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John P. Shanahan
University of Nevada, Las Vegas

Phillip W. Patton
University of Nevada, Las Vegas

Mark Rudin
University of Nevada, Las Vegas

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Dose Coefficient (DC) Methodology Report

J. Shanahan, P. Patton, and M. Rudin
University of Nevada, Las Vegas
Department of Health Physics

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Introduction

A research consortium comprised of representatives from several universities and national laboratories will be established as part of this project to generate internal and external dose coefficients for radionuclides produced in spallation neutron sources. Information obtained from this multi-year study will be used to support the siting and licensing of future accelerator-driven nuclear initiatives within the U.S. Department of Energy complex, including the Spallation Neutron Source (SNS) and Accelerator Production of Tritium (APT) Projects. Calculated dose coefficients will also be used to fill data gaps for several hundred radionuclides that exist in Federal Guidance Reports 12 and 13, as well as, Publications 68 and 72 of the International Commission on Radiological Protection (ICRP).

Dose coefficients allow simple determination of radiation dose associated with various radiation exposure scenarios, and ultimately, assessing the health risks to workers in a nuclear facility. Expressed in Sv Bq^{-1} , dose coefficients estimate the committed dose equivalent to an organ or tissue per unit intake, the committed effective dose equivalent per unit intake, the dose equivalent rate per unit air concentration of radionuclide, or the effective dose equivalent rate per unit air concentration of radionuclide.

The objectives in the first year of this project included:

- The formation of a Working Group whose member include: The University of Nevada, Las Vegas, Idaho State University, University of Florida, Georgia Institute of Technology, Tbilisi State University, and Oak Ridge National Laboratory (ORNL);
- The identification and prioritization of radionuclides produced during the spallation process based on a liquid mercury target;
- Develop a reproducible methodology to calculate both internal and external dose coefficients for these selected radionuclides;
- Calculate dose coefficients for the selected radionuclides that are not yet published in existing radiation safety databases.

Intended Users

The purpose of this report is to present the methodology developed to calculate internal and external dose coefficients for radionuclides produced in the spallation process. Much of the information regarding computer codes in this report comes from various technical manuals and professional papers. References are provided at the beginning of each section for documentation and for the user who requires more specific information. The report also includes the results of applying the methodology to determine dose coefficients for five radionuclides. This effort identified potential areas of concern that will need to be addressed when the methodology is used in the future to generate additional dose coefficients. The Appendices provide student generated notes on the loading of software and more user specific instructions on how to use the various computer codes.

Radionuclide Prioritization

The DC Working Group decided initially to concentrate efforts on generating dose coefficients for those radionuclides that could be produced from the spallation of a liquid mercury target for which no dose coefficients currently exist. Over 520 radionuclides were identified as possible byproduct materials, all of which have the potential to be involved in various radiation exposure scenarios involving workers. Prioritization of the 520 radionuclides included tabulating the list according to half-life and obtaining further physical information on each radionuclide (e.g., mode of decay, etc.), and determining which radionuclides currently have no dose coefficients published in the literature. The Working Group recommended focusing on those radionuclides with half-lives between one and ten minutes. Radionuclides from the list with half-lives less than one minute and greater than ten minutes will be considered at a later date. The prioritization effort identified 86 radionuclides from the original list of 520 that will be considered for this phase of the project.

DC Methodology

The methodology developed by the DC Working Group to calculate both internal and external dose coefficients for radionuclides produced from a spallation sources was adopted from the methodology used to develop Federal Guidance Report 13 (U.S. EPA 2002) and is presented in Figure 1. In this methodology, relevant nuclear decay data is extracted from ENSDF (Evaluated Nuclear Structure Data File) and used by the computer code EDISTR to calculate the mean energies and absolute intensities of all principal radiations associated with the radioactive decay of a nuclide. The executables of DECDAT (Decay Data) arrange the output of EDISTR into the proper format for inclusion into the nuclear decay data libraries within DCAL (Dose and Risk Calculation software). DCAL consists of a series of computational modules for the calculation of dose and risk coefficients. The DCAL system also includes extensive libraries of biokinetic, anatomical, and dosimetric data representing the current state of the art. Specific information regarding each step of the methodology is described below.

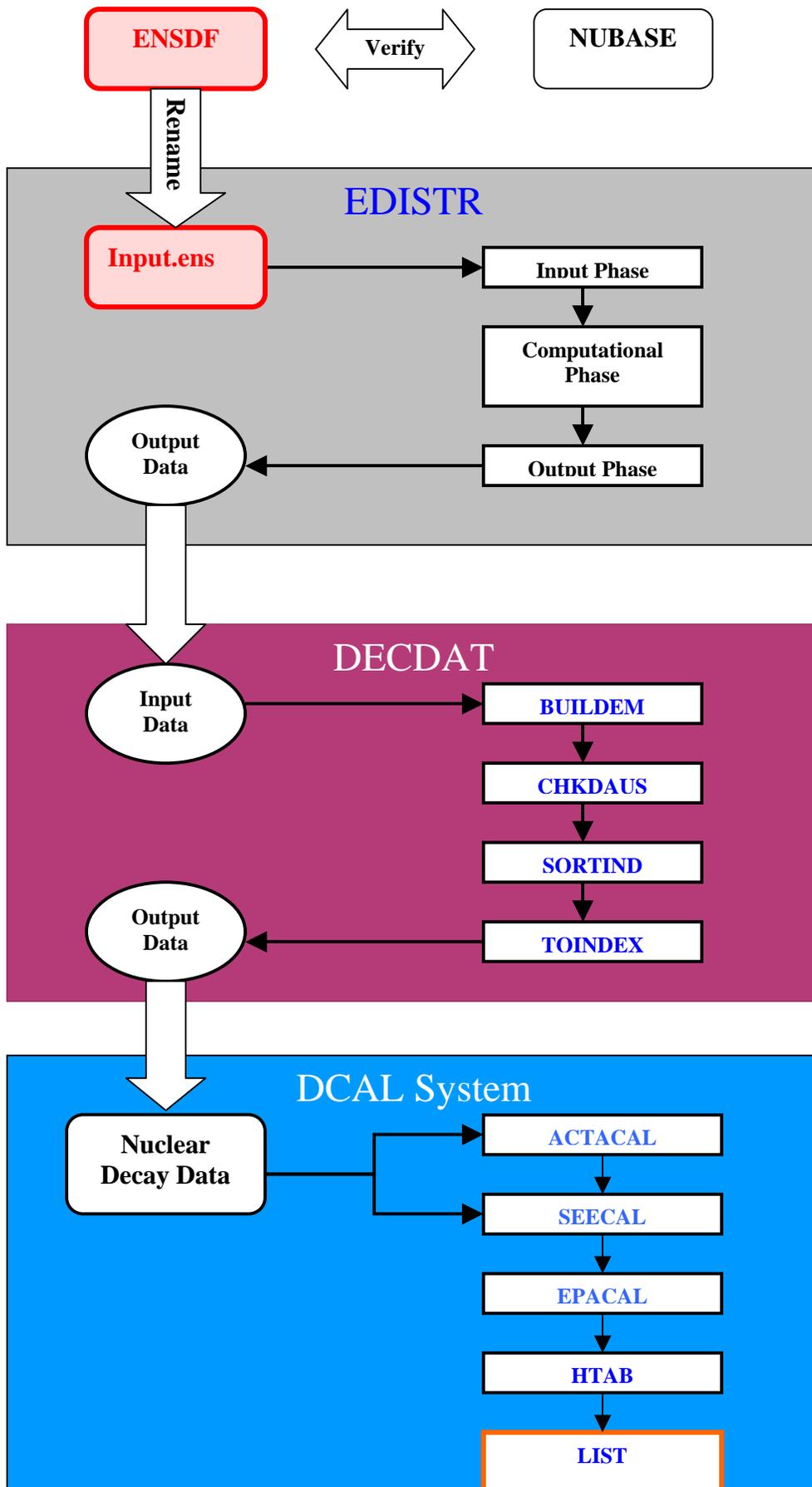


Figure 1. Dose Coefficient Working Group Methodology Flow Sheet

Evaluated Nuclear Structure Data File (ENSDF) - (Tuli 1987)

The National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (<http://www.nndc.bnl.gov>) maintains this computer-based file for the International Nuclear Structure and Decay Data Network. An ENSDF contains evaluated nuclear structure information (e.g., modes of decay, half-life, Q-values, spin, parity, etc.) for selected radionuclides with mass numbers (A) less than 263. For radionuclides with $A \geq 45$, this information is documented in the journal *Nuclear Data Sheets*. For radionuclides with $A < 45$, the data in ENSDF is based on compilations published in the journal *Nuclear Physics*. The information in ENSDF is updated by mass chains with a present cycle time of approximately six years.

Input.ens File - (Dillman 1980)

ENSDF is organized into data sets (i.e., adopted levels, gamma; decay data sets; reaction data sets), each of which consists of a number of 80-column card-image records. A decay data set for a particular radionuclide will be downloaded from the NNDC website and placed into the EDISTR directory (The EDISTR code is explained in detail below). Once in the directory, the file is renamed Input.ens and gets utilized by EDISTR as a basic radioactive decay data set specific to the radionuclide of interest when the code is executed. Examples of Input.ens files are shown in Figure 2.

As seen in Figure 2, for every record in an Input.ens file except the END record, columns 1 through 5 contain a two-to-five character string consisting of the mass number and, immediately following, the chemical symbol of the nuclide for which nuclear structure information is being given elsewhere on the card image. The END record is blank in every column and simply cues the computer that the end of the data set has been reached.

The first record in each data set is always the IDENTIFICATION record and indicates, by means of a key-word label string of characters, the type of data to be found in the data set. For our purposes, we are interested only in the DECAY data sets, that is, those data sets that give information on the radioactive decay of a nuclide. A DECAY data set IDENTIFICATION record contains, among other things, a field (columns 10 through 39) consisting of three parts - the decaying nucleus, the type of decay, and the word DECAY - separated by one or more blanks. The decaying nucleus is specified by the mass number followed by the chemical symbol of the parent. The EDISTR computer program uses the data in this three-part field to assign a mass number, atomic number, and decay type to the parent nuclide. The only other item read from the IDENTIFICATION record (columns 75 through 80) is the date (year/month/day) the data set was entered into ENSDF.

Following the IDENTIFICATION record is a NORMALIZATION record, designated by the letter N in column 8, and a PARENT record, designated by the letter P in column 8. For a PARENT record, Columns 1 through 5 are the mass number and chemical symbol of the parent nuclide, whereas, in most other types of records, columns 1 through 5 are the mass number and chemical symbol of the daughter nuclide because the radioactive decay gives information on the level structure, etc., of the daughter nuclide.

Following the NORMALIZATION and PARENT records is the main body of the data set, composed of LEVEL, ALPHA, B-, EC, B+, and GAMMA records, which describe the measured or deduced properties such as spins, gamma-ray energies, etc. These records are associated with the level that decays (for GAMMA records) or the level that is populated (for B-, EC, B+, or ALPHA records). Thus, each LEVEL record is followed by a group of B-, EC, B+, or ALPHA records describing charged-particle decay into the level and GAMMA records describing gamma-ray decay out of the level. Table 1 was developed to serve as a quick reference for all records in an ENSDF or Input.ens file.

```

3HE      3H B- DECAY                                87NP      200007
3HE N                                1.0      1.0
3H P 0.0                1/2+                12.32 Y   2      18.590    2
3HE L 0.0                1/2+                STABLE
3HE B 18.594            8 100.0                3.02

99TC      99TC IT DECAY                                NDS01      200107
99TC N 0.8906            240.8906  240.999963 6
99TC L              0      9/2+
99TC L  140.5110107/2+
99TC G 140.511            1 100                M1+E2      +0.129 35      0.114 3
99TC L  142.6836111/2-
99TC G 2.1726            4                E3                1.60E10 111.4
99TC G 142.63            3 0.021      2 M4                39.9

15N      15O B+ DECAY                                1991AJ01      91NP      200204
15O P 0                1/2-                122.24 S 16      2754.0    5
15N N 1                1                1
15N L 0                1/2-
15N E                99.900310 0.0997 10 3.6377 8      100

125TE      125I EC DECAY                                1976MI18,1990IW04 99NDS      199907
125I P 0.0                5/2+                59.400 D 10      185.77    6
125TE N 1.0                1.0
125TE L 0.0                1/2+
125TE L 35.4922            5 3/2+                1.48 NS 1
125TE E 150.27            6                100            5.4171 5
125TE G 35.4922            5 6.68      13M1+E2      0.029      +3-2      14.0

```

Figure 2. Example Input.ens files for selected radionuclides. Note that the ENSDF decay data set and the Input.ens file have the same format and contain the same information for a particular radionuclide.

It should be noted that data files may not contain all of the information outlined above for a specific radionuclide. When this is the case, the EDISTR code will assume default values for the missing information for calculation purposes. Specific information concerning the default values the reader is referred to ORNL/TM-6689 (Dillman 1980). It is also noted that information contained in these data files may be located and verified utilizing a Nuclear Science Reference (NSR) search. This utility is also available on the NNDC website (<http://www.nndc.bnl.gov/nndc/nsr/>) and can direct the user to appropriate reference material specific to a radionuclides' evaluation.

Another reference tool used by previous investigators to verify ENSDF information is the NUBASE database (Audi et al. 1997). This database can be downloaded from the Internet (http://www-csnm.in2p3.fr/amdc/nubase_en.html) and runs under a DOS operating platform. It contains experimentally known nuclear properties, and some that have been estimated from extrapolation, for 3010 nuclides in ground-state, 669 of them in first and 58 in second isomeric states: mass, isomeric excitation energy, half-life, spin, parity, decay modes and intensities. All the information is properly referenced and this tractability allows any user to check the recommended data. Any work that will use that file should make reference to the *Nuclear Physics* paper and not to the electronic data file.

Table 1. Summary of the Records Found in an ENSDF Decay Data Set or Input.ens File.

Record		Information Extracted from ENSDF
Identification		Nucleus Identification Data Set Identification Date entered into ENSDF
Normalization	N	Multiplier for converting relative photon intensities to photons per 100 decays of the parent through this decay branch Multiplier for converting relative transition intensity to transition per 100 decays of the parent through this decay branch. The branching ratio multiplier for converting intensity per 100 decays through this branch to intensity per 100 decays of the parent nucleus
Parent	P	Energy of the decaying level in KeV Spin, parity, or both. Half-life value.
Level	L	Level energy in KeV Spin, parity, or both. Half-life value Metastable-state level
Gamma	G	Energy of photon in KeV Relative photon intensity Multipolarity of transition For a mixed multipole transition, the mixing ratio delta. The total conversion coefficient. The relative total transition intensity
Beta minus	B	The end point energy of the Beta transition in KeV Intensity of the Beta decay branch in percentage of total beta decay. Log fit for the transition Uniqueness classification for the Beta decay
EC (or B+)	E	The energy for Electron Capture to the level, if measured The intensity of the Beta plus decay branch in percentage of the total Electron Capture Beta plus decay The intensity of the Electron-Capture branch in percentage of the total Electron Capture and Beta plus decay. Log fit for EC and Beta plus The total Electron Capture and Beta plus-decay intensity in percentage Uniqueness classification for the EC or Beta plus decay
Alpha	A	The Alpha energy in KeV The Alpha-decay branch as percentage of the total alpha decay

EDISTR - (Dillman 1980)

The EDISTR computer code was initially developed to compile a nuclear decay database for internal radiation dosimetry calculations by the Biomedical Effects and Instrumentation Section of the Health and Safety Research Division of ORNL. The EDISTR code uses an Input.ens file (a basic radioactive decay data set) to calculate the mean energies and absolute intensities of all principal radiations associated with the radioactive decay of a nuclide. The principal calculations performed by EDISTR are the determination of (1) the average energy of beta particles in a beta transition, (2) the beta spectra as a function of energy, (3) the energies and intensities of X rays and Auger electrons generated by radioactive decay processes, (4) the bremsstrahlung spectra accompanying beta decay and monoenergetic Auger and internal conversion electrons, and (5) the radiations accompanying spontaneous fission.

Functional Phases

The Program EDISTR is divided into three functional phases: (1) the input phase, in which the input data are prepared and put into a suitable format for computational purposes, (2) the computational phase, in which the computations required to implement the theory outlined below are completed, and (3) an output phase, in which the results of the computational phase are prepared for print.

Input Phase

In the input phase there are a series of subroutines to read the data contained in an Input.ens file and convert it to a format directly usable by the computational phase of EDISTR. The output data of these subroutines are stored in a random-access file, MASTER.DAT. Because data can be input for several nuclides (and perhaps several modes of decay for a single nuclide) a second random-access file, SUBMAS.DAT, is also created by these subroutines. SUBMAS.DAT indexes the records of MASTER.DAT so that records of a particular type and for a particular nuclide may be accessed rapidly.

Computational Phase

The bulk of the "number-crunching" calculations are made in the computational phase of EDISTR. Theoretical methods are outlined below (Methods of Solution) and are implemented during the computational phase. The input data for all parts of the computational phase come from the MASTER.DAT and SUBMAS.DAT random-access files.

METHODS OF SOLUTION

1. Alpha decay. Kinetic energies of the alpha particles and the associated recoil nuclei are computed using conservation of energy and momentum principles. The input data consist of the ground state Q value, the various excitation energies of the levels in the daughter nuclide at which the alpha transitions end, and the corresponding alpha intensities.
2. Beta decay. The average energies of the beta particles and the emitted continuous spectra are calculated using the Fermi theory of beta decay with the input of additional data to determine the forbiddenness of the beta spectra.
3. Electron-Capture decay. The distribution of primary vacancies created in the various atomic shells and sub shells as a result of the electron-capture process are calculated using the K/L/M capture ratios.

4. Internal conversion of gamma rays. This is a process by which the energy of a transition between two states of a nucleus is transferred to an orbital electron. The distribution of the primary vacancies in the various atomic shells and the energies and intensities of conversion electrons are calculated.
5. X-ray and Auger-electron intensities and energies. Intensities of X rays and Auger electrons are obtained using the numbers of primary vacancies in the various sub shells for electron capture or for internal conversion of electrons.
6. Spontaneous fission. The fission decay fraction, the number of neutrons emitted per fission, the mass number of the parent nuclide, and the atomic number of the parent nuclide are used to compute intensities and energies for spontaneous fission fragments, neutrons, beta particles, prompt gamma rays, and delayed gamma rays.
7. Bremsstrahlung radiation. Bremsstrahlung spectra associated with beta particles and monoenergetic conversion and Auger electrons are calculated.

Output Phase

The output phase of program EDISTR consists of calls to three subroutines, TABIPU, TABDEC, and TABBRE. In general, these subroutines take the output data from the computational phase, which have been written to temporary or scratch files, and compile the results so that they can then be printed. The results maybe viewed using any text editor and opening the decay file in the output directory of EDISTR.

Decay Data (DECDAT) - (Eckerman 2001)

The DECDAT directory contains a series of MS-DOS executables to take the output of EDISTR (i.e., the decay file) and generate nuclear decay data files suitably formatted for use by DCAL. These files are then placed into the nuclear decay data library within the DCAL code for tabulation of dose coefficients. DCAL is a comprehensive software system for the calculation of tissue dose and subsequent health risk from radionuclides taken into the body or residing within environmental media. A brief description of the executables within the DECDAT directory is given below.

INPUTDAT.DAT

This file serves as a template and is read by the BUILDEM.EXE application. The file simply directs the executable to the name of the EDISTR output file for the indicated radionuclide.

BUILDEM.EXE

BUILDEM.EXE reads INPUTDAT.DAT and then selects the EDISTR output file to create the files DECDATA.IDX, DECDATA.RAD, and DECDATA.BET in a format that can be read by DCAL.

CHKDAUS.EXE

CHKDAUS.EXE checks on the inclusion of all daughter products in DECDATA.IDX file. This executable also writes an output file MISSDAUS.DAT that flags the user to missing daughter information. The reader should note that a daughter might be missing need not be an error.

SORTINDEX.EXE

The SORTINDEX.EXE application sorts the DECDATA.IDX file alphabetically by radionuclide name.

TOINDEX.EXE

The TOINDEX.EXE application converts the DECDATA.IDX to the DECDATA.NDX. The conversion is a matter of replacing the name of daughter products by their record number in DECDATA.NDX. Note: if a daughter product is missing the code sets its records number to -999. Such entries should be deleted if the judgment is reached that the daughter is of no dosimetric significance.

Once the user has finished and corrected for, if necessary, any missing daughter product information the only remaining task is to rename the data files. The root name of the files with the extensions of NDX, RAD, and BET get changed from DECDATA to ICRP38 and placed into the nuclear decay data library within DCAL.

Dose and Risk Calculation (DCAL) Code - (Eckerman et al. 2001)

Background

DCAL is designed for use on a personal computer (PC) or scientific workstation. DCAL is intended for users who have experience with the PC/DOS operating environment, scientific computing, and the field of radiation dosimetry. The system consists of a series of computational modules (written in FORTRAN) driven by an interactive interface written in Professional BASIC. There are two modes of operation of DCAL: an interactive mode designed for evaluation of a given exposure case; and a batch mode that allows non-interactive, multiple-case calculations on a PC or scientific workstation. The Dosimetry Research Group (now the Biosystems Modeling Team within the Advanced Biomedical Science and Technology Group) at ORNL developed DCAL under the sponsorship of the U.S. Environmental Protection Agency. DCAL has been used in the development of two Federal Guidance Reports (Federal Guidance Reports 12 and 13) (EPA 1993; EPA 1999) and several publications of the International Commission on Radiological Protection (ICRP), specifically in the computation of age-specific dose coefficients for members of the public (ICRP 1989, 1993, 1995a, 1995b, 1996). The senior author (K. F. Eckerman) is the chairman of the ICRP's Task Group on Dose Calculations.

DCAL contains two nuclear decay data libraries that were initially documented in ORNL/TM-12350 (Eckerman et al. 1993). The "ICRP38" collection consists of data for 825 radionuclides that appeared in Publication 38 (ICRP 1983), plus an additional 13

radionuclides evaluated during the preparation of a monograph for the Medical Internal Radiation Dose (MIRD) Committee of the Society of Nuclear Medicine (Weber et al. 1989). The MIRD collection contains data for 242 radionuclides of interest to the medical community.

The ICRP38 and MIRD nuclear data libraries each consist of three data files. These triplets of files have the root name "ICRP38" or "MIRD" with extensions NDX, RAD, and BET. The file with extension NDX is an index file that serves as the entry point into the other two larger files. The file with extension RAD contains data on the unique or average energy and the intensity of each emitted radiation while the file with extension BET contains, for beta emitters, the beta spectra.

Overview

DCAL performs biokinetic and dosimetric calculations for the case of acute intake of a radionuclide by inhalation, ingestion, or injection into blood at a user-specified age. For the intake of the radionuclide, the user may compute either equivalent or absorbed (low and high LET) dose rates as a function of time following intake. Selection of the equivalent dose option allows the generation of a table of age-specific dose coefficients, i.e., committed equivalent doses to organs and committed effective doses per unit intake, such as those published in the ICRP's documents on doses to the public from intake of radionuclides (ICRP 1989, 1993, 1995a, 1995b, 1996).

In addition, DCAL includes the evaluation of dose rate resulting from exposure to radionuclides distributed in environmental media that is, distributed in an airborne cloud, in water, on the ground surface, or distributed to various depths in the soil. The computational module utilizes the photon and electron dosimetric data tabulated in Federal Guidance Report 12 (EPA 1993) to generate radionuclide specific coefficients

Dosimetric calculations proceed in three main steps: (1) Calculation of time-dependent activity of the parent radionuclide and any radioactive progeny present in anatomical regions (source regions) of the body, (2) Calculation of specific effective energies (SEE values) for specified source and target organs, and (3) Calculation of dose rates or equivalent dose rates, based on output generated in the first two steps. Dose coefficients may be computed after Step 3. A dose coefficient is an integrated organ dose or dose equivalent, or an effective dose per unit intake. The integration period is 50y for intake by the adult and to age 70 y for intake at a pre-adult age.

In its calculations of dose and risk, DCAL relies on libraries of biokinetic and dosimetric models, nuclear decay data, anatomic data, radiation risk models, survival data, cancer mortality and morbidity data, and other miscellaneous data as shown in Figure 3. These libraries of state-of-the-art models and data allow best available estimates of radiation dose and risk from internally deposited radionuclides, with minimal input by the user.

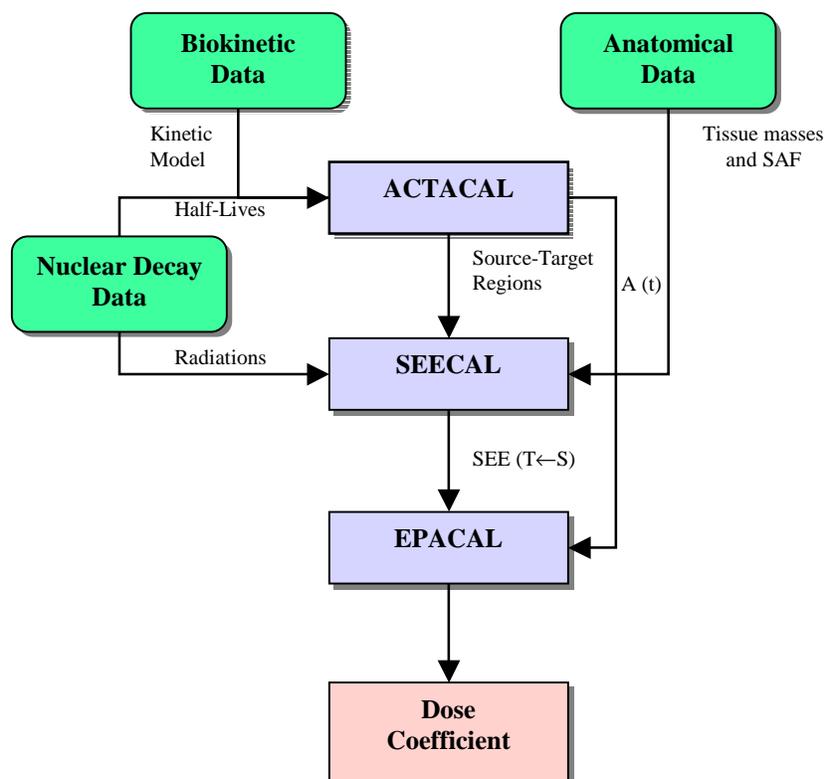


Figure 3. Schematic of DCAL system – adopted from ORNL/TM-2001/190 (Eckerman et al. 2001)

DCAL's main menu is organized in two parts (See table 2 below). The upper portion of the menu, denoted in blue, invokes the computational modules for calculation of dose and risk coefficients. The lower portion, denoted in green, includes a number of utilities and the batch calculation facility. A brief description of each module and utility found in DCAL's main menu is also provided in the table. Calculations must be carried out in a particular order and as they precede the selection bar will generally be positioned at the next step in the algorithm. Thus, for example, the calculation of a dose coefficient for the inhalation of ^3H vapor in the workplace would first proceed by invoking ACTACAL, then SEECAL, and EPACAL. The results of the calculation could be summarized by invoking the HTAB utility and viewed by selecting LIST.

External Dose Module

The DCAL system was developed largely to address the doses and risks resulting from the intake of radionuclides. However, the EXTCAL module has been integrated into DCAL to calculate the dose coefficients for external exposure to photons and electrons for submersion in contaminated air, immersion in contaminated water, and exposure to contaminated ground surfaces and volumes.

EXTCAL Calculations

To initiate calculations for an external dose coefficient, select EXTCAL from the DCAL's main menu. Following the credit display, the user will be prompted for specific information regarding the parameters of the external exposure (e.g. radionuclide, source media, distribution and depth). The results of these calculations will be contained in the work directory indicated at the bottom of the main menu, i.e., labeled by <F4> key. It should be noted that this module is only available to the nuclear decay data libraries that were provided with the software. Details on incorporating other radionuclides into these libraries will be addressed by the working group at a later date.

Table 2. DCAL's main menu and brief descriptions of the individual modules or utilities-adopted from ORNL/TM-2001/190 (Eckerman et al. 2001)

Module or Utility	Purpose
ACTACAL	The starting point for all calculations involving the intake of a radionuclide. The module calculates the activity as a function of time residing within organs and tissues of the body given a unit intake at an indicated age.
SEECAL	Computes the dose rate in the target tissues per unit activity residing in the source organs, the SEE values, for the radionuclides identified by ACTACAL and reference individuals of ages 0-, 1-, 5-, 10-, 15 years, and the adult as needed for the commitment period
EPACAL	Calculates the dose rate in the target organs given the activity as a function of time generated by ACTACAL and the SEE values for the source target pairs computed by SEECAL. The committed dose is computed as the time integral of the dose rate
RISKCAL	Computes the health risk given the absorbed dose rate files for the reference individual, assuming an age-dependant intake function. External exposures are age invariant.
EXTCAL	This computational module computes the external dose coefficient for a user-provided radionuclide and environmental medium.
LIST	Utility to view the output files in the indicated work directory.
PLOTORG	This utility provides a graphical display of the activity or dose rate data. The activity of each member of the decay chain is displayed.
HTAB	This utility generates a tabulation of the committed dose for the target organs for each reference individual considered in the calculation.
MODDEF	This utility facilitates the creation of systemic biokinetic data files and of absorption from the gastrointestinal tract, the f_1 parameter.
MRTVIEW	This utility computes the age and gender specific force of mortality for naturally occurring cancers based on the US 1990 decennial mortality data (years 1989 – 1991).
DBATCH	This is DCAL's batch calculation facility
HELP	This menu item provides the user to various data files and help files regarding the DCAL system.

Analysis of Dose Coefficient Methodology

Internal dose coefficients for inhalation and ingestion scenarios were determined using the methodology described above for 5 of the 86 radionuclides identified by the DC Working Group. The five radionuclides selected for this report are presented in Table 3 as well as the source of the nuclear decay data sets. Source information can be found and is documented in the journal *Nuclear Data Sheets*.

Table 3. Radionuclides included for evaluation in current study.
Ingestion and inhalation of particulates

Atomic Number	Nuclide	Physical Half-Life	Source of the Nuclear Decay Data Set
26	Fe-61	5.98m	ENSDF
51	Sb-113	6.67m	ENSDF
55	Cs-123	5.94m	ENSDF
56	Ba-125	3.5m	ENSDF
62	Sm-139	2.57m	ENSDF

The NUBASE database (Audi et al. 1997) was utilized for these selected radionuclides to note primary and secondary decay chains, as well as, the status of an ENSDF for a particular radionuclide. This essentially allowed project personnel to identify “exotic” decay chains with complete decay data sets available for dose calculation purposes. It also allowed personnel to compare the information in the ENSDF database to another database to identify missing or inaccurate information in the decay data sets. Previous investigators (Endo and Yamaguchi 2001) effectively utilized this database to reexamine and update the decay data sets for the 817 radionuclides that are listed in ICRP publication 38, 6 additional isomers, and 162 additional radionuclides with half-lives ≥ 10 min. not listed in ICRP #38.

The effective dose coefficients for workers for the five radionuclides are presented in Table 4. The results are presented in the same format as ICRP publications 68 and 72. It should be noted that the ICRP will report results to two significant figures and table 4 contains the output results from DCAL which are given in three significant figures. As shown in Table 4, dose coefficients for inhalation of $1\mu\text{m}$ and $5\mu\text{m}$ particulates and ingestion are presented along with the f_1 values and absorption types.

Table 4. Effective dose coefficients for Workers
Ingestion and inhalation of particulates

Nuclide	t _{1/2}	Type	Effective dose coefficient (Sv Bq ⁻¹)				
			f ₁	Inhalation, e _{inh} (50)		Ingestion	
				1µmAMAD	5µmAMAD	f ₁	e _{ing} (50)
Iron							
Fe-61	5.98m	F	0.1	6.77E-12	1.14E-11	0.1	2.26E-11
		M	0.1	8.74E-12	1.44E-11		
		S	0.1	8.96E-12	1.48E-11		
Antimony							
Sb-113	6.67m	F	0.1	5.62E-12	9.54E-12	0.1	1.68E-11
		M	0.01	7.41E-12	1.22E-11		
		S	0.1	7.65E-12	1.26E-11		
Cesium							
Cs-123	5.94m	F	1.0	5.62E-12	9.32E-12	1.0	1.96E-11
		M	1.0	7.29E-12	1.19E-11		
		S	1.0	7.47E-12	1.21E-11		
Barium							
Ba-125	3.5m	F	0.1	4.91E-12	7.67E-12	0.1	7.41E-12
		M	0.1	6.33E-12	9.68E-12		
		S	0.1	6.49E-12	9.90E-12		
Samarium							
Sm-139	2.57m	F	5E-4	3.00E-12	4.98E-12	5E-4	1.01E-11
		M	5E-4	3.44E-12	5.69E-12		
		S	5E-4	3.49E-12	5.77E-12		

Calculating external dose coefficients for environmental exposure scenarios for the 5 selected radionuclides were not performed at this time. The software version of DCAL did allow for these calculations to occur within the framework of the EXTCAL module but only for those radionuclides identified in FGR 13. In other words, these calculations could only be performed on those radionuclides included in the nuclear decay data libraries that came with the software package. The user's manual did provide instructions on how to calculate an external dose coefficient for radionuclides not listed in the nuclear decay data libraries once the appropriate data files were built (e.g. ICRP38.NDX, ICRP38.BET, and ICRP38.RAD). Not included in this version of the software package was the example file EXTLIST.INP, which would allow the user to setup a template in order to carry out these calculations.

Table 5 is a biokinetic comparison of current ICRP recommendations and the output from DCAL utilizing the ICRP 68 biokinetic subdirectory default parameters. Inhalation and ingestion f₁ values and absorption types are presented for the selected elements presented in this report. As seen from the table several f₁ values do not correspond to current ICRP recommendations. It is noted that DCAL does provide the

user with the flexibility to define or update existing biokinetic subdirectories and utilize these parameters during calculations.

Table 5. Biokinetic comparison of f_1 values: ICRP versus DCAL output (bio\i68).

Nuclide	Publication	Inhalation			Ingestion	
		Type	ICRP	DCAL	ICRP	DCAL
Iron	69	F	0.1	0.1	0.1	0.1
		M	0.1	0.1		
		S	0.01	0.1		
Antimony	69	F	0.1	0.1	0.1	0.1
		M	0.01	0.01		
		S	0.01	0.1		
Cesium	56	F	1.0	1.0	1.0	1.0
		M	0.1	1.0		
		S	0.01	1.0		
Barium	67	F	0.2	0.1	0.2	0.1
		M	0.1	0.1		
		S	0.01	0.1		
Samarium	30	All	5.0E-4	5.0E-4	5.0E-4	5.04E-4

Figures 4 and 5 present data for ^{123}Cs from the ENSDF and NUBASE databases, respectively. They are included in this report to illustrate the need to implement quality control measures to ensure the accuracy and credibility of the data. It is noted from the figures that both ENSDF and NUBASE report different half-life and Q values for the same radionuclide. These values are particularly important because EDISTR uses the Q-value to compute the energy of an alpha particle and the end point energy of a beta particle. It uses the half-life value to produce decay chain data as well as a reference to judge whether a daughter product is radioactive. Previous work (Endo and Yamaguchi, 2001) updated an ENSDF decay data sets when the values of half-life, branching fraction, excitation energy, and total decay energy differed by more than 1% from those of NUBASE.

^{123}Xe	^{123}Cs Electron Capture Decay 1981Ma01	199402
Published: 1993 Nuclear Data Sheets.		
^{123}Cs Parent: $E_x=0.0$; $J^\pi=1/2^+$; $T_{1/2}=5.94$ min 4 ; $Q_{g.s.\rightarrow g.s.}=4210$ 50 ; $\% \epsilon=100$		
History		
Type	Author	Citation
Full evaluation	S. Ohya and T. Tamura	Nuclear Data Sheets 70,531 (1993) 1-Jan-1993

Figure 4. ENSDF heading for Cs-123 EC decay data set. Note $t_{1/2}$ value of 5.94 min and a $Q_{g.s.\rightarrow g.s.}$ value of 4210 KeV.

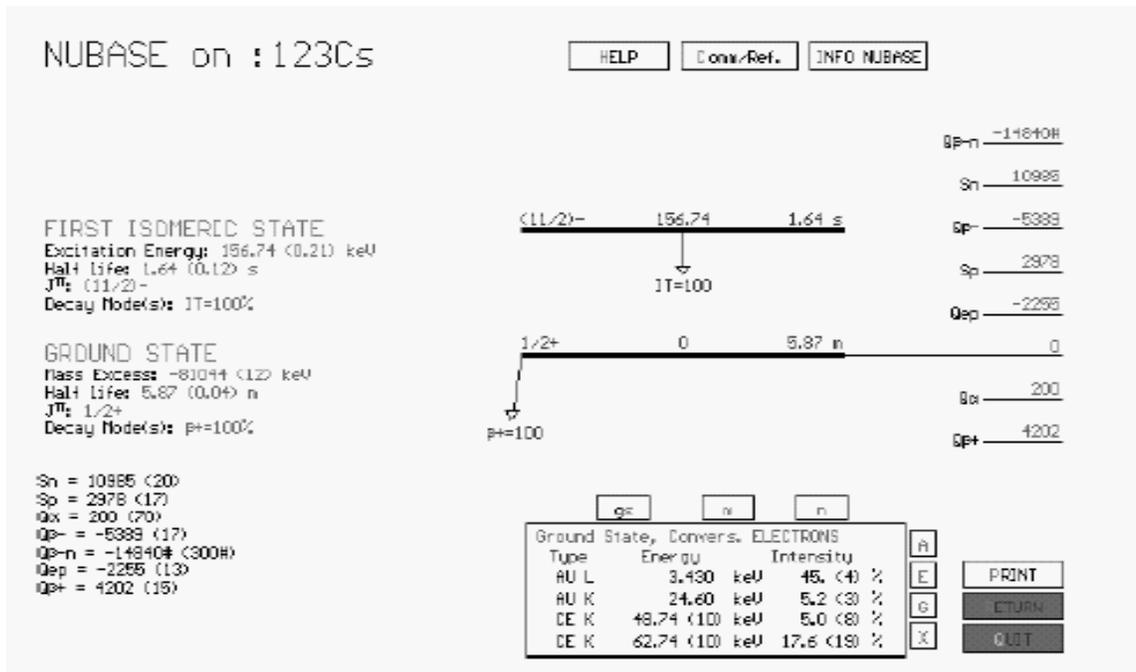


Figure 5. Radionuclide information sheet for Cs-123 from NUBASE. Note $t_{1/2}$ value of 5.87 min and a $Q_{g.s. \rightarrow g.s.}$ value of 4202 KeV. The reference (under Comm/Ref.) given for this radionuclide was the 1994 ENSDF (see fig. 2.).

It is interesting to note that the NUBASE information sheet for this particular radionuclide sites ENSDF as the reference source and yet reports a different half-life and Q value. In this particular case a more thorough evaluation of the literature would be required before a dose coefficient could be reported.

Conclusions

In general, the methodology to calculate an internal dose coefficient for radionuclides not listed in ICRP publications is in place at this time. There are however, several issues that need to be addressed by the working group before specific responsibilities are assigned to members. These issues include:

- The Y2K problem associated with the ENSDF and the ability of EDISTR to generate a beta spectrum;
- The use of the NUBASE or a similar database to confirm basic nuclear decay properties found in an ENSDF;
- Updating or creating an ENSDF to resolve conflicting reference information or missing daughter information;
- Updating or creating biokinetic files specific to the goals of the group;
- Establish guidelines for personnel as to what constitutes a significant dosimetric branching ratio;
- Complete the development of the methodology needed to calculate external dose coefficients.

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Appendix A

Installation Procedure

The reader should note that it has been assumed that all the codes are on one disk for these instructions.

1. DCAL
 - a. Insert CD
 - b. Open DOS window
 - c. Log into CD-ROM drive via the DOS prompt
 - i. Note: The command to log into the (D:) drive from the C:\ prompt is **C:\d:**
 - d. Once your logged into the (D:) drive type the following route and command:
 - i. **D:\Codes\Dcal\install**
 - ii. Follow the on screen directions.
 - e. Rename the following files in DCAL
 - i. C:\DCAL\DAT\NUC\ICRP38.RAD to ZICRP38.RAD
 - ii. C:\DCAL\DAT\NUC\ICRP38.BET to ZICRP38.BET
 - iii. C:\DCAL\DAT\NUC\ICRP38.NDX to ZICRP38.NDX
 - iv. You can use any variable you want as long as you can identify the file.
2. Ultra Edit – Note that Ultra Edit software is copyright protected. Trail versions of this software can be downloaded from <http://www.ultraedit.com>.
 - a. From the CD launch setup: **D:\Codes\Ultra Edit\setup**
 - b. Follow the on screen directions (English 32 bit)
 - c. Enter customer name.
 - d. Enter authorization code.
 - e. In Ultra Edit change/select the following settings
 - i. Advance—Configuration—Backup (select no backup)
 - ii. View—Display Ruler
3. EDISTR
 - a. Using the DOS prompt make a directory called DCF
 - i. **C:\md DCF**
 - b. Copy **D:\Codes\EDISTR\DCF** and paste it into **C:\DCF**
 - i. Once you have pasted the file, unzip it.
 - c. From the DOS prompt run the following two batch files to rename the files in EDISTR.
 - i. C:\edistr
 - ii. **C:\edistr name.bat**
 - iii. **C:\edistr runme.bat**
 - d. Edit the EDISTR batch file using Ultra Edit
 - i. C:\
 - ii. edit edistr.bat

- iii. Add two colons (::) to the beginning of the following lines.
 - 1. convert.exe
 - 2. count.exe
 - 3. index.exe
 - 4. copy1.exe
 - 5. betaspec.exe
- iv. Then save the changes to the file.
- e. Add the DECDAT folder on the DCAL CD to C:\EDISTR
 - i. Change the properties of **C:\edistr\decdat\inputdat.dat**
 - 1. Deselect the read only attribute
 - ii. Copy the inputdat file and rename it to inputdat.example
 - iii. Using Ultra Edit open the inputdat.dat file to create a working template (see example below)

Input data file for BUILDIT.BAS

Ac-228 6.15h B- ..\output\dAc228

Ac-223 2.10m A ..\output\dAc223

- iv. Note spacing requirements from inputdat.example
 - f. In EDISTR create an INPUT folder for ENSDF data downloads
 - i. C:\edistr\input
4. Decy_mode code
- a. From CD copy and paste to desktop or other appropriate location
 - b. Double click on icon to launch code
 - c. Follow the on screen directions

Appendix B - DC Working Group Procedure (Arndt and Campbell, 2002)

Procedure

- I. ENSDF: Nuclide information is obtained from the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory. NNDC maintains a database with nuclide information. The radionuclide information will be obtained using the Evaluated Nuclear Structure Data File (ENSDF).
 - A. Using the a web browser of choice access the Brookhaven website at <http://www.nndc.bnl.gov>
 - B. Click on the Evaluated Nuclear Structure Data File (ENSDF) link which is located in the “Data Retrievals, Data Files, Manuals, Proceedings, Programs, & Reports” section.
 - C. Click on the Quick Retrieval link to be taken to that area of the ENSDF page or scroll down to the appropriate location.
 - D. Enter the radionuclide of interest’s progeny (Ex. ^3He would be entered if the user was interested in ^3H) in the Quick Retrieval entry location.
 - i. Follow the quick retrieval instructions for the nuclide entry format.
 - E. Submit the request by clicking on the “Submit the request button” This will take the user to the nuclide retrieval page.
 - F. Click on the “Tables” link on the retrieval page. This will take the user to the data page.
 - G. Under the “Contents” heading on the data page click on the drop list button that will initially say “Adopted Levels.”
 - i. Activate the nuclide of interest decay mode. (Ex. For ^3He drop list 3H B- Decay Mode should be activated)
 - H. Under the “Download” heading click on the “ENSDF file for this data set”
 - I. Save this file to the input folder of EDISTR as the default file type which is *.ENS.
 - J. Repeat Steps G-I for nuclides that have more than one decay mode.
- II. EDISTR: The EDISTR program extracts and formats the data from the ENSDF file
 - A. Install EDISTR
 - i. Using the DOS prompt make a directory called DCF
 1. C:\md DCF
 - ii. Copy D:\Codes\EDISTR\DCF and paste it into C:\DCF
 1. Once you have pasted the file, unzip it.
 - iii. From the DOS prompt run the following two batch files to rename the files for edistr.
 1. C:\edistr
 2. C:\edistr>runme.bat
 3. C:\edistr>name.bat
 - iv. Edit the EDISTR batch file using a text editor such as Ultra Edit or the DOS edit function
 1. C:\ edit edistr.bat
 2. Add two colons (::) to the beginning of the following lines

- a. Convert.exe
 - b. Count.exe
 - c. Index.exe
 - d. Copy1.exe
 - e. Betaspec.exe
3. Then save the changes to the file
- B. Open the *.ENS file in a text editor such as Ultraedit and check the date of the ENSDF file. The date is in the format YYYYMM. The date needs to be 2001 or later. If the date needs to be changed, change the YYYY to 2001 change the MM to the year of the original date (ex 199502 should be changed to 200195)
 - C. If there were more than one decay mode, the ENS files need to be combined into one.
 - i. Copy and paste all of one into the other. There must be a blank line between the files. At the end of the entire file there must be two blank lines.
 - D. Copy the edited *.ENS file from the input folder into the edistr root folder.
 - E. Rename the copied ENS file as Input.ens
 - F. Run edistr from a Dos prompt this gives you a file called decay in the output folder of edistr
 - i. C:\edistr
 - G. Check to see if edistr ran properly by checking the decay file
 - H. Rename the decay file for record keeping. The new name should not exceed seven characters (Ex decay.out => decayH3).
 - I. Repeat steps B-H for all nuclides in the decay chain of interest.
- III. DECDAT: Decdat is a folder that contains some programs that prepare input files for DCAL.
- A. Install DECDAT
 - i. Copy the decdat folder from the DCAL CD to the edistr folder
 - ii. Be sure to deactivate the read only attribute of the folder.
 - B. Copy InputDat.dat to create a template InputDat.dat.tmp. The template is needed in order to conform to the spacing requirements.
 - C. Using a text editor such as Ultraedit open InputDat.dat.
 - i. Change the nuclide name to the one of interest in the format ZZ-AAA (note this input must be in the first seven columns of Inputdat)
 - ii. Change the half-life formatted with no space between the time and units.
 - iii. Change the decay mode to the corresponding decay mode B-, EC, A, B+
 - iv. Change the decay file reference
 1. This reference must start in column 26
 2. This reference must not exceed 18 characters
 3. ..\output\decayH3
 - D. InputDat needs to have at least three nuclide entries in order for buildem to work properly.
 - E. From a DOS prompt run Buildem
 - i. C:\edistr\decdat>buildem
 - ii. One can also run buildem through window by clicking on the buildem executable. By running buildem through windows the user is not notified if the program ended normally.

- iii. This program produces three files: Decdata.BET, Decdata.idx, and Decdata.Rad
- F. Open the three files created after running buildem and check to see if the daughter information and decay information is correct.
- G. From a Dos prompt run Chkdaus
 - i. C:\edistr\decdat>chkdaus
 - ii. One can also run Chkdaus through window by clicking on the buildem executable. By running Chkdaus through windows the user is not notified if the program ended normally.
 - iii. This program checks to see if all of the daughters in the chain of interest are included in the *.idx file.
 - iv. If there is notice given that there are daughters are missing return to ENSDF and retrieve the appropriate daughters and/or check to see if there is a mistake in the original ENSDF file.
- H. From a Dos Prompt run Sortind
 - i. C:\edistr\decdat>sortind
 - ii. One can also run Sortind through window by clicking on the buildem executable. By running Sortind through windows the user is not notified if the program ended normally
 - iii. This program sorts the idx file nuclides alphabetically and by mass.
- I. From a DOS prompt run ToIndx
 - i. C:\edistr\decdat>toindx
 - ii. One can also run ToIndx through window by clicking on the buildem executable. By running Toindx through windows the user is not notified if the program ended normally
 - iii. This program converts the idx file to a *.ndx file for DCAL
 - iv. Open the *.ndx file and check to see if all of the daughters are referenced correctly. If there is a daughter is missing 999 will be in the place of the daughter reference. One can return to ENSDF file and repeat the above steps or one can manually delete the 999s and replace with 0s. If one replaces the 999s with 0s, be sure that spacing requirements are followed.