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 modications, 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

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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 11	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[a]	(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[a]	(Not used)	No	Yes	Yes

[a]Represents multiple tissues considered explicitly in DCFPAK.

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 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, m^2 of soil for ground surface contamination, and m^3 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

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

[a]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.

a personal computer or work station and can be run interactively or in batch mode.

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;

2. 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;

8. 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).

<u>DFINHS.DAT</u>

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 µm.

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 µm, 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 µm or greater than 20 µm, DCFPAK assigns fractional depositions in these regions corresponding to a particle size of 0.1 µm or 20 µm, respectively.
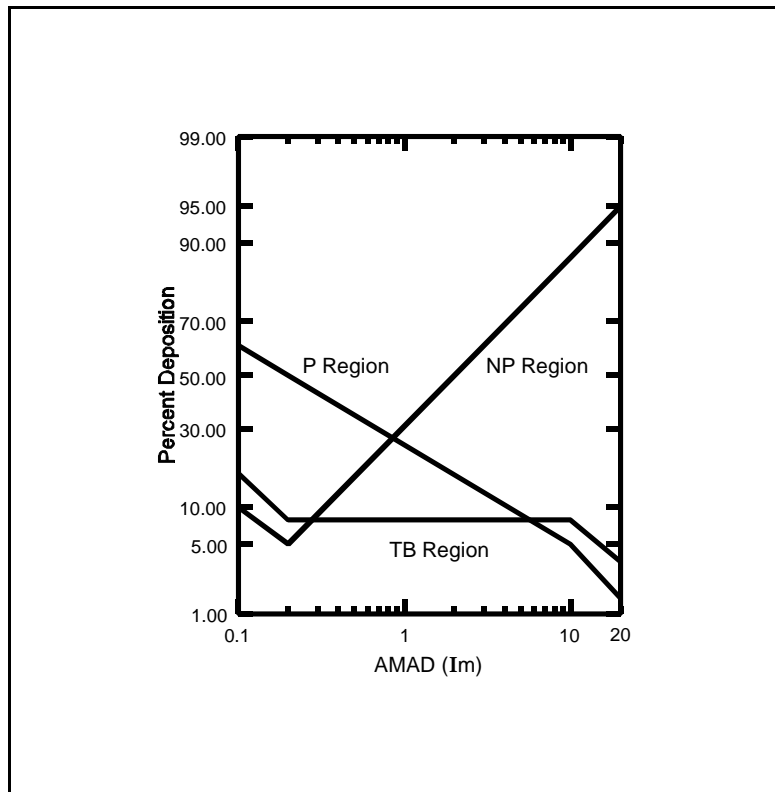

Figure 1 Deposition of particulate materials in the regions of the lung as a function of the activity median aerodynamic diameter (AMAD).

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.

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".

<u>DCFPAK.FOR</u>

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.

<u>PAKPARM.FOR</u>

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.

<u>DCFPAK.CMN</u>

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:

```
      common /dfacts/ organ(morg), df(mspec, mfact, morg),
flinh(mspec),
    :                f1orl(mspec), classo(mspec), iflag(mspec,
mfact),
    :                nint, next

 common /radat/ thalf(mspec), iu(mspec), nucnam(mspec),
    :             branch(mspec, mspec), lmr(mspec),
    :             ibr(mspec,mspec), nbr(mspec), nspec
```

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 (f_1) 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:

```
 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)
```

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
```

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.

<u>READEM.FOR</u>

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, F1ORAL, CLASS, F1INHI, 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 f1 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 f1 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, F1ORAL, 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

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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.

2. 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 acess 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

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APPENDIX A: Source Code Listings