} + \lambda_2, \tag{B-77}$$

$$a_{24} = \frac{(s_{22})(rs_{21})}{ms_2} + \frac{(1 - s_{22})(rw_{21})}{vw_2}, \tag{B-78}$$

$$a_{42} = \frac{(s_{12})(rs_{12})}{ms_1} + \frac{(1 - s_{12})(rw_{12})}{vw_1} \tag{B-79}$$

$$a_{44} = \frac{(s_{22})(rs_{20} + rs_{21})}{ms_2} + \frac{(1 - s_{22})(rw_{20} + rw_{21})}{vw_2} + \lambda_2, \tag{B-80}$$

with

$$s_{i2} = \frac{(kd_{i2})(ms_i)}{(kd_{i2})(ms_i) + vw_i} \tag{B-81}$$

for i = 1, 2.

The system of four equations indicated in (B-69) and (B-75) can be formulated as a single vector differential equation. This yields

$$\frac{d}{dt}\begin{bmatrix} x_{11}(t) \\ x_{12}(t) \\ x_{21}(t) \\ x_{22}(t) \end{bmatrix} = \begin{bmatrix} r_{11} \\ r_{12} \\ r_{21} \\ r_{22} \end{bmatrix} + \begin{bmatrix} -a_{11} & 0 & a_{13} & 0 \\ a_{21} & -a_{22} & 0 & a_{24} \\ a_{31} & 0 & -a_{33} & 0 \\ 0 & a_{42} & a_{43} & -a_{44} \end{bmatrix} \begin{bmatrix} x_{11}(t) \\ x_{12}(t) \\ x_{21}(t) \\ x_{22}(t) \end{bmatrix}. \tag{B-82}$$

More compactly, the preceding equation can be represented as

$$\frac{d}{dt}x(t) = R + Ax(t). \tag{B-83}$$

The system used in the example of the preceding section is used again. This system is assumed to be receiving an inflow of Cm245 and Pu241 into the surface-water component. Specifically,

$r_{11} = r_{12} = 0$, $r_{21} = 2.5 \times 10^{18}$ atoms/yr,

$r_{22} = 4.4 \times 10^{15}$ atoms/yr.

Further,

$\lambda_1 = 8.4 \times 10^{-5}\ yr^{-1}$, $\lambda_2 = 4.7 \times 10^{-2}$, $kd_{ij} = 1.0 \times 10^3$.

Now, from the equalities in (B-70) through (B-74) and (B-76) through (B-81), it follows that

$$a_{11} = 2.5 \times 10^{-3}\ yr^{-1}$$

$$a_{13} = 5.9 \times 10^{0}\ yr^{-1}$$

$$a_{31} = 1.4 \times 10^{-3}\ yr^{-1}$$

$$a_{33} = 8.7 \times 10^{2}\ yr^{-1}$$

$$a_{21} = a_{43} = 8.4 \times 10^{-5}\ yr^{-1}$$

$$a_{22} = 4.9 \times 10^{-2}\ yr^{-1}$$

$$a_{24} = 5.9 \times 10^{0}\ yr^{-1}$$

$$a_{42} = 1.4 \times 10^{-3}\ yr^{-1}$$

$$a_{44} = 8.7 \times 10^{2}\ yr^{-1}.$$

Thus, for this example, the R and A in (B-83) become

$$R = \begin{bmatrix} 0 \\ 0 \\ 2.5\text{x}10^{18} \\ 4.4\text{x}10^{15} \end{bmatrix}, \; A = \begin{bmatrix} -2.5\text{x}10^{-3} & 0 & 5.9\text{x}10^{0} & 0 \\ 8.4\text{x}10^{-5} & -4.9\text{x}10^{-2} & 0 & 5.9\text{x}10^{0} \\ 1.4\text{x}10^{-3} & 0 & -8.7\text{x}10^{2} & 0 \\ 0 & 1.4\text{x}10^{-3} & 8.4\text{x}10^{-5} & -8.7\text{x}10^{2} \end{bmatrix}. \tag{B-84}$$

The solution and asymptotic solution of the resultant system are very similar to the solutions represented in Figure B-6. In particular, the solutions for x_{11} and x_{12} are identical to the solutions graphed for x_1 and x_2 in Figure B-6. The solutions for x_{21} and x_{22} are similar to the solutions for x_1 and x_2 in Figure B-6 but are smaller by a factor of approximately 10^{-3}.

APPENDIX C

Special Topics

C-1. Introduction

The purpose of this appendix is to present background on various topics which have arisen in the study of the Pathways Model. The following areas are considered: existence and uniqueness of solutions to the radionuclide transport equations which underlie the Pathways Model, numerical approximation of solutions to the transport equations, asymptotic behavior of solutions to the transport equations, sensitivity analysis of the Pathways Model, and use of the Pathways Model in the analysis of a disposal site. The preceding topics are treated in Sections C-2, C-3, C-4, C-5 and C-6, respectively. In these sections, there is no attempt at a complete treatment. Rather, the intent is to make the reader aware of the topic and to provide references where additional information can be obtained.

C-2. Existence and Uniqueness of Solutions

The radionuclide transport equations which underlie the Pathways Model are of the form

$$dq_i/dt = h_i + \sum_{\substack{j=1\\ j\neq i}}^{n} k_{ij}q_j - \Big(k_{0i} + \sum_{\substack{j=1\\ j\neq i}}^{n} k_{ji}\Big)\, q_i \qquad \text{(C-1)}$$

for $i=1, \ldots , n$. If a system involving M zones and N radionuclides is under consideration, then $n = 4MN$. Further, if $1 \leq I \leq M$, $1 \leq J \leq N$, $1 \leq K \leq 4$, and

$$i = 4N(I-1) + 4(J-1) + K, \qquad \text{(C-2)}$$

then the function q_i represents the amount of radionuclide J in subzone K of zone I. The system of linear equations indicated in (C-1) can be reformulated in vector notation as

$$dq/dt = h + Kq, \qquad \text{(C-3)}$$

where q and h are column vectors of the q_i and h_i, respectively, and K is the matrix defined by

$$K = \begin{bmatrix} -\left(k_{01} + \sum_{\substack{j=1 \\ j\neq 1}}^{n} k_{j1}\right) & k_{12} & \cdots & k_{1n} \\ k_{21} & -\left(k_{02} + \sum_{\substack{j=1 \\ j\neq 2}}^{n} k_{j2}\right) & \cdots & k_{2n} \\ k_{n1} & k_{n2} & \cdots & -\left(k_{0n} + \sum_{\substack{j=1 \\ j\neq n}}^{n} k_{jn}\right) \end{bmatrix}. \qquad \text{(C-4)}$$

Normally, the matrix K appearing in (C-4) will be "banded" in the sense that all elements sufficiently far from the diagonal will be zero. The nature of this banded structure can be seen in the coefficient matrix associated with example 3 presented in Chapter 4.

Two fundamental questions can be posed with respect to the system appearing in (C-1) and (C-3): First, does the system have a solution? Second, if the system has a solution, is this solution unique? The answers to the preceding questions are contained in the following theorem:

Theorem. There exists a unique solution to the initial value problem

$$dq/dt = h + Kq, \; q(0) = q_0. \qquad \text{(C-5)}$$

Further, this solution can be expressed as

$$q(t) = e^{Kt}q_0 + \int_0^t e^{K(t-s)}h\,ds. \qquad \text{(C-6)}$$

Although the theorem is stated for h and K constant-valued, existence and uniqueness for solutions of the initial value problem in (C-5) can also be established when h and K are suitably restricted functions of t. However, the representation for the solution in this case will be more complicated than that given in (C-6). An investigation into some of the effects on the Pathways Model of making K a function of time is given in Brown and Helton (Bro81).

Systems of linear equations have been widely used and studied. Additional information can be found in numerous references. Included in these are the following: Atkins (At69), Funderlic and Heath (Fu71), Jacquez (Ja72), Rescigno and Segre (Re66), Rescigno and Beck (Re72), Sheppard (She62), and Shipley and Clark (Shi72). References with a more mathematical orientation include Casti (Cas77), Hirsch and Smale (Hir74), and Michel and Miller (Mi77).

C-3. Numerical Approximation of Solutions

An initial value problem for a vector differential equation can be expressed in the form

$$dq/dt = f[t, q(t)], \quad q(a) = q_0. \qquad \text{(C-7)}$$

The existence and uniqueness of solutions for such problems can be established in considerable generality with suitable restrictions on f. Such a result is given in the preceding section for linear equations. There, the function f is defined by

$$f[t, q(t)] = h + Kq(t). \qquad \text{(C-8)}$$

Sometimes it is also possible to give a closed-form representation for the solution. Such a representation is given in (C-6). However, such constructions generally do not provide a suitable way to obtain solutions to the original initial value problems.

In all but a few special cases, it is necessary to approximate numerically solutions to problems of the form indicated in (C-7). Basically, the idea is to go through a sequence of calculations that will yield a step-function which approximates the solution of (C-7) within some specified degree of accuracy. The description of numerical methods for the solution of initial-value problems for ordinary differential equations rapidly becomes very complicated. No attempt will be made to provide such a description here. Rather, the reader will be directed to various references where discussions of such methods can be found. There exist many introductory texts on numerical analysis which contain discussions of techniques for the solution of ordinary differential equations. Included in such texts are Conte and de Boor (Co80), Burden, Faires and Reynolds (Bu78), Dahlquist and Bjorck (Da74) and Isaacson and Keller (Is66). The preceding texts provide introductions to the solution of ordinary differential equations and also additional references. On a more advanced level, discussions and additional references can be obtained in Henrici (Hen62). Gear (Ge71), Stetter (St73), Lapidus and Seinfeld (La71), and Shampine and Gordon (Sha75).

The program PATH1 uses a package of solution techniques developed for application to initial value problems which involve systems of stiff, banded differential equations. Documentation is available in several technical reports by Hindmarsh (Hin72, Hin74, Hin75). Stiff systems arise when the real parts of the eigenvalues of the Jacobian matrix for the system are negative and greatly different in size. For constant coefficient, linear systems, the Jacobian is the same as the coefficient matrix. The system of equations which arises in the Pathways Model is usually stiff. Background on stiff systems can be obtained from Enright, Hull and Lindberg (En75), Curtis (Cu78) and Robertson (Rob78).

C-4. Asymptotic Behavior of Solutions

For the system in (C-1) and the equivalent matrix formulation in (C-3), the expression "asymptotic behavior" is used in reference to the performance of $q(t)$ as $t \rightarrow \infty$. For such systems, it is possible to obtain various characterizations of asymptotic behavior. The paper by Thron (Th72) provides a good discussion of such behavior. The result which is most useful in characterizing asymptotic behavior for the present study will be stated. However, several definitions are needed first. A compartment system is said to be open if material can move out of the system. Conversely, a system is said to be closed if it is not open; that is, a system is closed if material cannot move out of it. Finally, a system is said to be completely open if it is open and contains no closed subsystem.

Various physical systems are represented in Figures 2-1, 4-1, 5-1 and 6-1. When the Pathways Model is used to represent the movement of a decay chain through one of these physical systems, the resulting compartment system may or may not be completely open. If every member of the chain decays, then the resultant compartment system will be completely open in every case. This is because decay will generate a movement out of every compartment. Further, even if there are nondecaying members in the chain, the resultant compartment system will be completely open for the physical systems indicated in Figures 2-1, 4-1 and 5-1. This is because there is a physical flow out of every compartment. However, if the decay chain contains a nondecaying member, then the resultant compartment system will not be completely open for the physical system indicated in Figure 6-1. This results because there are no flows out of the compartments associated with a nondecaying chain member in zone 5.

The desired result on asymptotic behavior is now stated; a proof can be obtained in Thron (Th72).

Theorem. For any completely open compartment system satisfying (C-3), K^{-1} exists and a unique constant-valued solution is given by $q = -K^{-1}h$. Further, (i) if q is any solution to (C-3), then $\lim_{t \to \infty} q(t) = -K^{-1}h$ and (ii) if $h_i \geq 0$ for $i = 1, \ldots, n$ and $q(0) = 0$, then each component of $q(t)$ increases monotonically to the corresponding component of $-K^{-1}h$.

As indicated in the preceding theorem, the asymptotic solution to (C-3) can be obtained by computing a matrix inverse and performing a matrix multiplication. Proper choice of computational procedures for the performance of the indicated matrix operations can significantly reduce the amount of work required. For example, normal procedure is to determine the product $K^{-1}h$ without fully determining K^{-1}. Such considerations are discussed in Rice (Ri81) and other texts on numerical linear algebra. LINPACK (Do79) is a collection of high-quality numerical software which can be used for matrix computations. This package has been used to perform calculations of the type indicated in this section for the Pathways Model.

Additional discussion of the asymptotic behavior of the Pathways Model can be found in Helton, Brown and Iman (Hel81a).

C-5. Sensitivity Analysis

Due to the large number of variables which can be supplied to the Pathways Model as input and the great amount of uncertainty which often exists with respect to the proper selection of their values, it is important to be able to determine the effects of variables and their assumed ranges and distributions on the predictions made by the model. For such determinations, an approach to sensitivity analysis based on regression analysis has been found to be successful.

The overall approach is described in Iman, Helton and Campbell (Im78). Basically, the idea is (a) to start with a set of input variables with selected ranges and distributions, (b) to select model inputs from these variables according to their ranges and distributions, (c) to generate model output with the selected inputs, and (d) to assess the relationship between model input and output by stepwise regression. Special techniques found to be useful include (a) Latin hypercube sampling to select values of input variables (Mc79, Im80b), (b) the rank transform to reduce the effects of nonlinearity in the relationships between model input and output (Im79, Im80a), and (c) the PRESS (predicted error sum of squares) criterion to indicate overfit during regression analysis (Al71).

Application of the preceding techniques to the Pathways Model can be found in Helton and Iman (Hel80) and Helton, Brown and Iman (Hel81a).

C-6. Analysis of a Disposal Site

This section briefly indicates certain considerations which may arise in the use of the Pathways Model in the analysis of a disposal site. The possible nature of such an analysis is indicated in two papers by Cranwell and Helton (Cr81c, Cr81d). The performance of an analysis of a hypothetical waste repository constitutes one part of the risk methodology project from which the Pathways Model is derived. Background on this hypothetical site and its analysis can be obtained from Campbell et al. (Cam78) and Cranwell et al. (Cr81a, Cr81b). As review of the cited documents will indicate, the performance of such an analysis is a very involved process. First, it is necessary to consider a number of different potential occurrences (i.e., scenarios) at the repository. Second, much of the data needed to represent these occurrences is imprecisely known and often is described with ranges and distributions rather than specific values. Third, the analysis requires several different models and resultant data transfers between these models.

What all this leads to is that it is unlikely that the Pathways Model will be suitable for use in a repository analysis exactly as it is programmed and presented. What is much more likely is that various modifications will be necessary for its proper incorporation into an overall site analysis. This is precisely what was done for the disposal site analysis reported in Cranwell et al. (Cr81a).

Certain aspects of this analysis which involved the Pathways Model are now indicated. The Pathways Model operated between a model which predicted radionuclide discharge to the surface environment and a model which predicted human exposure to these radionuclides and resultant health effects. Thus, it was necessary to modify the Pathways Model to receive input generated by the preceding groundwater transport model and to generate input for the following dosimetry and health effects model. Implementing these transfers was complicated by the fact that the nature of the surface discharges and the resultant pathways calculations were dependent on the particular scenario under consideration. Further, the groundwater transport model was generating discharge rates to the surface environment which were step-functions. To handle such input rates to the surface environment, it was necessary to modify the manner in which the Pathways Model solved its underlying radionuclide transport equations. In particular, it was found to be more efficient to calculate a sequence of asymptotic solutions as indicated in Section C-4 than to use a differential equation solver to generate a time-dependent solution. Next, as many of the inputs to the Pathways Model were being varied, it was necessary to add a procedure for altering these values.

Also, to reduce the amount of information passed from the Pathways Model to the dosimetry and health effects model, the part of the Pathways Model which performs ingestion and inhalation calculations was moved to this latter model. Finally, once the preceding modifications had been implemented, all unused parts of PATH1 were deleted to reduce the amount of computer storage required to run the program. The result of all this modifying and paring was a computer program for the specific analysis being performed.

Although another analysis may not require the alterations indicated in the preceding paragraph, it is anticipated that the use of the Pathways Model in conjunction with other models to represent some complex system will normally require a certain amount of modification and adaptation.

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This report contains a series of sample problems and solutions for the Pathways-to-Man (PATH 1) model developed at Sandia National Laboratories for the Risk Methodology for Geologic Disposal of Radioactive Waste Project. With this document and the PATH 1 User's Manual (NUREG/CR-1636 Vol. 1), the user may familiarize himself with the computer program, its capabilities and limitations. When the user has completed this curriculum, he or she should be able to prepare data input for PATH 1 and have some insights into interpretation of the model output. This report is one of a series of self-teaching curricula prepared under a technology transfer contract for the U.S. Nuclear Regulatory Commission, Office of Nuclear Material Safety and Safeguards.

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