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DCFPAK: Dose Coefficient Data File Package for Sandia National Laboratory

K. F. Eckerman R. W. Leggett

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DCFPAK: Dose Coefficient Data File Package for Sandia National Laboratory

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ABSTRACT

The FORTRAN-based computer package DCFPAK (Dose Coefficient File Package) has been developed to provide electronic access to the dose coefficient data files summarized in Federal Guidance Reports 11 and 12. DCFPAK also provides access to standard information regarding decay chains and assembles dose coefficients for all dosimetrically significant radioactive progeny of a specified radionuclide. DCFPAK was designed for application on a PC but, with minor modifications, may be implemented on a UNIX workstation.

INTRODUCTION

The U.S. Environmental Protection Agency (EPA) has issued a series of "Federal Guidance" reports that provide the dosimetric information needed by government agencies to implement radiation protection programs in a consistent and adequately protective manner. This information is mainly in the form of "dose coefficients", or estimates of dose per unit exposure to individual radionuclides. These dose coefficients allow the user to relate concentrations of radionuclides in air, water, food, or soil to guidance for radiation dose to workers or members of the public.

Two Federal Guidance reports are currently in use. Federal Guidance Report No. 11 (Eckerman et al. 1988) provides dose coefficients, in the form of 50-year integrated dose equivalents, for acute ingestion or acute inhalation of radionuclides, based on the biokinetic and dosimetric models of ICRP Publication 30 (1979, 1980, 1981, 1988). Federal Guidance Report No. 12 (Eckerman and Ryman 1993) provides dose coefficients, in the form of dose per unit time-integrated exposure, for external exposure to radionuclides in air, water, or soil, based on state-of-the-art methods in external radiation dosimetry.

The tabulations in these two Federal Guidance reports include dose coefficients for the radionuclides considered in ICRP Publication 30, Limits for Intakes of Radionuclides by Workers (ICRP 1979, 1980, 1981, 1988). For each radionuclide and exposure mode, dose coefficients are provided for the seven organs or tissues assigned risk weighting factors in ICRP Publication 26 (1977): breast; lung; red marrow; bone surface; thyroid; gonads, representing the higher of the coefficients for ovaries and testes; and "remainder", representing the five remaining tissues receiving the highest doses. The tabulations include the effective dose equivalent, H_E, derived from the risk weighting factors and equivalent doses for these organs. In Federal Guidance Report No. 12, dose coefficients are also provided for skin because it is frequently the most highly irradiated organ for external exposure.

The software and data package DCFPAK (Dose Coefficient File Package) has been developed to allow electronic access to the full set of dose coefficients summarized in these two Federal Guidance reports and to facilitate consideration of dose coefficients for chains of radionuclides. In addition to the published dose coefficients, the DCFPAK libraries includes dose coefficients for 18 organs not addressed in Federal Guidance Report No. 11, and 17 organs not addressed in Federal Guidance Report No. 12 (Table 1). The additional dose coefficients were generated during the development of these two Federal Guidance reports but were excluded from the published tables to make the tables easier to use and to keep the reports at a reasonable length. For each radionuclide and exposure mode, the DCFPAK libraries include both the effective dose equivalent, H_E, based on the tissue weighting factors given in ICRP Publication 26 (1977), and the effective dose, E, based

Table 1. Tissues addressed in DCFPAK, Federal Guidance No. 11, and Federal Guidance No. 12.

Tissue	Abbreviation in . DCFPAK libraries	Listed in:		
		DCFPAK	Federal Guidance	Federal Guidance 12
Adrenal	Adrenal	Yes	No	No
Urinary Bladder Wall	Bld Wall	Yes	No .	No
Bone Surface	B Surface	Yes	Yes	Yes
Brain .	Brain	Yes	No	No
Breast	Breast	Yes	Yes	Yes
Esophagus	Esophagu	Yes	No	No
Stomach Wall	St Wall	Yes	No	· No
Small Intestine Wall	SI Wall	Yes	No	No
Upper Large Intestine Wall	ULI Wall	Yes	No	No
Lower Large Intestine Wall	LLI Wall	Yes	No	. No
Kidney	Kidney	Yes	No	No
Liver .	Liver	Yes	No	No .
Lung	Lung	Yes	Yes	Yes
Muscle	Muscle	Yes	No	No
Ovaries	Ovaries •	Yes	No	, No
Testes	Testes	Yes	No	No
Gonad*	(Not used)	No	Yes	Yes
Pancreas	Pancreas	Yes	No	No
Red Marrow	R Marrow	Yes	Yes	Yes
Skin .	Skin	Yes	No	Yes
Spleen	Spleen	Yes	No	No
Thymus	Thymus	Yes	· No	No
Thyroid	Thyroid	Yes	Yes	Yes
Uterus	Uterus	Yes	No	No
Remainder*	(Not used)	No	Yes	Yes

^{*}Represents multiple tissues considered explicitly in DCFPAK.

on the newer tissue weighting factors given in ICRP Publication 60 (1991). Tissue weighting factors recommended in ICRP Publication 26 and Publication 60 are compared in Table 2.

The DCFPAK libraries contain dose coefficients for each of nine modes of exposure to a given radionuclide: (1) ingestion; (2) inhalation; (3) submersion, meaning external exposure to (radiations emitted from) the radionuclide in air; (4) immersion, meaning external exposure to the radionuclide in water (from swimming); (5) external exposure to the radionuclide on the ground surface; and (6-9) external exposure to the radionuclide distributed to a depth of 1 cm, a depth of 5 cm, a depth of 15 cm, or an infinite depth in soil. The dose coefficients for internal exposures are 50-y integrated doses to organs following an acute intake and are given in units of Sv Bq⁻¹. The dose coefficients for external exposures are dose per unit time-integrated exposure. Dose coefficients for external exposures are in terms of Sv per Bq-s per unit volume of environmental medium (liter of air for submersion, liter of water for immersion, m² of soil for ground surface contamination, and m³ of soil for subsurface contamination of soil).

The dose coefficient for a given radionuclide and exposure scenario does not reflect ingrowth of chain members in the environment, but dose coefficients for ingestion and inhalation do reflect the contribution to dose from ingrowth of chain members in the body after intake of the parent radionuclide. For either internal or external exposure to a radionuclide, DCFPAK determines the radionuclide decay chain (if any) of that radionuclide, truncates the chain after the last potentially significant decay chain member, and assembles the dose coefficients for all potentially significant chain members. For internal exposure, DCFPAK truncates a chain if the cumulative energies for alpha, electron, and photon radiation over a 100-year period are changed less than 1% by the addition of subsequent chain members. The same procedure is followed for external exposures but with consideration restricted to electrons and photons.

The DCFPAK package, which is written in FORTRAN 77, was developed for use as a module of a radiological assessment package currently used at Sandia National Laboratory. However, DCFPAK is generic in nature and should be compatible with other FORTRAN-based radiological assessment packages. It was designed for use on a personal computer or work station and can be run interactively or in batch mode.

Table 2. Tissue weighting factors given in ICRP Publication 26 (1977) and ICRP Publication 60 (1991)^a.

	Tissue weighting factor (w _T)			
Organ or tissue	ICRP Pub. 26	ICRP Pub. 60		
Gonads	0.25	0.20		
Bone marrow (red)	0.12	0.12		
Colon	 -	0.12		
Lung	0.12	0.12		
Stomach		0.12		
Bladder		0.05		
Breast	0.15	0.05		
Liver		0.05		
Oesophagus		0.05		
Thyroid	. 0.03	0.05		
Skin		0.01		
Bone surface	0.03	0.01		
Remainder	0.30	0.05		

^{*}The values were developed for a reference population of equal numbers of both sexes and a wide range of ages. In the definition of effective dose they apply to workers, to the whole population, and to either sex.

For illustrative purposes DCFPAK was linked to a sample "driver" code called READEM (source code, READEM.FOR and executable file, READEM.EXE). READEM allows an interactive examination of DCFPAK's output for any of the 9 exposure modes and approximately 800 radionuclides addressed in this package.

The DCFPAK package consists of the following data libraries (data files) and software files:

- 1. nine libraries of dose coefficients, corresponding to the nine exposure modes listed above;
- a library of information on the half-lives, modes of decay, branching fractions, and decay products of all 838 radionuclides considered in these two Federal Guidance reports;
- 3. a "data access" module that accesses the 10 data files described above and returns the relevant information;
- 4. an include file containing information on dimensioning of arrays in DCFPAK;
- 5. two include files containing common blocks;
- 6. an include file that provides unit designations to be reserved for IO used by DCFPAK;
- 7. an "initialization" file that informs DCFPAK of the location of all data files and their record lengths;
- an illustrative driver code that serves the dual purpose of allowing an examination
 of available DCFPAK output and illustrating how to establish communication
 between the user's driver code and DCFPAK's data access module.

To access DCFPAK, the user must insert the following into his driver code: include statements that reference the files described in items 4-6 above, and a call statement, described later, that transfers the input variables describing the radionuclide, particle size, desired output, and other case-specific information to DCFPAK. The user's code and the source code DCFPAK.FOR must then be compiled and the resulting object files must be linked.

DATA FILES IN DCFPAK

Ten data files are included in DCFPAK. The data files are all "formatted direct-access files" consisting of ASCII characters, with all records in a given file of the same length and each record ending with an ASCII carriage-return (CR) and line-feed (LF) character. One of these data files contains information such as the half-time, decay modes, and branching fractions of the radionuclides and is used by DCFPAK to assemble the information on the decay chain for the parent radionuclide. The other nine data files contain dose coefficients corresponding to the nine exposure modes described earlier. A short description of each of the ten data files is given in the following.

DFEXTINT.NDX

This file is used by DCFPAK to assemble the information on the decay chain for the parent. The file contains 839 lines, including a header line with such information as the record format and one line of information for each of the 838 radionuclides addressed by DCFPAK. The line of information for a radionuclide contains the name and half-life of the radionuclide, the key (line number) of the radionuclide record in all other files, and a summary of decay properties of each radionuclide. For example, the line of information for Bi-212 gives the following information in the indicated order:

```
name of radionuclide (Bi-212);
half-life (60.55 m);
decay modes (B-A, indicating beta-minus and alpha);
beginning line number for Bi-212 in the inhalation dose coefficient file (2282);
record number for Bi-212 in the ingestion dose coefficient file (699);
record number for Bi-212 in each of the external dose coefficient files (690);
record number in DFEXTINT.NDX of decay product Po-212 (504);
branching fraction to Po-212 (6.4070E-01);
record number in DFEXTINT.NDX of decay product Tl-208 (762);
branching fraction to Tl-208 (3.5930E-01);
total energy (MeV) of emitted alpha particles (2.1741);
total energy (MeV) of emitted beta particles (0.4720);
total energy (MeV) of emitted photons (0.1855);
atomic weight (211.991271);
date of creation of the radioactive decay data (05-May-77).
```

DFINHS.DAT

This file is an expanded version of Table 2.1 of Federal Guidance Report No. 11. The file contains dose coefficients for the case of acute intake of a radionuclide by inhalation. The dose coefficients represent the dose over a 50-year period following intake (Sv Bq⁻¹ inhaled). Tabulated dose coefficients are for the default particle size 1 µm (activity median aerodynamic diameter, or AMAD), except for a few cases in which particle size is not relevant (e.g., for vapors). As described below, the tabulated dose coefficients are used to generate dose coefficients for any particle size specified by the user.

For each radionuclide, inhalation dose coefficients are included for each of the lung clearance classes applied to that radionuclide in ICRP Publication 30 (1977, 1980, 1981, 1988). The three main clearance classes are "D", "W", and "Y", where Class D refers to a clearance time of days, W to a clearance time of weeks, and Y to a clearance time of years from the pulmonary region of the lung. The occasionally used Class "V" refers to rapid clearance expected to occur for vapor forms of some elements. Three special clearance classes are used for carbon: "c", applied to labeled organic compounds, "m", applied to carbon monoxide, and "d", applied to carbon dioxide; differences in the three classes are associated mainly with differences in the relative amounts of deposited carbon exhaled and absorbed to blood and in the biokinetics of carbon after absorption to blood.

For each radionuclide, one or more lines of data are included for each clearance class. The first line includes the name of the radionuclide, the clearance class, the gastrointestinal absorption fraction (f_1 value) for material cleared to the gastrointestinal tract, a dose coefficient for each of the 23 tissues considered (Table 1), the effective dose equivalent, and the effective dose. For clearance class D, W, or Y (which apply to particulate matter), a second line of data provides the percentage of the dose coefficient for each organ that is attributable to deposition in the nasal-pharynx (N-P) and pulmonary (P) regions of the respiratory tract. As described below, these percentages are used by DCFPAK to calculate dose coefficients for particle sizes other than 1 μ m.

Dose coefficients for particle sizes other than 1 μm can be derived from the tabulated data for 1 μm as a result of the assumption in the underlying respiratory tract model (ICRP 1979) that the rate of clearance of material from the tract is independent of particle size. This assumption implies that the inhalation dose coefficient for a given radionuclide and clearance class is determined by the relative fractions of inhaled activity assigned to N-P, T-B, and P. Suppose, for example, that the user is considering inhalation of Be-10 of Class W and particle size 0.2 μm . For this particle size, the deposition fractions for N-P, T-B, and P are 0.05, 0.08, and 0.5, respectively (with the missing fraction, 0.37, assumed to be promptly exhaled). For particle size 1 μm , the deposition fractions for N-P, T-B, and P are 0.30, 0.08, and 0.25, respectively. According to the file DFINHS.DAT, for Be-10 of Class W and particle size 1 μm , 26% of the inhalation dose coefficient (DC) for breast, for example, is attributable to activity deposited in N-P and 41% is attributable to activity deposited in P. Therefore, 33% is attributable to activity deposited in T-B. The dose coefficient for the breast for 0.2 μm would be

 $[(0.05/0.30) \times (0.26 \times DC)] + [(0.08/0.08) \times (0.33 \times DC)] + [(0.5/0.25) \times (0.41 \times DC)] = 1.1933 \times DC,$

i.e., 1.1933 times the dose coefficient for particle size 1 µm.

For a given particle size in the range 0.1-20 μ m, deposition fractions for the regions N-P, T-B, and P are based on the piecewise linear curves shown in Fig. 1 (after Fig. 5.1 of Part 1 of ICRP Publication 30 (1979)). For particle sizes less than 0.1 μ m or greater than 20 μ m, DCFPAK assigns fractional depositions in these regions corresponding to a particle size of 0.1 μ m or 20 μ m, respectively.

The esophagus was not depicted explicitly in the dosimetric human phantom used in ICRP Publication 30 and was not considered as a target organ in that document. However, the esophagus is addressed in DCFPAK because dose to the esophagus is considered in the calculation of the effective dose, E. Because internal dose calculations are not available for the esophagus, the thymus has been used as a surrogate. The esophagus was recently introduced into ORNL's human phantom and was considered explicitly in the external dose coefficients tabulated in Federal Guidance No. 12 and in DCFPAK.

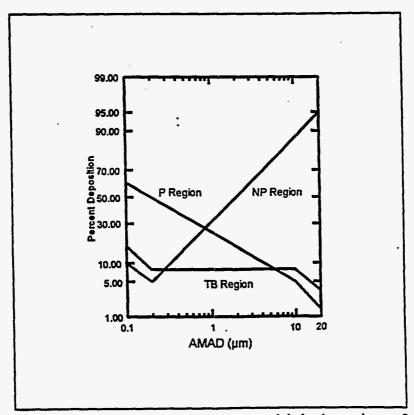


Figure 1 Deposition of particulate materials in the regions of the lung as a function of the activity median aerodynamic diameter (AMAD).

For radionuclides addressed in Part 1 of ICRP Publication 30 (1979), an inhalation dose coefficient of 0.0 is given for brain. This is because the brain was not included in the human phantom used in the ICRP dosimetry until after the completion of Part 1, and because there is no suitable surrogate for brain among the organs addressed.

DFINGS.DAT

This file is an expanded version of Table 2.2 of Federal Guidance Report No. 11. The file contains dose coefficients for the case of acute intake of a radionuclide by ingestion. The dose coefficients represent the dose over a 50-year period following acute intake (Sv Bq⁻¹ ingested).

With a few exceptions, one line of data is given for each radionuclide. That line includes the name of the radionuclide, the gastrointestinal absorption fraction (f_1 value) for ingested activity, a dose coefficient for each of the 23 tissues considered (Table 1), the effective dose equivalent, and the effective dose. For a few radionuclides, one or more additional lines of dose coefficients are given, corresponding to alternate f_1 values used for certain forms of the radionuclide. For example, for radioisotopes of strontium, one line of dose coefficients corresponds to the f_1 value of 0.3 used for strontium compounds other than titanate and a second line gives dose coefficients for the f_1 value of 0.01 applied to strontium titanate.

For the reasons given in the discussion of inhalation dose coefficients, an ingestion dose coefficient of 0.0 for brain is given for each of the radionuclides addressed in Part 1 of ICRP Publication 30 (1979). Also, for reasons discussed above, ingestion dose coefficients for the thymus are applied to the esophagus.

FGR12F31.DAT

This file is an expanded version of Table III.1 of Federal Guidance Report No. 12. The file contains dose coefficients for the case of external exposure to the radionuclide in air (submersion). The units are dose per time-integrated air concentration (Sv per Bq-s L⁻¹ air).

One line of data is given for each radionuclide. That line contains the name of the radionuclide, a dose coefficient for each of the 23 tissues considered (Table 1), the effective dose equivalent, and the effective dose.

FGR12F32.DAT

This file is an expanded version of Table III.2 of Federal Guidance Report No. 12. The file contains dose coefficients for external exposure to the radionuclide in water ("immersion"), from swimming. The units are dose per time-integrated water concentration (Sv per Bq-s L-1 water).

One line of data is given for each radionuclide. That line contains the name of the radionuclide, a dose coefficient for each of the 23 tissues considered (Table 1), the effective dose equivalent, and the effective dose.

FGR12F33.DAT

This file is an expanded version of Table III.3 of Federal Guidance Report No. 12. The file contains dose coefficients for external exposure to the radionuclide on the ground surface. The units are dose per time-integrated surface concentration (Sv per Bq-s m⁻²).

One line of data is given for each radionuclide. That line contains the name of the radionuclide, a dose coefficient for each of the 23 tissues considered (Table 1), the effective dose equivalent, and the effective dose.

FGR12F34.DAT

This file is an expanded version of Table III.4 of Federal Guidance Report No. 12. The file contains dose coefficients for external exposure to the radionuclide distributed to a depth of 1 cm in the soil. The units are dose per time-integrated concentration (Sv per Bq-s m⁻³).

One line of data is given for each radionuclide. That line contains the name of the radionuclide, a dose coefficient for each of the 23 tissues considered (Table 1), the effective dose equivalent, and the effective dose.

FGR12F35.DAT

This file is an expanded version of Table III.5 of Federal Guidance Report No. 12. The file contains dose coefficients for external exposure to the radionuclide distributed to a depth of 5 cm in the soil. The units are dose per time-integrated concentration (Sv per Bq-s m⁻³).

One line of data is given for each radionuclide. That line contains the name of the radionuclide, a dose coefficient for each of the 23 tissues considered (Table 1), the effective dose equivalent, and the effective dose.

FGR12F36.DAT

This file is an expanded version of Table III.6 of Federal Guidance Report No. 12. The file contains dose coefficients for external exposure to the radionuclide distributed to a depth of 15 cm in the soil. The units are dose per time-integrated concentration (Sv per Bq-s m⁻³).

One line of data is given for each radionuclide. That line contains the name of the radionuclide, a dose coefficient for each of the 23 tissues considered (Table 1), the effective dose equivalent, and the effective dose.

FGR12F37.DAT

This file is an expanded version of Table III.7 of Federal Guidance Report No. 12. This file contains dose coefficients for external exposure to the radionuclide distributed to an infinite depth in the soil. The units are dose per time-integrated concentration (Sv per Bq-s m⁻³).

One line of data is given for each radionuclide. That line contains the name of the radionuclide, a dose coefficient for each of the 23 tissues considered (Table 1), the effective dose equivalent, and the effective dose.

DCFPAK SOFTWARE

The DCFPAK software files, written in FORTRAN 77, are described below. In the following descriptions, the code that calls DCFPAK's data access module will be referred to as the "user's driver code".

DCFPAK.FOR

This is the FORTRAN source code for the data access module that accesses the data files and returns the relevant information. It should be compiled on the user's system.

PAKPARM.FOR

This "include" file should be referenced by the user's driver code, along with the include file DCFPAK.CMN described below. The file contains the following two lines of FORTRAN code that determine the dimensioning of arrays in DCFPAK:

```
integer mspec, morg, mfact
parameter(mspec = 25, morg = 25, mfact = 9)
```

Here, MSPEC is the maximum length of the decay chain, MFACT is the maximum number of dose factors types, and MORG is the maximum number of organs in the dose factor file.

DCFPAK.CMN

This include file should be referenced by the user's driver code in any routines that access dosimetric information for the chain members. As noted above, PAKPARM.FOR should also be included in these routines. The file contains the common blocks that will contain the information extracted from the data files by DCFPAK:

The common block DFACTS contains the dose coefficients. The variables in the dimension statements are defined in the include file PAKPARM.FOR. The definitions of the variables in this block are as follows:

ORGAN: A character(*9) array of organ names of maximum length MORG. The 23 organs addressed by DCFPAK are listed in Table 1.

DF: A real variable array of dose coefficients by chain member, exposure pathway, and organ.

F1INH: Real variable array of gastrointestinal uptake (f_1) values for inhalation, by chain member.

F1ORL: Real variable array of gastrointestinal uptake (f₁) values for ingestion, by chain member.

CLASSO: A character(*1) array of clearance class notation for the inhalation coefficients of the chain members.

IFLAG: An array of logical flags, by chain member and pathway, set to true in each case for which DCFPAK returns a coefficient in DF array.

NINT: Integer variable for the number of chain members that are used in the evaluation of inhalation and ingestion intakes (i.e., the length of the chain, or truncated chain, used in the calculation).

NEXT: Integer variable for the number of chain members that must be considered for external exposures.

The common block RADAT, shown above, contains information on the decay chain under consideration. The definitions of the variables in this block are as follows:

THALF: A character(*8) array of the half-life of each chain member.

IU: A character(*2) array of the units of the half-life of each chain member.

NUCNAM: A character(*7) array of the names of the chain members.

BRANCH: A two-dimensional real array (upper triangular matrix) of branching fractions, with an entry representing the fraction of the decays of the ith chain member forming the jth chain member.

LMR: A double precision array of decay constants (d⁻¹) for the chain members.

NBR: An integer array containing the number of chain members that decay directly to the specific chain member.

IBR: An integer array containing the indices of the chain members which form the specific chain member. For example, (ibr(I, ispec), I=1, nbr(ispec)) are the indices of the precursor of member ispec.

NSPEC: The length of the decay chain.

BATCH.CMN

This include file should be referenced by the user's driver code. The file contains two lines of code, including a common block with a logical flag that determines whether DCFPAK is operated in an interactive or a non-interactive mode:

```
logical dbatch
common/dcalbat/dbatch
```

The DBATCH logical variable inserted into the user's code should be set to "false" for the interactive mode and "true" for the non-interactive mode. Setting the DBATCH logical variable to "true" eliminates output to the screen that occurs in the interactive mode.

IOLIST.CMN

This include file should reside in the same directory as the file DCFPAK.FOR when the latter is compiled. This four-line file contains the unit designations for the IO used by DCFPAK:

The unit designations in IOLIST.CMN must be reserved for DCFPAK input and output; that is, they must differ from unit designations in the user's driver code. In addition to these units, DCFPAK uses unit 40.

DCFPAK.INI

This "initialization" file should be placed in the directory where the software is run. The file informs DCFPAK of the location of all data files and their record lengths. This file enables the user to place DCFPAK's data files in a directory distinct from that used for code output. The following is a sample version of DCFPAK.INI. The real version should show the actual path to each file indicated in the second field:

```
'snlindex.ndx', 'c:\snl\dcf\dfextint.ndx', 125
'ingestsf.dfs', 'c:\snl\dcf\dfings.dat' , 240
'inhalesf.dfs', 'c:\snl\dcf\dfinhs.dat' , 232
'submrsin.dfs', 'c:\snl\dcf\fgr12f31.dat', 232
'imersion.dfs', 'c:\snl\dcf\fgr12f32.dat', 232
'grsurf00.dfs', 'c:\snl\dcf\fgr12f33.dat', 232
'grvol 01.dfs', 'c:\snl\dcf\fgr12f34.dat', 232
```

```
'grvol_05.dfs', 'c:\snl\dcf\fgr12f35.dat', 232
'grvol_15.dfs', 'c:\snl\dcf\fgr12f36.dat', 232
'grvolinf.dfs', 'c:\snl\dcf\fgr12f37.dat', 232
'EOF', ' ' <- end of file marker</pre>
```

The first field is the file name within DCFPAK, and the second field is the full name of the file, including its path. For example, the record

'snlindex.ndx', 'snl\dcf\dfextint.ndx'

indicates that the file 'snlindex.ndx' is to be read as snl\dcf\dfextint.ndx, where "snl\dcf" is the path to the directory containing the file. The user should not edit the first field and should limit the path in the second field so that the field length does not exceed 64. The third field is the integer value for the record length for the file to be used in the FORTRAN open statement.

Not all FORTRAN compilers define the record length in the same manner when opening direct access files. DCFPAK was developed using the Microsoft FORTRAN compiler, which uses the physical length of the record less 2 bytes corresponding to the carriage return (CR)- line feed (LF) that separate formatted direct records. The integer values in the third field above specify the RECL parameter for the Microsoft compiler. Some other compilers (e.g, Lahey) specify RECL as the length of the physical record, which includes the 2 bytes associated with the CR-LF. For such compilers, DCFPAK.INI should be edited to increase the integer values indicated above by 2. For additional information, see the comments included in the files after the EOF marker.

READEM.FOR

This is the source code for a sample driver code that accesses DCFPAK and returns to the screen the decay chain and dose coefficients for the chain members, based on the user's input. This code is included for illustrative purposes.

READEM.EXE

This is the executable file for READEM.FOR.

CONNECTING DCFPAK TO THE USER'S DRIVER CODE

The DCFPAK data files and software are distributed in a self-extracting ZIP file named SNL.EXE. After extraction, the DCFPAK package can be connected to the user's driver code as follows:

- Step 1: Copy the file snl.exe into a directory, preferably the directory that contains the user's driver code.
- Step 2: Type "snl" and hit the "Enter" key. This extracts all data and software files. The data files may be moved to another directory. The new address of the data files must be specified in the file DCFPAK.INI.
- Step 3: In the user's driver code, insert include statements referencing the include files PAKPARM.FOR, DCFPAK.CMN, BATCH.CMN, and IOLIST.CMN as illustrated in the sample driver source code, READEM.FOR.
- Step 4: Insert the following "call" into the user's drive code, as illustrated in READEM.FOR:

CALL DOSECOF (NUKE, FIORAL, CLASS, FINHI, AMAD, IPATH)

to obtain the information for radionuclide NUKE. The dose conversion factor information is returned in the common blocks discussed above. The variables NUKE and IPATH must be specified. If the other variables are not specified, default values are supplied by DCFPAK. If the library has multiple sets of dose coefficients (e.g., corresponding to different fl values for a radionuclide), then DCFPAK will assign the most conservative set of coefficients. To obtain a particular set of coefficients one can specify the fl values for inhalation and ingestion as well as the clearance class for inhalation. These variables are described in the following section. Illustrative read statements are given in the sample driver source code, READEM.FOR.

- Step 5: As discussed in the following section and illustrated in READEM.FOR, insert data input statements into the user's driver code to define the radionuclide (NUKE), the operative exposure pathway (IPATH), and optional input if used.
- Step 6: Insert the calls "CALL OPENEM" and "CALL CLOSEM" into the user's driver code in appropriate places for opening and closing the data files, respectively, as illustrated in READEM.FOR.
- Step 7: Compile DCFPAK.FOR and the user's driver code, and link the resulting object files.

INPUT TO THE USER'S DRIVER CODE

Prior to calling the routine DOSECOF, a call should be made to the routine NUKEOK to determine if the nuclide of interest is contained in DCFPAK's data files. Thus, the user's code should include the following call:

CALL NUKEOK(NUKE, OK)

The variables are defined as:

NUKE: This character*7 variable represents the name of the radionuclide of interest. The naming convention for radionuclides follows standard practice (e.g., Co-60, Cs-137, Tc-99m). DCFPAK includes a character*7 function CHECK, which is called to place the nuclide name in the proper format.

OK: This is a logical variable which is set to true if the nuclide is present in the data files and is otherwise returned as false.

If the nuclide is present in the data files, then the user's driver code should access the data files through the call to DOSECOF described above:

CALL DOSECOF (NUKE, F10RAL, CLASS, F1INHI, AMAD, IPATH)

The user's driver code should be set up so that the variables in this call are input variables, even though default values are supplied by DCFPAK for most of these variables. The variables are defined in the following.

NUKE: This variable was defined above.

F1ORAL: This is a real variable representing the value of the f_1 parameter (gastrointestinal uptake factor) associated with the ingested chemical form of the radionuclide. f_1 represents the fraction of the ingested material reaching blood in the absence of radioactive decay. For most radionuclides, a single f_1 value is applied to all chemical forms. However, for uranium, plutonium, and a few other elements, separate f_1 values are applied to relatively soluble and relatively insoluble compounds. If F1ORAL is set to zero, DCFPAK will return the ingestion coefficients for the chemical form that has the highest effective dose.

F1INHI: This is a real variable representing the gastrointestinal uptake factor for inhaled material that moves from the respiratory tract to the gastrointestinal tract. If F1INHI is set to zero, DCFPAK will assign the default value to F1INH1 associated with the radionuclide and the CLASS variable.

CLASS: This is a character*1 variable that specifies the clearance class for inhaled forms of the radionuclide. The dose coefficients are based on the lung model of ICRP Publication 30, and the variable has values of "D", "W", "Y", and "V". Class D refers to a clearance time of days, W to a clearance time of weeks, and Y to a clearance time of years. The less frequently used Class "V" refers to rapid clearance such as occurs for vapor forms of some elements. If CLASS is not supplied, DCFPAK will select the classification of the chemical form giving the highest effective dose.

AMAD: This is a real variable representing the activity median aerodynamic diameter of the aerosol. If unspecified, a default AMAD of 1 µm is applied. If specified, DCFPAK calculates coefficients for the user's supplied AMAD. DCFPAK applies the value of AMAD to all chain members.

IPATH: This is a logical array (size 9) used to flag the type of dose coefficients that are of interest to the user. IPATH should be set to "true" to return tables of dose coefficients for all nine exposure models addressed by DCFPAK.

In addition to assembling the decay chain and the corresponding dose coefficients, DCFPAK can be used to compute the activities of the chain members as a function of time. The calculations assume a unit activity of the chain parent at time zero and no initial activity of other chain members. To make use of this capability, the following call should be inserted into the user's driver code after a call to DOSECOF:

CALL BIRCH(ISPEC, T, A, AINT)

The variables are defined as follows:

ISPEC: This input variable is the index number of the chain member of interest. ISPEC ranges from 1, the chain parent, to NSPEC, the last radioactive member of the chain.

T: This input variable is the time (d) for which the activity of chain member ISPEC is to be computed.

A: This output variable of the routine BIRCH is the activity of ISPEC at time T assuming that one unit of activity was present at T=0 for the parent and all daughter activities at that time were zero.

AINT: The output variable is the time integrated activity of ISPEC during the period of length T, assuming that one unit of activity was present at T=0 for the parent and all daughter activities were zero at T=0. The unit is days. The number of nuclear transformations of ISPEC per Bq of the parent during this period would be 8.64E04 x AINT.

To produce activities for multiple chain members and/or multiple times, the call may be looped over ISPEC and/or T. For long decay chains and short times the computed values A and AINT may exhibit numerical noise for some chain members due to loss of significance in the computations. Although these artifacts can be seen when tabulating values as a function of time, they are typically of no dosimetric consequence. An extended precision version of this routine is available from the authors but was not used in DFCPAK because its computations are considerably slower than those of the present version.

Before any calls to BIRCH, the routine DOSECOF must be called to assemble the decay chain. The user should see READEM.FOR for an illustrative implementation.

The user should examine the source code READEM.FOR for an example of how the routines of DCFPAK should be called.

DEMONSTRATION CODE

The READEM code included with this software package is an interactive code that can be used to examine available DCFPAK output. To run the code, type "readem" and press <Enter>. You will be prompted for the name of the radionuclide, the inhalation clearance class (a default is provided, as explained earlier), and the particle size (a default value of 1 µm is provided). In this demonstration code, default values are used for the other variables in the call DOSECOF. After responding to the three prompts described above, you will be shown the half-lives, branching fractions, and cumulative alpha, beta, and gamma energies of each member of the (non-truncated) decay chain for that radionuclide. Press <Enter> to see inhalation dose coefficients for the parent radionuclide, press <Enter> again to see inhalation dose coefficients for the next decay chain member in the truncated chain, and so forth. Repeatedly pressing <Enter> will take you through the dose coefficients for all members of the truncated chain, for all nine exposure modes addressed in DCFPAK.

Following the listing of the dose coefficients assembled for the chain, you will be asked to provide a time at which the activities of the chain members should be computed. If this computation is not desired, enter a time of zero; you will then be prompted to enter the next radionuclide. Entering the time (in days) will produce a tabulation of the activity and time-integrated activity for the chain members, as derived by the routine BIRCH. This computation is carried out only for the chain members that have been judged by DCFPAK to be significant in the dosimetry.

To exit READEM, press <Enter> when prompted for the next radionuclide.

INSTALLATION ON UNIX WORKSTATION

The following additional steps allow a user to run READEM on a UNIX (SUN) workstation:

- 1. Convert all files extracted from SNL.EXE (with the exception of convert2unix, wdaf, and wdaf.f) from DOS format to UNIX format. A batch file named convert2unix is included as an example of the necessary unix commands to convert the files.
- Rewrite the data files as direct access files since the direct access attribute is lost in conversion from DOS to UNIX. A short FORTRAN program named wdaf (write direct access files) is included as an example of how to rewrite the files to restore the direct access attribute.
- 3. Replace the extension "for" on the files readem for, dcfpak for, and pakparm for with extension "f".
- 4. Replace the variable "nargs" in readem.f with "iargc".
- 5. Replace "len_trim" with "lnblnk" in readem.f and dcfpak.f.
- 6. Compile the package as

f77 -03 -native -libmil -o readem readem.f dcfpak.f \$LIB

REFERENCES

Eckerman, K. F.; Ryman, J. C. Federal Guidance Report No. 12: External Exposure to Radionuclides in Air, Water, and Soil. EPA-402-R-93-081. Washington, DC: U.S. Environmental Protection Agency; Office of Radiation and Indoor Air; 1993.

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International Commission on Radiological Protection. Annals of the ICRP 1. ICRP Publication 26. Oxford: Pergamon Press; 1977.

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International Commission on Radiological Protection. Limits for intakes by workers. ICRP Publication 30. Oxford: Pergamon Press; Part 3: 1981.

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APPENDIX A: Source Code Listings

A1. INCLUDE FILES

INCLUDE FILE PAKPARM. FOR

The following parameter values give the maximium dimensions of the arrays in the dose factor package. To increase the problem size edit this file and recompile all routines.

mspec is the maximium number of nuclides in a chain mfact is the maximium number of dose factors types morg is the maximium number of organs in the dose factor file.

integer mspec, morg, mfact parameter (mspec = 25, morg = 25, mfact = 9)

INCLUDE FILE DCFPAK.CMN

INCLUDE FILE BATCH.CMN

 SNL batch flag logical dbatch common/dcalbat/dbatch

INCLUDE FILE IOLIST.CMN

integer idex, ingx, inhx, i31, i32, i33, i34, i35, i36, : i37, olog parameter (idex = 10, ingx=11, inhx=12, i31=13, i32=14, : i33=15, i34=16, i35=17, i36=18, i37=19, olog=20)

A2. PROGRAM DCFPAK.FOR

DCFPAK: Dose Coefficient File Package ORNL/TM-13347
K.F. Eckerman and R.W. Leggett
Oak Ridge National Laboratory

The following is DCFPAK's source code. The routines are presented in alphabetical order by function; the order is:

- 1. computational subroutines,
- 2. screen routines,
- 3. functions routines.

The code was written in FORTRAN 77 using the Microsoft FORTRAN

Compiler 5.1. Microsoft's LEN_TRIM function has been used,

however at the end of the listing is a replacement function that

can be activated by uncommenting the statements.

K.F. Eckerman July 1, 1996.

Routine call tree for DCFPAK

CHAIN

BIRCH <------ Can call after DOSECOF

BATMAN

EXPF1

EXPFUN

EXPEUN

CLS

FRWARD

IBINRY

ICUTOFF

LEN_TRIM

ORDER

PATH

PAUSEIT

PRINTM

CLS

RECVER

TIMEST

CLS

DEPFRAC

IBINRY

LEN_TRIM

NEWDES

SORTEM

ZEROM

Call cross-reference

BATMAN called by: BIRCH

BIRCH called by: CHAIN

CHAIN called by: DOSECOF

CHECK called by: CHEKAB NUKEOK

CHEKAB called by: NUKEOK

CHEKMN called by: NUKEOK

CLS called by: CHAIN DOSECOF PRINTM

DEPFRAC called by: DOSECOF

EXPF1 called by: BATMAN

EXPFUN called by: BATMAN EXPF1

FILEINI called by: OPENEM

FRWARD called by: CHAIN

IBINRY called by: DOSECOF FRWARD READEM NUKEOK

ICUTOFF called by: CHAIN

LCASE called by: FILEINI

LEN_TRIM called by: CHAIN CHEKAB DOSECOF FILEINI

LCASE LTRIM CASE

LTRIM called by: CHECK TABLEM

NEWDFS called by: DOSECOF

ORDER called by: CHAIN

PATH called by: CHAIN

thin ourica by. Chair

PAUSEIT called by: CHAIN

PRINTM called by: CHAIN

RECVER called by: CHAIN

SORTEM called by: NEWDFS

TIMEST called by: CHAIN

ZEROM called by: DOSECOF

The user's code should call the following routines

OPENEM <-- to open the data files

NUKEOK <-- to check the the nuclide name is valid.

DOSECOF <-- to assemble the decay chain

CLOSEM <-- to close the data files

1. Computational Routines

* 5 m

block data

include 'pakparm.for'
include 'dcfpak.cmn'

```
data organ /'Adrenals ', 'Bld Wall ', 'B Surface', 'Brain
                 'Breasts ', 'Esophagus', 'St Wall ', 'SI Wall ',
                 'ULI Wall ', 'LLI Wall ', 'Kidneys ', 'Liver ',
                 'Lungs ', 'Muscle ', 'Ovaries ', 'Pancreas ', 'R Marrow ', 'Skin ', 'Spleen ', 'Testes ', 'Thymus ', 'Thyroid ', 'Uterus ', 'H sub E ',
    end
subroutine batman(b0, zk, zkt, an1, an2, t, n)
    include 'pakparm.for'
    call variables.
    double precision b0, zk, zkt, an1, an2, zero
    integer n
    dimension b0 (mspec), zkt (mspec), zk (mspec)
    local variables.
    double precision s1, s2, ss1, ss2, prod, expfun, expf1
    integer i, j, k
    parameter (zero=0.0d0)
    include 'iolist.cmn'
    an1 - zero
    an2 - zero
    do 50 i = 1, n
      if (b0(i) .ne. zero) then
         s1 = zero
         s2 = zero
         ss1 = zero
         ss2 = zero
         do 40 j = i, n
            prod = zkt(n) / zk(n) + zk(j) / zkt(i)
             do 30 k = i, n
                if (k \cdot ne. j) prod = prod * zk(k) / (zkt(k) - zkt(j))
 30
             continue
             if (prod .lt. zero) then
                s1 = s1 + dabs(prod) * expfun(-zkt(j) * dble(t))
                ss1 = ss1 + dabs(prod) * expf1(zkt(j), dble(t))
             else
                s2 = s2 + prod \cdot expfun(-zkt(j) \cdot dble(t))
                ss2 = ss2 + prod * expf1(zkt(j), dble(t))
             end if
         continue
 40
         only positive values are retained; negatives are zero
         if (s2 .qt. s1) an1 = an1 + b0(i) • (s2 - s1)
         if (ss2 .gt. ss1) an2 = an2 + b0(i) • (ss2 - ss1)
      end if
 50 continue
    return
```

```
end
   subroutine birch (imem, t, rx1, rx2)
   include 'pakparm.for'
   include 'dcfpak.cmn'
   integer mpath, max
   common/calcul/ max(mspec), mpath(mspec, mspec)
   call variables.
   integer imem
   local variables.
   integer i, j, mark, jpath, ipath, nmem, m
   double precision zkt, zk, b, b0, an1, an2, x1, x2, zerod
   dimension b(mspec), b0(mspec), zkt(mspec), zk(mspec), mark(mspec),
            jpath (mspec), ipath (mspec)
   parameter(zero = 0.0, zerod = 0.0d0)
   Trace the pathway backwards from Imem to decide which elements
   of the Mpath matrix to choose.
   rx1 = zero
   rx2 = zero
   x1 - zerod
   x2 = zerod
   do 30 i = 1, nspec
    mark(i) = 1
    b(i) = dble(branch(i, i))
30 continue
31 nmem - 1
   jpath(1) - imem
   if (max(imem) .eq. 0) goto 35
33 imem - mpath (mark (imem), imem)
    nmem = nmem + 1
    jpath(nmem) = imem
     if (max(imem) .gt. 0) goto 33
35 do 40 i = 1, nmem
    ipath(i) - jpath(nmem - i + 1)
40 continue
   imem = ipath(nmem)
   do 50 i = 1, nmem
     b0(i) = b(ipath(i))
      zkt(i) = lmr(ipath(i))
      if (i .1t. nmem) then
        zk(i) = dble(branch(ipath(i), ipath(i + 1))) • zkt(i)
        zk(i) = zkt(i)
      end if
50 continue
   call batman(b0, zk, zkt, an1, an2, t, nmem)
   x1 = x1 + an1
   x2 = x2 + an2
60 do 80 i = 1, nmem
     b(ipath(i)) - zerod
```

```
if (i .gt. 1) then
          if (mark(ipath(i)) .ne. max(ipath(i))) then
            m - ipath(i)
            mark(m) = mark(m) + 1
            do 70 j = 1, m - 1
             mark(j) = 1
             b(j) = dble(branch(j, j))
  70
            continue
            goto 31
          end if
        end if
   80 continue
      imem = ipath (nmem)
      rx1 = sngl(x1)
      xx2 = sngl(x2)
      return
      end
      subroutine chain (nuke)
    routine: chain
   author: k. f. eckerman
             04/06/89: 09/25/91: 08/06/92: 02/28/95:06/04/96
   date:
   purpose: assemble decay chain. the name of the parent nuclide should
             be passed to the routine as namen(1) in the common block
              /chains/. upon return the chain members will be contained
              in namen, and ndau is the length of the chain.
      include 'pakparm.for'
      include 'dcfpak.cmn'
      include 'batch.cmn'
• common block /chaind/.
      character*7 named, nuke
      real fhold
      integer iptb, iparb, ibrch, ipar, ipt, n
      logical eob, pob
     common/chaind/named(mspec), fhold(mspec), iptb(mspec),
                   iparb (mspec), ipt, ibrch, ipar, eob, pob
     common/energy/ealpha(mspec), ebeta(mspec), egamma(mspec)
      dimension eat(mspec), ebt(mspec), egt(mspec)
     local variables.
character*78 text
      character*8 t12
      character*2 t12u
      double precision zln2, timest
      parameter(zln2=0.693147181d0, zero=0.0)
      include 'iolist.cmn'
      initialize chain parameters
      ibrch = 0
      ipar = 1
     nspec = 1
     eob = .true.
     pob = .false.
```

```
nucnam(1) - nuke
    do 11 i = 1, mspec
       do 10 j = 1, mspec
          branch(i, j) = zero
 10
       continue
 11 continue
    assign one unit of activity to the parent, rest are zero
    branch(1, 1) = 1.0
    lmr(1) = 0.0d0
 20 call frward
    if (nspec .le. 0) then
      i = len trim(nucnam(1))
      write(*,'(1x,(a),'' is not in data base!'')') nucnam(1)(:i)
      return
    endif
    call recver
    if (.not. eob) goto 20
    nspec = nspec - 1
    if (pob) call order
    do 100 i = 1, nspec
       if (nucnam(i)(:2) .eq. 'Sf') then
          lmr(i) = 0.000
          lmr(i) = zln2 / timest(thalf(i), iu(i))
       end if
100 continue
    t12 = thalf(1)
    t12u = iu(1)
    text = nucnam(1) (:len_trim(nucnam(1))) // ' Decay Chain:'
    text = text(:len_trim(text)) // ' Half-lives and Branching'
text = text(:len_trim(text)) // ' Fractions'
    if (.not. dbatch) then
       write(*,*) text(:len_trim(text))
       write(olog, '(/a)') text(:len trim(text))
       call printm
       if (nspec .gt. 5) call cls
    end if
    call path
    timess = 36525.0
    if (.not. dbatch) then
    text = ': Activity, Transformations, & Cumulative Energies (MeV) a
   :t 100y'
    write(*,*) nucnam(1)(:len_trim(nucnam(1))), text(:len_trim(text))
    write(olog, *) nucnam(1) (:len_trim(nucnam(1))), text(:len_trim(text))
                     Nuclide T1/2
    write(*,'(''
                                          A(t)/Ao intA/Ao(d) Ealph
    .a Ebeta Egamma'')')
    write(olog, '('' Nuclide T1/2 .
                                              A(t)/Ao intA/Ao(d) Ea
    .lpha Ebeta Egamma'')')
    end if
    ea = zero
    eb = zero
```

eg = zero

```
do 50 ispec = 1. nspec
     if (nucnam(ispec)(:2) .eq. 'Sf') goto 50
     call birch(ispec, timess, rx1, rx2)
     ea = ea + rx2 • ealpha(ispec)
     eb = eb + rx2 * ebeta(ispec)
     eg = eg + rx2 • egamma(ispec)
     if (.not. dbatch) then
        write(*,'(i4, 1x, a7, 1x, a8, a2, 1p2d12.5, 3e9.2)') ispec,
        nucnam(ispec), thalf(ispec), iu(ispec), rx1, rx2, ea, eb, eg
        write(olog, '(14, 1x, a7, 1x, a8, a2, 1p2d12.5, 3e9.2)') ispec,
        nucnam(ispec), thalf(ispec), iu(ispec), rx1, rx2, ea, eb, eg
     end if
     eat(ispec) - ea
     ebt(ispec) = eb
     eqt(ispec) = eq
50 continue
  if (nucnam(nspec) (:2) .eq. 'Sf') then
      nint = icutoff(eat, ebt, egt, 0, nspec-1)
      next = icutoff(eat, ebt, eqt, 1, nspec-1)
      nint = icutoff(eat, ebt, egt, 0, nspec)
      next = icutoff(eat, ebt, egt, 1, nspec)
   if (nspec .eq. 1) then
      nint = 1
      next = 1
   end if
   if (.not. dbatch) call pauseit
   do 70 jspec = 2, nspec
      n = 0
      do 60 ispec = 1, nspec
         if (nucnam(ispec) (:2) .eq. 'Sf') goto 60
         if (branch(ispec, jspec) .gt. 1.0E-6) then
            n = n + 1
            ibr(n, jspec) = ispec
         end if
      continue
      nbr(jspec) = n
70 continue
   return
   end
   subroutine chekab ( nuke )
   routine: chekab
   author: M. Cristy
             05/05/93
   date:
   purpose: if nuclide not found, checks whether "a" & "b" isomers
   character*7 nuke, nukeab, nukea, nukeb, check
   character*6 thalf1, thalf2
```

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parameter (nnuke = 9)
      dimension nukeab(nnuke), nukea(nnuke), nukeb(nnuke),
                 thalf1(nnuke), thalf2(nnuke)
     data nukeab /'Eu-150 ', 'In-110 ', 'Ir-186 ', 'Nb-89 ',
    data nukeab /'Eu-150', 'In-110', 'Ir-186', 'Nb-89',
.'Np-236', 'Re-182', 'Sb-120', 'Sb-128', 'Ta-178'/
data nukea /'Eu-150a', 'In-110a', 'Ir-186a', 'Nb-89a',
.'Np-236a', 'Re-182a', 'Sb-120a', 'Sb-128a', 'Ta-176a'/
data nukeb /'Eu-150b', 'In-110b', 'Ir-186b', 'Nb-89b',
.'Np-236b', 'Re-182b', 'Sb-120b', 'Sb-128b', 'Ta-178b'/
data thalf1/'12.62h', '69.1m', '15.8h', '66m', '115E3y',
     .'12.7h', '15.89m', '10.4m', '9.31m'/
    data thalf2/'34.2y', '4.9h', '1.75h', '122m', '22.5h', '64.0h', '5.76d', '9.01h', '2.2h'/
do 10 i = 1, nnuke
        if (nuke .eq. nukeab(i)) then
          write(*,9110) nuke, nukea(i), thalf1(i), nukeb(i), thalf2(i)
          write(*,'(a\)')' Input nuclide or <Enter> to guit)-> '
          read(*, 1(bn, a7)) nuke
          nuke = check( nuke )
          if (len_trim(nuke) .eq. 0) stop
          return
        endif
  10 continue
      return
9110 format( 4x, 'Nuclide ',a, 'has 2 isomers: '/20x,a,' with halflife ',a
  ./16x, 'and ',a,' with halflife ',a/4x,
    .'Re-input entire name with appropriate "a" or "b" designation',/)
   subroutine chekmn( nuke )
      routine: chekmn
      author: M. Cristy
      date: 05/05/93, revised 8/16/93
     purpose: if "m" isomer is requested, checks whether "n" isomer
                also exists.
      character*7 nuke, nukem, nuken
      character*6 thalfm, thalfn
      character*1 meta
      dimension nukem(3), nuken(3), thalfm(3), thalfn(3)
      data nukem /'Ir-190m', 'Sb-124m', 'Tb-156m'/
      data nuken /'Ir-190n', 'Sb-124n', 'Tb-156n'/
      data thalfm/'1.2h', '93s', '24.4h'/
      data thalfn/'3.1h', '20.2m', '5.0h'/
      data nnuke /3/
      do 20 i = 1, nnuke
        if (nuke .eq. nukem(i)) then
          write(*, 9110) nuke, nukem(i), thalfm(i), nuken(i), thalfn(i)
          write(*, 9120) nukem(i), nuken(i)
           read(*, '(a1)') meta
           if (meta.eq.' '.or. meta.eq.'m'.or. meta.eq.'M') then
             elseif (meta.eq.'n' .or. meta.eq.'N') then
               nuke = nuke(1:6) // 'n'
```

```
return
           A2 [A
            goto 10
        endif
       endif
 20 continue
     return
9110 format(4x, 'Nuclide ',a,' has 2 metastable isomers: '/20x,
   :a,' with halflife ',a/16x,'and ', a,' with halflife ',a)
9120 format(4x, 'Input <Enter> to accept ',a,', or input "n" for ',a,
   : ': ',/)
    end
     subroutine closem
    include 'iolist.cmn'
    close(idex)
    close(inax)
    close(inhx)
    close(i31)
    close(132)
    close(133)
    close(i34)
    close(135)
    close(i36)
    close(137)
    close(olog)
    return
    end .
     subroutine depfrac (amad, d3, d4, d5)
    author: k. f. eckerman
              08/20/93
    purpose: routine computes the deposition fractions in the three
              regions of the lung: nasal-pharynx (d3), tracheo-bronchial
               (d4) and pulmonary (d5).
    p(t) = 1.0 - 0.5*((((0.019527*t + 0.000344)*t + 0.115194)*t +
                         0.196854) *t + 1.0) ** (-4)
    ppt(w) = -(w - ((0.010328*w + 0.802853)*w + 2.515517) /
                 (((0.001308*w + 0.189269)*w + 1.432788)*w + 1.0))
    ww(x) = sqrt(-2.0*alog(x))
    Nasal-pharvnx region
    if (amad .eq. 0.0) then
       d3 = 0.30
    elseif (amad .le. 0.1) then
       d3 = 0.1
     elseif (amad .ge. 20) then
       d3 = 0.95
    elseif (amad .gt. 0.1 .and. amad .lt. 0.2) then
```

```
u0 = -0.698970
  u1 = -1.00
   t0 = ppt(ww(0.05))
  t1 = ppt(ww(0.10))
  t = t0 + (t1 - t0) / (u1 - u0) * (alog10(amad) - u0)
   if (t .ge. 0.0) then
     d3 = p(t)
   else
     d3 = 1.0 - p(-t)
   end if
elseif (amad .ge. 0.2 .and. amad .le. 10.0) then
  u0 = -0.698970
  u1 = 0.301030
   t0 = ppt(ww(0.05))
   t1 = ppt(ww(0.5))
   t = t0 + (t1 - t0) / (u1 - u0) * (alog10(amad) - u0)
   if (t .ge. 0.0) then
     d3 = p(t)
   else
     d3 = 1.0 - p(-t)
  end if
elseif (amad .gt. 10.0 .and. amad .lt. 20.0) then
  u0 = 1.0
  u1 = 1.301030
  t0 = ppt(ww(0.875))
  t1 = ppt(ww(0.95))
  t = t0 + (t1 - t0) / (u1 - u0) * (alog10(amad) - u0)
  if (t .ge. 0.0) then
     d3 = p(t)
   else
     d3 = 1.0 - p(-t)
  end if
end if
TB region
if (amad .eq. 0.0) then
  d4 = 0.08
elseif (amad .le. 0.1) then
  d4 = 0.17
elseif (amad .ge. 20) then
  d4 = 0.035
elseif (amad .gt. 0.1 .and. amad .lt. 0.2) then
  u0 = -0.698970
  u1 = -1.0
  t0 = ppt(ww(0.08))
  t1 = ppt(ww(0.17))
  t = t0 + (t1 - t0) / (u1 - u0) * (alog10(amad) - u0)
  if (t .ge. 0.0) then
     d4 = p(t)
  else
     d4 = 1.0 - p(-t)
  end if
elseif (amad .ge. 0.2 .and. amad .le. 10.0) then
  d4 = 0.08
elseif (amad .gt. 10.0 .and. amad .lt. 20.0) then
  u0 = 1.0
  u1 = 1.30130
```

t0 = ppt(ww(0.08))

```
t1 = ppt(ww(0.035))
      t = t0 + (t1 - t0) / (u1 - u0) + (alog10(amad) - u0)
      if (t .ge. 0.0) then
         d4 = p(t)
      else
         d4 = 1.0 - p(-t)
      end if
   end if
   Pulmonary region
   if (amad .eq. 0.0) then
      d5 = 0.25
   elseif (amad .le. 0.1) then
      d5 = 0.6150
   elseif (amad .ge. 20.0) then
      d5 = 0.015
   elseif (amad .gt. 0.1 .and. amad .lt. 0.2) then
      u0 = -0.698970
      u1 = -1.00
      t0 = ppt(ww(0.5))
      t1 = ppt(ww(0.615))
       t = t0 + (t1 - t0) / (u1 - u0) \cdot (alog10(amad) - u0)
       if (t .ge. 0.0) then
         d5 = p(t)
       else
         d5 = 1.0 - p(-t)
      end if
   elseif (amad .ge. 0.2 .and. amad .le. 10.0) then
      u0 = -0.698970
      u1 = 1.0
       t0 = ppt(ww(0.5))
       t1 = ppt(ww(0.05))
       t = t0 + (t1 - t0) / (u1 - u0) + (alog10(amad) - u0)
       if (t .ge. 0.0) then
          d5 = p(t)
       else
          d5 = 1.0 - p(-t)
       end if
    elseif (amad .gt. 10.0 .and. amad .lt. 20.0) then
      u0 = 1.0
       u1 = 1.301030
      t0 = ppt(ww(0.05))
       t1 = ppt(ww(0.015))
       t = t0 + (t1 - t0) / (u1 - u0) * (alog10(amad) - u0)
       if (t .ge. 0.0) then
          d5 = p(t)
       else
          d5 = 1.0 - p(-t)
       end if
    end if
50 continue
    return
    end
```

```
subroutine dosecof(nuke, flo, class, fli, amad, ipath)
routine: dosecof
author: k.f. eckerman
         05/20/96
data:
purpose: assemble the decay chain and extract the dose coefficients
         for the chain members.
input variables
            parent of the chain in standard notation; e.g., Cs-137
  nuke
  f1o
            f 1 value for oral intakes (defaults to highest effective
             dose
            inhalation clearance class for parent. decay products
  class
             will be of this class if possible or class with highest
             effective dose.
  fli
             f 1 value for inhalation. coefficients are actually
            picked by class.
             amad for the aerosol in um.
  amad
  ipath(1)
            pathway logical flag of size 9. 1 inhalation,
            2 ingestion, 3 submersion, 4 immersion, 5 ground surface,
             6 1 cm thick soil sample, 7 5 cm, 8 15 cm, 9 infinite.
output
output is through the common blocks in the include file dcfpak.cmn
as shown below.
common /dfacts/ organ(morg), df(mspec, mfact, morg), flinh(mspec),
                 flor1 (mspec), classo (mspec), iflag (mspec, mfact),
                 nint, next
             character*9 array of organ names.
  organ
  df 
             dose factors array by chain member, pathway, and organ
             array of f_1 values for inhalation by chain member
  flinh.
             array of f 1 values for ingestion by chain member
  florl
  classo
             array of class notation for inhalation by chain member
             logical flags for dose factor by chain member and pathway
  iflag
  nint
             length of chain for internal factors
  next
             length of chain for external factors
 common /radat/ thalf(mspec), iu(mspec), nucnam(mspec),
                branch (mapec, mapec), lmr (mapec),
                ibr(mspec, mspec), nbr(mspec), nspec
  thalf
             half-life of chain members
             units of the half-lives
  iu
             names of the chain members
  nucnam
  branch
             branching fraction
             decay constant in 1/d
  lmr
  ibr
             branch pointer
  nbr
             number of branches for chain members
  nspec
             length of chain
include 'pakparm.for'
include 'dcfpak.cmn'
include 'batch.cmn'
character*7 nuke, nuclide
character*1 clshld, class, cx
```

```
if we have a particulate factor then read the next record
     integer ipt, ibinry, idep
     logical ipath(9)
                                                                                                 to get the contribution of the deposition in the NP and P
      dimension dx(4, 25), f1hld(4), clshld(4), idep(4, 25, 2), ifi(7)
                                                                                                 region to the organ dose.
     include 'iolist.cmn'
                                                                                                 if (cx .eq. 'D' .or. cx .eq. 'W' .or. cx .eq. 'Y') then
      data ifi /i31. i32. i33. i34. i35. i36. i37/
     if (.not. dbatch) call cls
                                                                                                    irec = irec + 1
                                                                                                    read(inhx, '(17x, 25(i5, i4))', rec = irec)
      zero out the dose factor array
                                                                                                        (idep(itry, j, 1), idep(itry, j, 2), j = 1, 25)
                                                                                        ٠
                                                                                                 end if
      call zerom
                                                                                                 clshld(itrv) = cx
                                                                                                 if (len trim(nuclide) .gt. 0 .and. nuclide .ne. nuke) then
     assemble the decay chain
                                                                                                    goto 60
                                                                                                 elseif (len trim(nuclide).eq.0 .or. nuclide.eq.nuke) then
      call chain (nuke)
                                                                                                    if (class .eq. clshld(itry) .and.
                                                                                                                 fli .eg. flhld(itrv)) then
      first do the external coefficients for the next chain members
                                                                                                     calculate the factors for this amad if <> 1 um
      do 20 ispec = 1, next
        nuke = nucnam(ispec)
                                                                                                     if (amad.ne.1.0) call newdfs (itrv.d3.d4.d5.dx.iden)
         ipt = ibinry( nuke )
                                                                                                      do 30 1 - 1, 25
        if (ipt .ne. 0) then
            read(idex, '(a7, a8, a2, a6, 315)', rec=ipt) nuke, t, ix, mode,
                                                                                                         df(ispec, 1, j) = dx(itry, j)
                                                                                      30
                 inh, ing, iex
                                                                                                      continue
                                                                                                      flinh(ispec) = flhld(itry)
            if (iex .ne. 0) then
               do 10 ip = 3, 9
                                                                                                      classo(ispec) = clshld(itry)
                 if (ipath(ip)) then
                                                                                                      goto 80
                    iflag(ispec, ip) - .true.
                                                                                                    elseif (class .eq. clshld(itry)) then
                    read(ifi(ip-2), (a7, 1p25e9.0), rec = iex)
                       nuclide, (df(ispec, ip, j), j = 1, 25)
                                                                                                     calculate the factors for this amad if <> 1 um
     :
  10
              continue
                                                                                                     if (amad.ne.1.0) call newdfs (itry,d3,d4,d5,dx,idep)
            end if
         end if
                                                                                                      do 40 i = 1, 25
  20 continue
                                                                                                         df(ispec, 1, j) = dx(itrv, j)
                                                                                      40
                                                                                                      continue
      now do the inhalation and ingestion coefficients
                                                                                                      flinh(ispec) - flhld(itry)
                                                                                                      classo(ispec) = clshld(itrv)
      if (amad .ne. 1.0) call depfrac (amad, d3, d4, d5)
                                                                                                      goto 80
      do 200 ispec = 1, nint
                                                                                                    else
         nuke = nucnam(ispec)
                                                                                                      if (dx(itry, 25) .gt. dmax) then
         ipt = ibinry( nuke )
                                                                                                         dmax = dx(itry, 25)
         read(idex, '(a7, a8, a2, a6, 315)', rec=ipt) nuke, t, ix, mode, inh,
                                                                                                         imax - itry
              ing, iex
                                                                                                      end if
c
                                                                                                    end if
c
         inhalation
                                                                                                 else
                                                                                                  goto 60
         if (ipath(1).and. inh .ne. 0) then
                                                                                                 end if
           imax - 0
                                                                                      50
                                                                                              continue
           dmax = 0.0
           irec - inh - 1
                                                                                              calculate the factors for this amad if <> 1 um
           iflag(ispec, 1) = .true.
           do 50 itry = 1, 4
                                                                                      60
                                                                                              if (amad.ne.1.0) call newdfs (imax, d3, d4, d5, dx, idep)
              irec = irec + 1
              read(inhx, '(a7, 1x, a1, e8.0, 25e9.0)', rec=irec, end=60)
                                                                                              do 70 1 = 1, 25
                          nuclide, cx, flhld(itry),
                                                                                                 df(ispec, 1, j) = dx(imax, j)
     :
                          (dx(itry, j), j = 1, 25)
                                                                                      70
                                                                                              continue
                                                                                              flinh(ispec) = flhld(imax)
```

```
classo(ispec) = clshld(imax)
       end if
       continue
80
       ingestion
       if (ipath(2) .and. ing .ne. 0) then
         imax = 0
         dmax = 0.0
         irec = ing - 1
         iflag(ispec, 2) - .true.
         do 100 itry = 1, 4
            irec = irec + 1
            read(ingx, '(a7, e8.0, 25e9.0)', rec = irec, end = 110)
                        nuclide, fihld(itry), (dx(itry, j), j = 1, 25)
            if (len_trim(nuclide) .gt. 0 .and. nuclide .ne. nuke) then
            elseif (len trim(nuclide).eq.0 .or. nuclide.eq.nuke) then
             if (flo .eq. flhld(itry)) then
                 do 90 j - 1, 25
                    df(ispec, 2, j) = dx(itry, j)
 90
                 continue
                 florl(ispec) = flo
                 goto 130
             else
                 if (dx(itry, 25) .ge. dmax) then
                    dmax = dx(itry, 25)
                    imax = itrv
                 end if
             end if
            else
             goto 110
            end if
100
         continue
110
         do 120 j = 1, 25
           df(ispec, 2, j) = dx(imax, j)
120
         continue
         florl(ispec) = flhld(imax)
       end if
       continue
200 continue
    return
    subroutine fileini(fnpath, target, nlen, nulog, nuini, program)
Author: K. F. Eckerman
 Opens file 'program'.ini and finds the full file name, including path,
 for the file target and its record length nlen. See the ini file for
 additional comments.
 target = file name passed to this subprogram
 firstd = standard file name read from file 'program'. INI
 fnpath = file name including path
```

c

C

```
character*(*) fnpath, target, program
     character*12 fnini, fnstd, lcase
     integer nulog
     logical test
    parameter (maxfil = 40)
     fnini = program(1:len trim(program)) // '.ini'
     inquire (file = fnini, exist = test)
     if (.not. test) goto 20
     open(nuIni, file=fnini, status='old')
     target = lcase(target)
    do 10 i = 1, maxfil
      read(nuIni, *, end=15) fnstd, fnpath, nlen
       if (fnstd(:3) .eq. 'EOF') goto 15
      if(lcase(finstd) .eq. target) goto 20
 10 continue
  15 write(nuLog, 9110) target(:len trim(target)), fnini(:len trim(fnini))
     write( • ,9110) target(:len trim(target)), fnini(:len trim(fnini))
    close(nuIni)
     stop 1
  20 close(nuIni)
     return
9110 format(* **** FATAL ERROR in function FileIni: Unable to find the
    :file ', a, ';'/6x,'check ',a,' for proper assignments ****'}
     subroutine frward
   routine: frward
  author: k. f. eckerman
             01/14/92
   date:
   purpose: read down a branch of a decay chain.
     include 'pakparm.for'
     include 'dcfpak.cmn'
     character*7 named
     real fhold
     integer iptb, iparb, ibrch, ipar, ipt
     logical eob, pob
     common/chaind/named(mspec), fhold(mspec), iptb(mspec),
                   iparb(mspec), ipt, ibrch, ipar, eob, pob
     common/energy/ealpha(mspec), ebeta(mspec), egamma(mspec)
     functions referenced.
     integer ibinry
     character*8 t, mode
     character*7 nuke, d1
     character*2 ix
     integer j
     include 'iolist.cmn'
     get parent record.
```

```
if (ipar .eq. 1) then
      nuke = nucnam(ipar)
      ipt = ibinry(nuke)
      if (ipt .eq. 0) then
         nspec = 0
         return
      endif
   endif
10 if (ipt .1t. 999) then
      read(idex, '(a7, a8, a2, a6, 315, 3(i4, e11.0), 3f7.0, e11.0, 1x, a9)',
         rec-ipt) nuke, t, ix, mode, inh, ing, iex, id1, f1,
         id2, f2, id3, f3, ea, eb, eg, amu, endsf
   else
     id1 = 0
     f1 = 0.0
     id2 = 0
     f2 = 0.0
     id3 = 0
     f3 = 0.0
     nuke = 'Sf'
     ea = 0.
     eb = 0.
     eg = 0.
     t = 1 1
     ix - ' '
   end if
   ids = 999 denotes "sf" which is not a daughter product, thus set
   the ids to zero if "sf".
   if (id1 .eq. 999 .and. id2 .ne. 0) then
      if (id3 .eq. 0) then
         fhld = f1
         ihld = id1
         f1 = f2
         id1 = id2
         f2 = fhld
         id2 - ihld
      else
         fhld = f1
         ihld = id1
         f1 = f2
         id1 = id2
         f2 = f3
         id2 = id3
         f3 = fhld
         id3 = ih1d
      end if
   end if
   if (id2 .eq. 999 .and. id3 .ne. 0) then
      ihld = id2
      fhld - f2
      1d2 = 1d3
      f2 - f3
      id3 = ihld
      f3 = fhld
   end if
```

```
if processing a branch then check to see if d1 has already
   been included in nucnam, if so only fix up branch(ipar, past) and
   terminate chain, i.e., chain has converged.
   if (pob) then
      if (id1 .gt. 0 .and. id1 .1t. 999) then
         read(idex, 50, rec = id1) d1
      elseif (idl .eq. 999) then
         d1 - 'sf'
      end if
      do 15 j = 1, nspec - 1
       if (d1 .eq. nucnam(j)) goto 16
15
      continue
      goto 17
      have already handled this daughter; chain has converged.
      set end of chain and return.
      branch(ipar, j) - f1
      nucnam(ipar) - nuke
      thalf(ipar) - t
      ealpha(ipar) - ea
      ebeta(ipar) - eb
      egamma(ipar) = eg
      iu(ipar) = ix
      nspec = nspec + 1
      return
   end if
   need to treat this chain member.
17 nucnam(ipar) = nuke
   thalf(ipar) - t
   ealpha(ipar) - ea
   ebeta(ipar) = eb
   egamma(ipar) = eg
   iu(ipar) = ix
   nspec = nspec + 1
   branch (ipar, nspec) = f1
   no further daughters in chain - set end of chain
   if (id1 .ne. 0) then
     further daughters, treat id1 and check for possible branches.
     if (id2 .ne. 0 ) then
       set end of branch to false, increment branch counter, store
       pointer of parent, and record number of second or third daughter
       while following current chain. routine recver will direct
       recovery of branches.
       eob = .false.
       ibrch = ibrch + 1
```

iptb(ibrch) - id2

```
fhold(ibrch) = f2
       iparb(ibrch) = ipar
       if (id2 .ne. 999) then
          read(idex, 50, rec = id2) named(ibrch)
          named(ibrch) ='Sf'
       end if
     endif
     third daughter, branch info held as above.
     if (id3 .ne. 0) then
       eob = .false.
       ibrch = ibrch + 1
       iptb(ibrch) = id3
       fhold(ibrch) = f3
       iparb(ibrch) = ipar
       if (id3 .ne. 999) then
          read(idex, 50, rec = id3) named(ibrch)
          named(ibrch) - 'Sf'
       end if
     endif
     ipar - nspec
     if (ipt .ne. 999) goto 10
   endif
   return
50 format (a7, a8, a2, a8, i7, i5, i6, i4, 3(i4, e11.0), f7.0, 2f8.0, a10)
   end
   subroutine newdfs (1, d3, d4, d5, dx, idep)
   routine: newdfs
   author: k.f. eckerman
             10/23/93
   purpose: compute h_e and e for d3, d4, d5 depositions
   dimension dx(4, 25), idep(4, 25, 2), dsort(12), isort(12)
   data isort / 1, 4, 7, 8, 9, 10, 11, 12, 16, 19, 21, 23/
   calculate the inhalation coefficient for this new depositions
   do 10 1 = 1, 23
      f = d3 \cdot float(idep(i, j, 1)) / 0.30 +
          d5 * float(idep(i, j, 2)) / 0.25 +
          d4 • (float(100 - idep(i,j,1) - idep(i,j,2))) / 0.08
      dx(i, j) = 0.01 \cdot f \cdot dx(i, j)
10 continue
   compute the effective dose equivalent (weighting factors of icrp-26)
   and the effective dose (weighting factors of icrp-60) for the new
   depostions.
   he = 0.25 \cdot \max(dx(i, 15), dx(i, 20)) + 0.15 \cdot dx(i, 5) +
        0.12 \cdot dx(i, 13) + 0.12 \cdot dx(i, 17) + 0.03 \cdot dx(i, 22) +
        0.03 \cdot dx(1, 3)
```

```
do 20 \frac{1}{1} = 1, 12
      dsort(j) = dx(i, isort(j))
20 continue
   call sortem (dsort, 12)
  he = he + 0.06 \cdot (dsort(12) + dsort(11) + dsort(10) + dsort(9) +
       dsort (8))
  e = 0.20 \cdot \max(dx(i,15), dx(i,20)) + 0.05 \cdot dx(i,5) +
      0.12 \cdot dx(1.10) + 0.12 \cdot dx(1.17) + 0.12 \cdot dx(1.13) +
       0.12 \cdot dx(i,7) + 0.05 \cdot dx(i,2) + 0.05 \cdot dx(i,12) +
       0.05 \cdot dx(i,6) + 0.05 \cdot dx(i,22) + 0.01 \cdot dx(i,3) +
       0.01 * dx(1.18)
  hr = (14. \cdot dx(1,1) + 1400. \cdot dx(1, 4) + 640. \cdot dx(1, 8) +
        310. • dx(i,11) +28000. • dx(i, 14) + 100. • dx(i,16) +
        180. • dx(i,19) + 20. * dx(i, 21) + 80. • dx(i,23)) /
        30744.
   e = e + 0.05 \cdot hr
   dx(i, 24) = he
   dx(1, 25) = e
   return
   end
   subroutine openem
  routine: openem
   author: k.f. eckerman
   date:
             10/23/93
   purpose: open index and dose coefficient files.
   character*64 fpath
   character*12 target
   character*8 prog
   include 'iolist.cmn'
   open(olog, file = 'df_read.log')
   prog = 'dcfpak'
   target = 'snlindex.ndx'
   call fileini(fpath, target, nlen, olog, 41, prog)
   open(idex, file-fpath, access-'direct', recl-nlen, form-
       'formatted', status='old')
   target = 'ingestsf.dfs'
   call fileini(fpath, target, nlen, olog, 41, prog)
   open(ingx, file-fpath, access-'direct', recl-nlen, form-
       'formatted', status='old')
   target = 'inhalesf.dfs'
   call fileini(fpath, target, nlen, olog, 41, prog)
   open(inhx, file=fpath, access='direct', recl=nlen, form=
      'formatted', status='old')
   target = 'submrsin.dfs'
   call fileini(fpath, target, nlen, olog, 41, prog)
   open(i31, file=fpath, access='direct', recl=nlen, form=
       'formatted', status='old')
   target = 'imersion.dfs'
   call fileini(fpath, target, nlen, olog, 41, prog)
   open(i32, file=fpath, access='direct', recl=nlen, form=
  : 'formatted', status='old')
```

```
target='grsurf00.dfs'
    call fileini(fpath, target, nlen, olog, 41, prog)
    open(i33, file=fpath, access='direct', recl=nlen, form=
       'formatted', status='old')
    target = 'gryol 01.dfs'
    call fileini(fpath, target, nlen, olog, 41, prog)
   open(i34, file-fpath, access-'direct', recl=nlen, form-
     'formatted', status='old')
   target = 'grvol 05.dfs'
    call fileini(fpath, target, nlen, olog, 41, prog)
   open(i35, file=fpath, access='direct', recl=nlen, form=
      'formatted', status='old')
    target = 'grvol 15.dfs'
    call fileini(fpath, target, nlen, olog, 41, prog)
    open(i36, file=fpath, access='direct', recl=nlen, form=
   : 'formatted', status='old')
   target = 'grvolinf.dfs'
   call fileini(fpath, target, nlen, olog, 41, prog)
   open(i37, file=fpath, access='direct', recl=nlen, form=
       'formatted', status='old')
    end
    subroutine order
  routine: order
  author: k. f. eckerman
           04/06/89
  date:
  purpose: order the chain so daughter index > parents.
    include 'pakparm.for'
    include 'dcfpak.cmn'
    common/energy/ealpha(mspec), ebeta(mspec), egamma(mspec)
    character*8 thold
    character*7 nuke
    character*2 ix
    real rsave, csave
    integer i, j, ip, jp, ipass, move
    dimension rsave (mspec), csave (mspec)
    include 'iolist.cmn'
    move # of elements to move
    ipass = 0
100 move = 0
    ipass = ipass + 1
    if (ipass .gt. 4*nspec) then
      write(olog,'('' Failure in routine order: greater than'', i3,
     '' passes for '', a7, ''.'')') ipass, nucnam(1)
      write(*,'('' Failure in routine order: greater than'', i3,
      '' passes for '', a7, ''.'')') ipass, nucnam(1)
      stop 1
    endif
```

```
do 10 i = 1, napec
      do 10 i = 1. i-1
          if (branch(i, j) .ne. 0.) then
            in = i
            10 = 1
            move = 1
            go to 15
          endif
10 continue
   if no elements to move then return
15 if (move .eg. 0) return
   nuke = nucnam(ip)
    thold = thalf(ip)
   ea = ealpha(ip)
   eb = ebeta(in)
   eg = egamma(ip)
   ix = iu(ip)
   do 20 j = 1, nspec
      rsave(i) = branch(ip, i)
20 continue
   do 30 i = ip - 1, jp, -1
      nucnam(i + 1) - nucnam(i)
      thalf(i + 1) = thalf(i)
      ealpha(i + 1) = ealpha(i)
      ebeta(i + 1) = ebeta(i)
      egamma(i + 1) = egamma(i)
      iu(i + 1) = iu(i)
      do 30 1 = 1, nspec
         branch(i + 1, j) = branch(i, j)
30 continue
   nucnam(jp) - nuke
    thalf(ip) - thold
   iu(ip) = ix
   ealpha(jp) = ea
    ebeta(1p) = eb
    egamma(1p) = eg
   do 40 j = 1, nspec
      branch(jp, j) = rsave(j)
40 continue
   do 50 i = 1, nspec
      csave(i) = branch(i, ip)
50 continue
   do 60 j = ip - 1, jp, -1
    do 60 i = 1, nspec
      branch(i, j + 1) = branch(i, j)
60 continue
    do 70 i - 1, nspec
      branch(i, jp) = csave(i)
70 continue
   Yes we do have backward point gotos in FORTRAN, sorry!
   goto 100
    end
```

```
subroutine path
   author: K.F. Eckerman
            04/06/89
   date:
   purpose: initialize mpath and max matrices
            Adopted from A. Birchall, Health Phys. 50, 3, 309-397, 1986.
   include 'pakparm.for'
   include 'dcfpak.cmn'
   integer max, mpath
   common/calcul/ max(mspec), mpath(mspec, mspec)
   initializes mpath and max matrics.
   do 10 i = 1, nspec
     max(i) = 0
     do 10 j = 1, nspec
     mpath(i,j) = 0
10 continue
  do 20 j = 2, nspec
do 20 i = 1, j - 1
     if (branch(i, j) .ne. 0.) then
       max(j) = max(j) + 1
   mpath(max(j), j) = i
     end if
20 continue
   return
   end.
   subroutine pauseit
   routine: pause
   author: K.F. Eckerman
   date: 10/23/93
   purpose: pause w/o line feed
   character*1 dumy
   write(*, '(a\)')' Hit <Enter> to continue.'
   read(*, '(bn, a1)') dumy
   return
   end
```

```
subroutine printm
  routine: printm
  author: k. f. eckerman with modifications by j. c. ryman
  date:
            01/15/92
  purpose: print the decay chain
     include 'pakparm.for'
     include 'dcfpak.cmn'
     local variables.
     character*7 nuke, rlist
     integer i, j, k, nlist, jlist
     dimension jlist(mspec), nuke(mspec), rlist(mspec)
     include 'iolist.cmn'
    write(*, 8001)
    write(olog, 8001)
     if (nspec .eq. 1) then
       write(*, 8002) nspec, nucnam(1), thalf(1), iu(1)
       write(olog, 8002) nspec, nucnam(1), thalf(1), iu(1)
    else
        do 20 i = 1, nspec
          if(nucnam(i)(:2) .eq. 'Sf') goto 20
          nlist - 0
          do 10 j = 1, nspec
             if (i .ne. j .and. branch(i,j) .ne. 0.0) then
nlist = nlist + 1
                jlist(nlist) = j
                 nuke(nlist) = nucnam(j)
                write (rlist(nlist), '(1pe7.1)') branch(i,j)
                 do 5 k = 4, 6
                   rlist(nlist)(k:k) = rlist(nlist)(k+1:k+1)
                 continue
                rlist(nlist)(7:7) = '
              endif
 10
          continue
          write(*, 8002) i, nucnam(i), thalf(i), iu(i),
                         (rlist(j), jlist(j), nuke(j), j = 1, nlist)
          write(olog, 8002) i, nucnam(i), thalf(i), iu(i),
                         (rlist(j), jlist(j), nuke(j), j = 1, nlist)
       continue
       if (nspec .gt. 5) pause
     endif
     clear screen and return
     if (nspec .gt. 5) call cls
     return
     formats
8001 format(' ',3x,'Nuclide Halflife f1',7x,'Nuclide f2',7x,
    : 'Nuclide f3',7x,'Nuclide')
```

```
8002 format(' ',i2,1x,a7,1x,a8,a2,:,3(1x,a6,'->',i2,1x,a7))
     subroutine recver
   routine: recver
   author: k. f. eckerman
   date:
             04/06/89
   purpose: recover info on branches in the chain that were detected
             by frward and direct the reading of the new branch.
     include 'pakparm.for'
     include 'dcfpak.cmn'
     character*7 named
     real fhold
     integer iptb, iparb, ibrch, ipar, ipt
     logical eob, pob
     common/chaind/named(mspec), fhold(mspec), iptb(mspec),
                   iparb (mspec), ipt, ibrch, ipar, eob, pob
• local variables.
     character*7 nuke
     integer i
     include 'iolist.cmn'
     no branches to treat, set end of branch to true and return.
   1 if (ibrch .eq. 0) then
        eob = .true.
      elseif (iptb(ibrch) .eq. 999) then
         eob - .true.
      else
        consider remaining branches. recover parent's
        index at branch (ipar) and daughter's record number (ipt).
        decrement branch counter and return.
        pob = .true.
        ipar = iparb(ibrch)
        ipt = iptb(ibrch)
        nuke = named(ibrch)
        need to check to see of the daughter of the branch has already
        a member of the chain.
        do 10 i = 1, nspec - 1
           if (nuke .eq. nucnam(i)) goto 15
 10
        continue
        nucnam(nspec) = nuke
        branch(ipar, nspec) = fhold(ibrch)
        ibrch = ibrch - 1
        ipar - nspec
        return
        if already a chain member set r, decrement the branch counter
        and look for another branch to process.
```

```
15
      branch(ipar,i) - fhold(ibrch)
      ibrch = ibrch = 1
      go to 1
    endif
    return
    end
    subroutine sortem (ar, n)
    routine: sortem
   author: k.f. eckerman
    date: 10/23/93
   purpose: sort array a into descending numerical order
    dimension ar(*)
    do 20 j = 2, n
      a = ar(j)
      do 11 i = j-1, 1, -1
         if(ar(i) .le. a) goto 12
         ar(i+1) = ar(i)
      continue
 11
      i = 0
      ar(i+1) = a
 20 continue
    return
    end
    subroutine nukeok (nuke, ok)
    character*7 nuke, check
    logical ok
    function check ensure proper format of user input
    nuke = check( nuke )
    call chekmn( nuke )
    find the nuclide in the index file
    ipt = ibinry( nuke )
    if (ipt .eq. 0) then
       call chekab( nuke )
      ipt = ibinry( nuke )
    end if
    if pointer ipt is zero, the nuclide is not in the index file
    else we have a valid nuclide to process
    if (ipt .eq. 0) then
```

```
ok = .false.
  else
     ok = .true.
   end if
   return
   end
   subroutine zerom
   author: k.f. eckerman
   date: 10/23/93
   purpose: set the dose coefficient arrays to zero
   include 'pakparm.for'
   include 'dcfpak.cmn'
   logical ifalse
   dimension dzero(morg*mspec*mfact), ifalse(mspec*mfact)
   equivalence (df(1,1,1), dzero(1)), (iflag(1,1), ifalse(1))
   parameter(zero = 0.0)
   do 10 i= 1, morg * mspec * mfact dzero(i) = zero
10 continue
   do 20 i = 1, mspec * mfact
      ifalse(i) = .false.
20 continue
   return
   end
   2. Screen Routines
   subroutine cls
   author: k. f. eckerman
           12/08/93
   routine to clear screen
   write(*,*) char(27),'[2J'
   return
   end
    subroutine curright(icol)
   author: k. f. eckerman
   date: 12/08/93
   move the cursor icol columns right on the display.
```

```
character*2 col
write(col, '(i2.2)') icol
write(*,'(a\)') ' ' // char(27) // '[' // col //'C'
return
end
 subroutine curpos(irow, icol)
author: k. f. eckerman
date: 12/08/93
move cursor to the indicated row and column.
character*2 row, col
write(row, '(12.2)') irow
if (icol .ne. 0) then
   write(col, '(i2.2)') icol
else
   col ='01'
end if
write(*,'(a\)') ' ' // char(27) // '[' // row // ';' // col // 'H'
return
3. Function Routines
character*(*) function check(nuke)
function: check
author: r.j. westfall
date:
          07/20/89
purpose: convert chemical symbol in nuclide name to proper
          notation, e.g.; Kr-85m, etc.
character*(*) nuke
character*7 ltrim
remove any leading blanks from nuke
nuke = 1trim( nuke )
ensure first character is upper case.
if (nuke(:1) .ge. 'a' .and. nuke(:1) .le. 'z')
: nuke = char(ichar(nuke(:1)) - 32) // nuke(2:7)
 ensure second character, if present, is lower case.
if (nuke(2:2) .ge. 'A' .and. nuke(2:2) .le. 'Z')
    nuke = nuke(:1) // char(ichar(nuke(2:2)) + 32) // nuke(3:7)
```

```
ensure metastable notation, if present, is lower case.
    do 30 j = 4, 7
      if (nuke(j:j) .ge. 'A' .and. nuke(j:j) .le. 'Z')
   : nuke = nuke(:j-1) // char(ichar(nuke(j:j)) + 32) // nuke(j+1:)
 30 continue
    check = nuke
    end
    double precision function expf1 (lm, t)
    author: k. f. eckerman
    date: 10/04/94
    purpose: routine to compute [1.0 - exp(-lm * t)] / lm.
    double precision lm, t, lmt, one, two, expfun, eps
    logical first
    parameter (one = 1.0d0, two = 2.0d0)
    data first/ .true./
    if (first) then
       eps = one
       eps = eps / two
10
       if (eps + one .gt. one) goto 10
       eps = dsqrt(eps)
       first = .false.
    end if
    lmt = lm \cdot t
    if (lmt .lt. eps) then
       expf1 = t * (one - lmt / two)
       expf1 = (one - expfun(-1mt)) / lm
    end if
    return
    end
    double precision function expfun (t)
    author: k. f. eckerman
    date: 10/04/94
    purpose: routine to compute exp (t).
    double precision t, zero, upval
    parameter(zero = 0.0d0, upval = 180.d0)
    if (t .lt. -upval) then
       expfun = zero
    else
       expfun - dexp(t)
    end if
    return
    end
```

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```
integer function ibinry ( target )
   function: ibinry
   author: k.f. eckerman
            06/20/88
   date:
   purpose: locate record sort by target key
   integer nstart, nlast, left, right, try
   character*7 target, al
   logical first
   save first, nstart, nlast
   include 'iolist.cmn'
   initialization.
   data first /.true./
   if (first) then
      read (idex, '(214)', rec = 1) nstart, nlast
      first - .false.
   left - nstart
   right - nlast
   begin attempts to find target.
10 try = -int((left + right) / 2)
   read (idex, '(a7)', rec = try) al if (a1 .1t. target) then
      left = try + 1
   elseif (al .gt. target) then
      right = try - 1
   else
      ibinry - try
      return
   end if
   continue search unless left > right then set ibinry to zero and
   let calling deal with the unidentified target.
   if (left .1t. right + 1) then
      goto 10
   else
      ibinry = 0
      return
   end if
   end
   integer function icutoff(eat, ebt, egt, igamma, nspec)
   dimension eat(*), ebt(*), egt(*)
```

ea = eat(nspec)

```
eb = ebt(nspec)
     eg = egt(nspec)
     if (ea .gt. 0. .and. igamma .eq. 0) then
        do 10 i = nspec-1, 1, -1
           if (eat(i) .1t. 0.99 * ea) then
              ia = 1 + 1
             goto 15
           end if
        continue
  10
        ia = 1
     else
        ia = 0
     end if
  15 if (eb .gt. 0.) then
        do 20 i = nspec-1, 1, -1
           if (ebt(i) .1t. 0.99 * eb) then
              ib = i + 1
              goto 25
           end if
        continue
         ib - 1
     else
        1b = 0
     end if
  25 if (eg .gt. 0.) then
        do 30 i = nspec-1, 1, -1
           if (egt(i) .1t. 0.99 * eg) then
             ig = i + 1
              goto 35
           end if
        continue
  30
        ig = 1
     else
        ig = 0
     end if
  35 icutoff = max0(ig, max0(ia, ib))
     return
     end
     character*(*) function lcase (a)
*---
     author: k. f. eckerman
     date: 10/04/94
     purpose: convert character variable a to lower case.
     character*(*) a
     lcase = a
     do 10 i = 1, len trim(lcase)
        ix = ichar(lcase(i:i))
        if (ix .gt. 64 .and. ix .lt. 91) then
           lcase(i:i) = char(ix + 32)
        end if
  10 continue
     return
```

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```
end
  character*(*) function ltrim(a)
  function: ltrim
  author: K.F. Eckerman
  date: 10/23/93
  purpose: trim leading blanks from string a
  character*(*) a
  logical ok
  ok - .false.
10 if (a(1:1) .ne. ' ') ok = .true.
  if (.not. ok) then
     n = len_trim(a) - 1
do 20 i = 1, n
       a(i:i) = a(i+1:i+1)
     continue
     a(n+1:n+1) = '
     goto 10
   end if
  1trim - a
  return
  end
   double precision function timest (t, ix)
   author: k. f. eckerman
            10/04/94
   date:
   purpose: function returns time in days given time string t and its
             units ix.
   function arguments.
   character*2 ix
   character*8 t
   double precision tp
   read(t, '(E8.0)') tp
   if (ix .eq. 'us') then
      tp = tp / 8.64d+10
   elseif (ix .eq. 'ms') then
      tp = tp / 8.64d+07
   elseif (ix .eq. 's ') then
      tp = tp / 8.64d + 04
   elseif (ix .eq. 'm ') then
      tp = tp / 1.44d+03
   elseif (ix .eq. 'h ') then
      tp = tp / 24.d0
   elseif (ix .eq. 'y ') then
      tp = tp • 365.25d0
   endif
```

A3. ILLUSTRATIVE PROGRAM READEM. FOR

program readem

```
    READEM illustrates the manner-the electronic files of dose coefficients

for Sandia National Laboratory can be accessed in FORTRAN. The procedure

    uses the index file DFEXTINT.NDX to coordinate the reading of the

    coefficients from their respective files.

• The coefficient files are:
   ICRPINGS.DAT - FGR 11/ICRP-30 ingestion intakes.
   ICRPINHS.DAT - FGR 11/ICRP-30 inhalation intakes.
   FGR12F31.DAT - FGR 12 Table III.1 for air submersion.
   FGR12F32.DAT - FGR 12 Table III.2 for water immersion.
   FGR12F33.DAT - FGR 12 Table III.3 for ground surface contamination.
    FGR12F34.DAT - FGR 12 Table III.4 contaminated soil slab 1 cm thick.
   FGR12F35.DAT - FGR 12 Table III.5 contaminated soil slab 5 cm thick.
   FGR12F36.DAT - FGR 12 Table III.6 contaminated soil slab 15 cm thick.
   FGR12F37.DAT - FGR 12 Table III.7 contaminated soil infinite thickness.

    All files are formatted direct access files. The RECL specification in

the FORTRAN open statement is read from the file DCFPAK.INI. See that file
* for further discussion regarding specifications for different compllers.
The file FGR1112.IDX contains the following information:
• The first record gives the record numbers of the first and last data
record, format (214) which are 2 and 839. The format of records 2 through
839 is (a7,a8,a2,a6,315,3(14,e11.0),3f7.0,e11.0,1x,a9)
Variable
                   Description
                                           Format
· nuke
                   Name of nuclide
• t12
                   Halflife
                                             a8
* ix
                   Halflife units
                                             a2
                   Decay Modes
mode
                                             a6
# inh
                   Record # for inhalation
                                             15
· ing
                   Record # for ingestion
                                             15
• iex
                   Record # for external
                                             15
* id(1)
                   Record # of daughter
                                             14
* f(1)
                   Branching fraction
                                             e11
* id(2)
                   Record # of daughter
                                             14
                   Branching fraction
* f(2)
                                             e11
# id(3)
                   Record # of daughter
                                             14
* f(3)
                   Branching fraction
                                             e11
* Ealpha
                   Emitted alpha energy
                                             £7.0
```

£7.0

£7.0

· e11

a9

author: k.f. eckerman date: 06/04/96: 06/27/96

Emitted electron energy

Emitted photon energy

Atomic mass

Date of ENDSF

include 'pakparm.for' include 'dcfpak.cmn' include 'batch.cmn' character*7 nuke character*5 amadx

Eelectron

Ephoton

* AMU

· ENDSE

```
character*1 class, ucase
   logical ipath(9), ok
   include 'lolist.cmn'
   dbatch - .false.
   numarg = nargs()
   if (numarg .gt. 1) dbatch - .true.
   this loop sets all pathway flags to true; i.e., we want dose
   cofficients for all pathways.
   do 1 i = 1, 9
1 ipath(i) = .true.
   write(*,'(1x,'' View dose coefficients'')')
   write(*,'(3x,'' K.F. Eckerman and R.W. Leggett'')')
   write(*, '(3x, '' Oak Ridge National Laboratory'')')
  write(*,'(3x,'' Oak Ridge, TN 37831-6383'',/)')
   open direct access files and write text to screen
   call openem
   label 10 is the subject of a backward pointing goto
10 write(*,'(a\)')' Input nuclide (e.g.; Ba-137m or <Enter> to quit)-
   read(*,'(bn, a7)') nuke
   if (len_trim(nuke) .ne. 0) then
      call nukeok to determine if nuke in data bases
      call nukeok (nuke, ok)
      if (.not. ok) then
         write(*,'(1x, (a),'' is not in index file!'')')
                   nuke(:len_trim(nuke))
         write(*,*)
         write(*,*)
         call pauseit
      else
         if no inhalation class is indicated then the class with the
         higest effective dose will be assumed.
         write(*,'(a\)')' Clearance class (D, W, Y, V or " ")-> '
         read(*,'(bn, a1)') class
         class = ucase (class)
         read in amad as a character and then do a internal read
         write(*,'(a\)')' Input AMAD (default 1 \mum) -> 'read(*, '(bn, a5)') amadx .
         if (len_trim(amadx) .eq. 0) then
            amad = 1.0
         else
```

```
read(amadx, '(f5.0)') amad
        end if
        lets get some factors
        floral = 0.0
        flinhi = 0.0
        call dosecof(nuke, floral, class, flinhi, amad, ipath)
        call tablem to print factors to screen
        call tablem (amad)
      compute activity of chain members as at user specified times
     write(*,*) ' Activity and Integrated Activity of Chain Members'
       write(*,'(a\)')
       'Input time of interest (d); zero to quit --> '
        read(*,'(bn, e10.0)') t
       if (t .eq. 0.) goto 40
       write(*,'(5x,''Nuclide T1/2
                                           A(t)/Ao intA/Ao(d)'')')
        do over the maximum length of the retained chain members
        do 30 ispec = 1, max(mint, next)
          call birch(ispec, t, a, aint)
          write(*,'(5x, a7, 1x, a8, a2, 1p2e12.5)') nucnam(ispec),
                thalf(ispec), iu(ispec), a, aint
30
       continue
       goto 20
      clear screen and goto 10 to get another nuclide.
40
     call cls
     go to 10
   endif
   close all files
   call closem
   subroutine tablem (amad)
   author: k.f. eckerman
   data: 05/20/96
   purpose: write dose coefficients to screen.
   include 'pakparm.for'
   include 'dcfpak.cmn'
   character*60 head
```

```
character*20 titles(mfact)
character*18 units(mfact)
character*8 t, 1trim, buffer
character*5 buff5
data titles / 'Inhalation
                                         ', 'Ingestion
                                         ', 'Immersion
                *Submersion
                                         ', '1 cm Soil Slab
                 *Ground Surface
                                         ', '15 cm Soil Slab
                '5 cm Soil Slab
                'Infinite Thick Soil ' /
                                     ', '(Sv/Bq)
data units / '(Sv/Bg)
                '(Sv per Bq s m^-3)', '(Sv per Bq s m^-3)',
                '(Sv per Bq s m^-2)', '(Sv per Bq s m^-3)',
                '(Sv per Bq s m^-3)', '(Sv per Bq s m^-3)',
                '(Sv per Bq s m^-3)' /
 do 100 ifact = 1, mfact
    if (ifact .le. 2) then
       nupper - nint
       nupper - next
    end if
    do 50 ispec = 1, nupper
       if (iflag(ispec, ifact)) then
           call cls
           head = 'Dose Coefficients' // titles(ifact) (:len_trim( titles(ifact))) // '' // units(ifact)
:
           ip = (80-len trim(head))/2
           call curpos (\overline{2}, ip)
           write(*,*) head(:len_trim(head))
           write(*,*)
           t = ltrim(Thalf(ispec))
           call curright(6)
           if (ifact .eq. 1) then
             write(buffer, '(1pe8.1)') flinh(ispec) write(buff5, '(f5.2)') amad
             write(*,*) nucnam(ispec) //
                         ' T1/2 = ' // t(:len_trim(t)) // ' ' //
:
                         iu(ispec) // 'Class: ' // classo(ispec) .
:
                        // f 1 = 1 // buffer // AMAD (µm) = 1
:
                         // buff5
:
           elseif (ifact .eq. 2) then
  write(buffer, '(1pe8.1)') florl(ispec)
             write(*,*) nucnam(ispec) //
                         ' T1/2 - ' // t(:len_trim(t)) // ' ' //
                         iu(ispec) // ' f 1 = 7 // buffer
           else
             write(*,*) nucnam(ispec) //
                         * T1/2 = * // t(:len_trim(t)) // * * //
                         iu(ispec)
           end if
           write(*,'(/,t7,''Organ'',t20,''h_T'',t32,''Organ'',t45,
                     ''h_T'',t57,''Organ'',£70,''h_T'',/,
t7, ''----'',t18,''----'',
t32,''----'',t68,''----'',
t57,''----'',t68,''----'')')
:
           write(*,'(3(6x,a9,2x,1pe8.2))') (organ(j),
```

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