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Code for Internal Dosimetry (CINDY) Part 1: Conceptual Representation

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CODE FOR INTERNAL DOSIMETRY (CINDY)
PART 1: CONCEPTUAL REPRESENTATION

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Pacific Northwest Laboratory
Richland, Washington 99352

DOCUMENTATION STATUS

The complete documentation package for the CINDY computer code will consist of the following parts:

Part 1: Conceptual Representation

Part 2: User's Guide

Part 3: Advanced User's Guide

Parts 1 and 2 have been prepared for the initial release of the CINDY code. This report (Part 1) describes the code as it is expected to be configured when all capabilities have been implemented. In some cases described features are not yet implemented; these cases are indicated in the text. However, the report should provide useful information in understanding and evaluating the current version of CINDY. As additional models and methods are identified for inclusion in the CINDY program, updates to this set of reports will be prepared and distributed. Comments and suggestions regarding documentation for the CINDY code are appreciated. This initial version of the documentation and the CINDY code have undergone extensive field testing and completion of a Final Internal Development Review (FIDR) with resolution of all comments. The Advanced User's Guide (Part 3) is planned to be made available during 1991.

EXECUTIVE SUMMARY

The computer code CINDY (Computerized Internal Dosimetry Software Package) has been developed by Pacific Northwest Laboratory to address the Department of Energy (DOE) Order 5480.11 by providing the capabilities to calculate organ dose equivalents and effective dose equivalents using the approach contained in International Commission on Radiological Protection (ICRP) Publication 30. The code assists in the interpretation of bioassay data, the evaluation of committed and calendar-year doses from intake or bioassay measurement data, and the preparation of reports, consistent with revised DOE orders. The code is easy to use and is generally applicable to DOE sites. Flexible biokinetics models are used to determine organ doses for annual, 50-year, calendar-year, or any other time-point dose necessary for chronic or acute intakes.

The CINDY code is an interactive computer program that prompts the user to describe the cases to be analyzed and calculates the necessary results for the type of analysis being performed. Four types of analyses may be specified:

- **Intake Assessment Mode** - estimate intake based on bioassay data using weighted or unweighted least-squares regression between measured and expected bioassay values calculated, based on reference man or other models
- **Dose Assessment Mode: Specified Time Periods** - estimate organ dose equivalents and effective dose equivalents for specified time periods and committed effective dose equivalents for given intakes
- **Dose Assessment Mode: Calendar Year Doses** - estimate organ and effective dose equivalents for the present calendar year and future annual increments for given intakes
- **Bioassay Projection Mode** - estimate organ burdens and urinary and fecal excretion rates from given intakes.

Evaluation of radiation doses and excretion rates involves numerical solution of the differential equations describing intake of activity (by inhalation, ingestion, absorption, or wounds), metabolism and translocation (involving various body organs and systems), and elimination from the body. The equations programmed are those recommended by the ICRP and NCRP and other

closely related or slightly modified versions of the same models. CINDY obtains precise solutions to these differential equations used to determine radionuclide amounts in model compartments over time. The heart of the CINDY package is the numerical solver used to evaluate the intake, metabolism, and excretion of radionuclides. Differential equations are solved using the LSODES package (from the ODEPACK collection developed at Lawrence Livermore National Laboratory).

Results of the analyses can be displayed on the screen in tabular or graphical form, tables and graphs can be printed, and data files and reports can be saved for later retrieval. All saved files (input and output) are marked by a unique identifier for the subject individual, allowing easy access to the necessary information for a given analysis.

This report is the first part of a three-part series documenting the CINDY computer code, and describes the general features and conceptual models implemented in the code. The user information is presented in part two (User's Guide) and the technical details of the program for advanced users are documented in part three (Advanced User's Guide).

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Although the contributions of these individuals is much appreciated, the authors take sole responsibility for the accuracy and quality of these documents.

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1.0 INTRODUCTION

The computer code CINDY (Code for Internal Dosimetry Software) addresses the Department of Energy (DOE) Order 5480.11 by providing the capabilities to calculate organ dose equivalents and effective dose equivalents using the approach in International Commission on Radiological Protection (ICRP) Publication 3D. Flexible biokinetic models are used to determine organ doses for annual, 50-year, calendar-year, or any other time-point dose necessary for chronic or acute intakes. The doses are expressed as organ dose equivalents, effective dose equivalents or committed dose equivalents, as appropriate to the specific calculation being performed. The code is developed to assist in the interpretation of bioassay data, evaluation of committed and calendar-year doses from intake or bioassay measurement data, and preparation of reports consistent with revised DOE orders. The code is easy to use and is generally applicable to DOE sites.

The CINDY software package has been developed as a tool to aid in the evaluation of internal exposures of workers. As with any computer program, there are limitations that must be recognized as to applicability and use of the various features provided. The code has been designed for use by knowledgeable health physicists familiar with the operation of a bioassay program for radiation worker exposures. The user is responsible for the quality and accuracy of the input information, and for interpretation of the results provided in the output reports. The results generated by the CINDY code are not intended to be used blindly without scrutiny.

The basis for the internal dosimetry analyses performed by the CINDY code is the set of metabolic models recommended by the ICRP. The ICRP models were developed to describe the dose received over a 50-year period. As such, they may not accurately represent the amount of activity in the body (or systemic organs) at shorter time periods. The ICRP was concerned only with the time integral of activity, and not with activity present at specific time points. The models are used in the CINDY code because better models are not generally available (with a few noted exceptions). In an attempt to add flexibility in implementing the models, the user is given the option of changing metabolic

model parameters defined by the ICRP. This will allow a user to tailor models to specific individual and bioassay data histories. However, the user is cautioned against using this option except for special cases that have well defined histories and data for the individual in question. Changing of biokinetic parameters to fit the bioassay data does not mean that the estimated intakes are closer to the truth. There is much uncertainty in the data, models, and parameters as applied to any individual.

This part of the CINDY software documentation package describes the dosimetry concepts and design features implemented by CINDY. Part 2 is the user's guide to operation of the code, and Part 3 is the advanced user's guide.

This report contains four main sections (in addition to the introduction and reference sections) plus three appendixes. A general overview of the concepts and methodology used in the CINDY code is given in Section 2.0. Section 3.0 presents the design features used in the development of the code, modified to reflect the actual implementation of the features. Section 4.0 describes the biokinetic models used to evaluate uptake, retention, and elimination of radionuclides in the body. Section 5.0 presents details of dosimetric evaluations. Appendix A contains a glossary of terms used in this report. Listings of the metabolic data contained in the CINDY data base are given in Appendix B, and a summary of the method used to solve the differential equation sets is given in Appendix C.

2.0 GENERAL CONCEPTS AND METHODOLOGY

The CINDY code is compatible with requirements of DOE Order 5480.11 (DOE 1988) for internal dosimetry evaluations. Internal dosimetry concepts implemented in CINDY are consistent with recommendations of the National Council on Radiation Protection and Measurements (NCRP) Reports 84 (NCRP 1985) and 87 (NCRP 1987) and the recommendations of the ICRP (1977, 1979-1982, 1986, 1988). The following paragraphs describe the dosimetry concepts and methods used in the CINDY code.

Radionuclides may enter internal organs and tissues of the body through several intake modes: inhalation, ingestion, absorption, and injection. Inhaled radionuclides are deposited in the respiratory tract according to particle size and breathing characteristics. Deposited material may be translocated to other sites in the respiratory tract or elsewhere in the body by mechanical and chemical processes that are dependent on the physicochemical characteristics of the material. Elimination of material from the respiratory tract may take place by mechanical clearance to the gastrointestinal (GI) tract, absorption into systemic circulation, deposition in lymph nodes, and radioactive decay. The retention of material in the respiratory tract varies with region and material. The ICRP has established three general lung retention categories: Class D, in which retention half-times are on the order of days; Class W, in which retention half-times are on the order of weeks; and Class Y, wherein material is assumed to be retained for years.

Ingested material is transported through the gastrointestinal tract. During this process some of the material may be absorbed into systemic circulation. Material that is not absorbed passes through the GI tract and is eliminated from the body by fecal excretion.

Absorbed or injected radionuclides are initially deposited into subcutaneous tissue and blood. This material may be immediately available for uptake into the systemic circulation; however, some of the deposited material may remain at the point of entry for some time before it is absorbed. Also, some of the injected material may be taken up and retained by regional lymph nodes. Material that enters into systemic circulation may be deposited in and

retained by various organs and tissues, depending on the metabolic characteristics of the material.

Elimination of radionuclides from the body occurs either through radioactive decay or by excretion. Fecal excretion contains radionuclides that are ingested but not absorbed in the gastrointestinal tract plus absorbed activity that has been metabolized and is present in bile. Urinary excretion contains radionuclides absorbed in the gastrointestinal tract (usually the stomach or small intestine) and transferred through the systemic fluids to the kidney and bladder. Material deposited in other organs of the body may eventually be transferred back to the systemic fluids and eliminated in the urine or feces.

The processes of uptake and deposition are assumed to result in the uniform distribution of activity in specified tissues called source organs. Radiations emitted by radionuclides in source organs may deposit energy in several organs or tissues of interest. These organs and tissues, called target organs, are usually specified as entire organs, but, in particular instances, may consist of specified groups of radiosensitive cells within an organ, for example, the cells on the surfaces of bones. The CINDY code contains a library of the specific effective energy absorbed in the target organs for each nuclear transformation occurring in a source organ.

Biokinetic models described by the ICRP in Publication 30 (ICRP 1979) and endorsed by the NCRP in Report 84 (NCRP 1985) are provided as default models in the CINDY code. Separate models describe the deposition and transport of material in the respiratory tract, the GI tract, and the systemic organs. Specification of systemic excretion functions is also allowed.

The distribution and movement of radionuclides in the body is a very complex process. For computational purposes, the ICRP has modeled these processes using a series of interlinked compartments that represent the organs and tissues of the body into which the radionuclide may be deposited. With certain exceptions (e.g., alkaline earth radionuclides in bone and iodine in thyroid), the models were simplified by not considering the recycling of a radionuclide from a compartment back into systemic circulation. This is achieved by a careful choice of compartment parameters. Thus, although the compartments do not correspond directly to physiological processes, the

results of the model (insofar as they are intended to be used) are in good agreement with observed data (ICRP 1988).

The equations that describe the model can be solved for any radionuclide over a given period of time to determine the number of nuclear transformations that occur in the compartment. Excretion of the radionuclide from the body is also modeled as a compartment, and thus, equations are written to describe the quantity of the radionuclide present in excreta over a time period of interest. It should be noted that the original intention of the ICRP was to estimate the dose received over a 50-year time period following initial uptake. The requirements of DOE Order 5480.11 necessitate estimation of doses and distribution of activity in the body over much shorter time periods (i.e., days to a few years). The models recommended by ICRP may not be representative of the distribution in the body over the shorter time periods.

After a radionuclide has been taken into the body, it is assumed to be translocated to body fluids at a rate determined by the rate constants for the different compartments of initial deposition. Its translocation to the other organs and tissues of the body occurs via a transfer compartment, representative of systemic circulation. The transfer compartment is assumed to be cleared by first-order kinetics with a half-time of 6 hours unless specified otherwise in the metabolic data. Transformations occurring in the transfer compartment are assumed to be uniformly distributed throughout the body.

Computations can be based on user-supplied intake quantities (activity) or user-supplied bioassay measurement results. If the user provides bioassay measurement results, the code computes the magnitude of a radionuclide intake that yields bioassay values in best agreement with the actually observed values, based upon the assumed biokinetic models and parameters as well as other intake assumptions. Changes in models or model-parameter values, or other assumptions, can be made as appropriate to develop better agreement between the data and the assumed model. However, the user is cautioned that a better fit to observed data may not mean that the estimates of intake or dose are closer to the truth.

The conceptual basis for the calculation of the dose equivalent from internally deposited radionuclides is provided by ICRP Publications 26 and 30 (ICRP 1977; ICRP 1979) and endorsed by the NCRP in NCRP Report 84 (NCRP 1985). The general committed dose equivalent formula, as presented in ICRP 30 (1979) is:

$$H_{t,n}(T + S) = 1.6 \times 10^{-13} U_{t,S,n} * SEE(T + S)_n \times 10^3 \quad (2.1)$$

where $H_{t,n}(T + S)$ = committed dose to tissue, T, from disintegrations of radionuclide, n, in source tissue, S, over time period, t, in Sv,

$U_{t,S,n}$ = the number of transformations over the period, t, of the radionuclide, n, in the source organ, S,

$SEE(T + S)_n$ = the specific effective energy for the radionuclide, n, suitably modified by the quality factor, absorbed in the target tissue, T, from each of the transformations of the radionuclide in source tissue, S, in MeV/g per transformation,

1.6×10^{-13} = the number of joules in 1 MeV,

10^3 = conversion factor from g^{-1} to kg^{-1} .

(Recall that a Sv is equivalent to energy deposition at the rate of 1 joule per kg suitably modified by dimensionless quality factors contained in SEE values.)

The number of radionuclide transformations (U) are calculated for applicable source organs (compartments) over the specified periods of interest using the biokinetic compartment model assumed to apply for the case. The SEE factors are then applied to the calculated U values to determine dose equivalent to target tissues. The total dose equivalent to a tissue is calculated as the sum of contributions from all source organs. The SEE values used by the CINOY program were obtained from Oak Ridge National Laboratory (ORNL) on magnetic tape. The values are specifically based on organ size data provided for Reference Man (ICRP 23 1975).

Assessment of dose equivalence to target organs enables an evaluation of compliance with nonstochastic occupational dose limits in DOE 5480.11.

Nonstochastic dose limits are intended to protect the worker from receiving internal doses to organs in excess of threshold values for deleterious effects. DOE 5480.11 also prescribes occupational dose equivalent limits for effective dose equivalent based on consideration of stochastic risks, that is, malignant and hereditary disease for which the probability of the effect occurring is considered to be a function of the dose equivalent.

The effective dose equivalent is the weighted sum of organ dose equivalents calculated using the formula:

$$H_E = \sum_T w_T H_{t,T} \quad (2.2)$$

where w_T is the weighting factor for target tissue T based on the proportion of risk (for cancer and hereditary defects) from uniform exposure of the whole body that is attributable to the organ, and $H_{t,T}$ is the dose equivalent for organ T over time period t. The target organ dose equivalents are weighted and summed over organs using weights indicated in Table 2.1.

TABLE 2.1. Organ Weighting Factors

<u>Organ or Tissues</u>	<u>Weighting Factor</u>
Gonads	0.25
Breasts	0.15
Red bone marrow	0.12
Lungs	0.12
Thyroid	0.03
Bone surfaces	0.03
Remainder ^(a)	0.30

(a) "Remainder" means the five other organs or tissue with the highest dose (e.g., liver, kidney, spleen, thymus, adrenal, pancreas, stomach, small intestine, upper large intestine, or lower large intestine). The weighting factor for each remainder organ or tissue is 0.06. The extremities, skin, and lens of the eye are excluded from the "remainder" organs or tissue for assessment of effective dose equivalent.

3.0 CINDY DESIGN FEATURES

This section describes the operational design features of the CINDY code. The objective for the code is to provide a tool for use by internal dosimetrists at DOE facilities for assessing occupational internal exposure cases and designing bioassay monitoring programs. A basic design assumption is that the code will be used under the direction of a competent professional internal dosimetrist. The CINDY code is only intended to provide information to aid the dosimetrist in evaluating possible exposures and dose; it is not intended that the results will be used blindly without scrutiny.

It is recognized that ongoing internal dosimetry programs at DOE facilities have been developed in response to particular needs of the facility. Thus, each facility has need for particular features in an internal dosimetry code. In recognition of this, CINDY incorporates features that enable the code to be adapted to a range of special user needs and applications; these features are discussed in more detail in Section 3.5 below.

3.1 OPERATING MODES

CINDY is an interactive program that prompts the user to describe the cases to be analyzed and calculates the necessary results for the type of analysis being performed. Four modes of operation may be specified:

- **Intake Assessment Mode** - estimates intakes based on bioassay data using weighted or unweighted least-squares regression between measured and expected bioassay values calculated, based on Reference Man or other models
- **Dose Assessment Mode: Specified Time Periods** - estimate organ dose equivalents and effective dose equivalents for specified time periods and committed effective dose equivalents for given intakes
- **Dose Assessment Mode: Calendar Year Doses** - estimate organ and effective dose equivalents for the present calendar year and future annual increments, for specified intakes
- **Bioassay Projection Mode** - estimates organ burdens and urinary and fecal excretion rates from given intakes.

The relationship between these modes is shown schematically in Figure 3.1. For example, evaluation of an internal exposure case might

FIGURE 3.1. CINDY Operating Modes

involve 1) the assessment of intake based on bioassay measurements performed after the intake (Intake Assessment Mode), 2) the calculation of the calendar year effective dose equivalent values for the intake (Dose Assessment Mode), and 3) the projection of expected bioassay results for future samples (Bioassay Projection Mode). The features of the code may also be exercised in a subject independent mode to allow calculation of dose factors (e.g., per unit intake) or for other analyses not tied to a specific individual.

The use of separate operating modes is intended to reduce the complexity of code runs. By allowing the user to select operating modes, only the required analyses will be evaluated. This is an important consideration because each mode involves a unique set of model solution times; selecting

operating modes will minimize the time taken by the code to perform calculations. Details of each of the operating modes are given in the following sections.

3.1.1 Intake Assessment Mode

The intake assessment mode involves estimation of the activity taken into the body by a specified mode (inhalation, ingestion, absorption, or wound), based on bioassay data for excretion rate or total activity in the body, lungs, or thyroid. For tritium the assessment is based on the concentration of tritium in the urine. The analysis involves estimation of expected bioassay values for a unit intake using the appropriate models. These unit intake function estimates are made at times corresponding to the times at which measurement data are provided. A statistical comparison is then made between the expected and measured values to provide an estimate of intake. Four methods are available in the CINDY program for estimation of the intake from bioassay data. All methods are based on the basic formula for weighted least-squares regression as follows.

$$I = \frac{\sum_{i=1}^n w_i R_i X_i}{\sum_{i=1}^n w_i R_i^2} \quad (3.1)$$

where I = estimated intake (pCi for acute intakes and pCi/d for chronic intakes)

X_i = bioassay measurement for the i th data point (pCi/d for excretion and pCi for retention)

R_i = fractional retention or excretion estimate (see Table 3.1 for units)

n = number of bioassay measurement points.

Units for the parameters in the formula are given in Table 3.1 for various analyses performed in the CINDY code.

TABLE 3.1. Typical Units for Parameters in Intake Estimate Analysis

<u>Calculation Description</u>	<u>Intake, I</u>	<u>Measurement, X_i</u>	<u>Unit Function, R_i</u>
Acute Intake:			
Excretion	pCi	pCi/d	1/d
Retention	pCi	pCi	-
Tritium excretion	pCi	pCi/L	1/L
Chronic Intake:			
Excretion	pCi/d	pCi/d	-
Retention	pCi/d	pCi	d
Tritium excretion	pCi/d	pCi/L	d/L

The four methods for intake estimation relate to four methods for defining the weighting factors, w_i . The methods can be summarized as follows:

1. Unweighted least-squares - The weighting factors are assumed to be constant and equal.
2. Ratio of the means - The weighting factors are assumed to be inversely proportional to the expected value (unit intake function).
3. Average of the slopes - The weighting factors are assumed to be inversely proportional to the square of the expected value.
4. User defined weights - The user supplies estimates of the inverse of the weighting factors.

Unweighted Least-Squares

The unweighted least-squares regression analysis is expressed by the following equation:

$$I = \frac{\sum_{i=1}^n X_i R_i}{\sum_{i=1}^n R_i^2} \quad (3.2)$$

where terms are as previously defined. This method may be used when all measurement values are expected to have similar accuracy and all are significantly above the detection limits of the measurement method.

Ratio of the Means

The ratio of the means method is based on the assumption that the variance of the expected value is proportional to the magnitude of the expected value. The weights are expressed as follows:

$$w_i = \frac{1}{k \ I \ R_i} \quad (3.3)$$

where k is a constant of proportionality. Substitution of Equation (3.3) into Equation (3.1) results in the following expression for the intake estimate (Draper and Smith 1981):

$$I = \frac{\sum_{i=1}^n X_i}{\sum_{i=1}^n R_i} \quad (3.4)$$

As can be seen from this expression, the intake estimate is just the ratio of the sum of the measured values to the sum of the unit intake function values. This is equivalent to the ratio of the means of the measured values and the unit intake function values (proportional to the expected values), hence, the name "ratio of the means" method. Note also that from Equation (3.4), the sum of the measured values is equal to the sum of the expected values:

$$\sum_{i=1}^n X_i = \sum_{i=1}^n I \ R_i \quad (3.5)$$

This method is appropriate when the error of the measurement is expected to be proportional to the expected value.

Average of the Slopes

The average of the slopes method is derived from Equation (3.1) by defining the weights as inversely proportional to the square of the unit intake function values:

$$w_i = \frac{1}{k I^2 R_i^2} \quad (3.6)$$

The resulting expression for the intake estimate is as follows (Draper and Smith 1981):

$$I = \frac{\sum_{i=1}^n X_i / R_i}{n} \quad (3.7)$$

This expression gives the average of the ratios of measurement value to unit intake function value, which is equivalent to the average of the slopes of the equation

$$X_i = I R_i \quad (3.8)$$

This method is appropriate when the error of the measurement is expected to be proportional to the square of the expected value.

User-Defined Weights

The user has the option of identifying a statistical parameter with each measurement data point. The fourth method (user-defined weights) uses this statistical parameter as an inverse weight in Equation (3.1):

$$w_i = \frac{1}{V_i} \quad (3.9)$$

where V_i is the user-supplied statistical parameter value for bioassay measurement i . This method allows the user to implement almost any weighting

method desired based on predetermined weights. In evaluating the intake estimate using this method, only the data points having a defined value for V_i are used in the calculation.

Measurement Uncertainty Estimate

The expected values corresponding to each measurement can be estimated from the intake estimate and the unit intake factors using Equation (3.8). A measure of the uncertainty in the measurement values, relative to the model, is provided by the following expression based on the difference between the measured and expected values:

$$S_I = \frac{\left[\sum_{i=1}^n \frac{(X_i - I R_i)^2}{R_i} \right]^{1/2}}{(n-1) \sum_{i=1}^n R_i} \quad (3.10)$$

This uncertainty measure is used in the CINDY code to estimate an average intake when estimates are available from two or more bioassay sample types:

$$I_a = \frac{\sum_{i=1}^n I_i / S_i}{\sum_{i=1}^n 1 / S_i} \quad (3.11)$$

where I_a = intake estimate average for all bioassay measurement types

I_i = intake estimate based on data for bioassay type i

S_i = uncertainty measure for intake estimate for bioassay type i ,
dimensionless,

and units for I_a and I_i are as defined for I in Table 3.1. Bioassay excretion samples are taken to estimate the rate of elimination of radionuclides from the body following an intake. The desired form of the data is activity per day. However, actual data may come in a variety of forms and some analysis may be required by the dosimetrist. To aid in the analysis of the excretion

rate, the code will accept excretion data on total sample activity, sample activity concentration, period of collection, and volume or mass collected. For urinary measurements, the concentrations are expressed per unit volume, and for fecal measurements, the concentrations are expressed per mass. In the following discussion, volume units refer to urinary data and mass units refer to fecal data. The equations are identical for fecal excretion if mass units are substituted for volume units; handling of the analyses is the same for fecal and urinary cases. The actual activity units may be selected by the user (such as dpm, pCi, nCi, Bq, or μg). In the discussion below, units of dpm are used for illustration, although any other unit could be substituted. It should be emphasized that the user may override the analyses described here by supplying estimated 24-hour sample results and indicating a 24-hour sample period. Also, for tritium, no analyses of excretion rate are made because urine concentrations supplied by the user are used directly in the intake assessment (see metabolic models for tritium, Sections 4.6.5 and 4.7.4).

Two cases are considered in the CINDY code, depending on the form of the activity measurement (total sample activity or sample concentration). The period of collection is the most useful piece of information (in addition to the sample activity or concentration) because the period can be used directly to estimate the daily rate. The use of the input data is described for each of the two cases in the following sections.

3.1.1.1 Total Sample Activity Analysis

When the activity data is given in the form of total activity in the sample, information on the sample size and period of collection can be used to estimate the daily excretion. The estimation method to be used depends on availability of this additional data. The following possibilities exist.

Case 1A: Sampling period and volume unknown. The sample is assumed to represent 1 day of excretion and the intake rate is equal to the sample count:

$$\text{Intake Rate (dpm)} = \frac{(\text{Count, dpm})}{(1 \text{ day})} \quad (3.12)$$

Case 1B: Sampling period known (hours). The intake rate is given by

$$\text{Intake Rate (dpm/d)} = \frac{(\text{Count, dpm}) * (24 \text{ h/d})}{(\text{Period, h})} \quad (3.13)$$

Case 1C: Sample volume known and period unknown. The period can be estimated by comparison of the volume to the reference volume. The intake rate is, then,

$$\text{Intake Rate (dpm/d)} = \frac{(\text{Count, dpm}) * (\text{Ref. Vol., mL/d})}{(\text{Vol., mL})} \quad (3.14)$$

Case 1D: Sample volume and period known. Same as for case 1B (the volume is not used if the period is known).

3.1.1.2 Activity Concentration Analysis

For excretion data given as activity concentration, the following possibilities exist for availability of the sample volume and sampling time period.

Case 2A: Sample volume and period unknown. The intake rate is estimated assuming the measured concentration would continue for the entire day:

$$\text{Intake Rate (dpm/d)} = (\text{Count, dpm/mL}) * (\text{Ref. Vol., mL/d}) \quad (3.15)$$

Case 2B: Sample period known and volume unknown. The intake rate is estimated from the reference volume (the period is not used):

$$\text{Intake Rate (dpm/d)} = (\text{Count, dpm/mL}) * (\text{Ref. Vol., mL/d}) \quad (3.16)$$

Case 2C: Sample volume known and period unknown. The intake rate is estimated, assuming that the measured concentration would continue for the entire day (the volume is not used):

$$\text{Intake Rate (dpm/d)} = (\text{Count, dpm/mL}) * (\text{Ref. Vol., mL/d}) \quad (3.17)$$

Case 2D: Sample period and volume known. The intake rate is estimated as follows:

$$\text{Intake Rate (dpm/d)} = \frac{(\text{Count, dpm/mL}) * (\text{Vol., mL}) * (24 \text{ h/d})}{(\text{Period, h})} \quad (3.18)$$

As can be noted from the above cases and equations, the measured volumes and periods are used only when values are given for both parameters (volume and time period). The daily intake is evaluated using the same equation for cases 2A, 2B, and 2C.

In addition to the above evaluations, the CINDY code will perform a check of the input data and warn the user if the data are outside the normal range expected for sample volumes for the given sample period. Tests are performed using the supplied volume (mass) and time period (no tests are performed if volume and mass are not specified). When both volume and period are given, the volume is corrected to a daily volume by ratio of 24 hours to the given period:

$$\text{Daily Volume (mL)} = \frac{\text{Volume (mL)} * (24 \text{ h})}{(\text{Time Period, h})} \quad (3.19)$$

This daily volume is compared to the reference volume for the sex of the worker and the sample type. Default reference volumes are indicated in Table 3.2 (the user may change any of the reference volumes). If the estimated volume is not within 40% of the reference volume, a diagnostic warning is given to the user (interactively on the screen) stating that the given volume is suspect. The user has the option to change the input data, have the code correct the data, or add a comment to the data file about the data value. If the CINDY code is requested to correct the data, then the period of exposure will be modified by ratio of the volumes:

$$(\text{Corrected Time Period, h}) = \frac{24 \text{ h} * (\text{volume})}{(\text{reference volume})} \quad (3.20)$$

TABLE 3.2. Reference Volumes and Masses for Excretion Data

<u>Measurement Type</u>	<u>Worker Sex</u>	<u>Reference Amount</u>
Urinary	Male	1400 mL
	Female	1000 mL
Fecal	Male	135 g
	Female	110 g

If the time period is not given, the period is assumed to be 24 hours and the analysis is performed in the same manner. When the volume is not given, no tests on volume can be made.

3.1.2 Dose Assessment Mode: Specified Time Periods

CINDY allows for the estimation of dose received over any consistent set of intake modes and dose time periods. This type of analysis gives the user the ability to estimate doses for any commitment period, besides the standard 50-year time period on which many tabulations of dose factors are based. For example, a chronic intake for 7 months via ingestion could be analyzed to provide the dose received during the 7 months, the first year after start of exposure, and the total dose after each decade of exposure. If the input is supplied as a unit value (e.g., 1-pCi acute intake), the resulting values may be used as dose factors for hand calculations or for comparison with other compilations of dose factors.

The specific doses calculated for this mode of exposure are defined as follows:

- **Organ Dose Equivalent** - The dose equivalent received by an organ from the start of exposure to the time indicated.
- **Effective Dose Equivalent** - The effective dose equivalent received from the start of exposure to the time indicated. Note that the effective dose equivalent is calculated using the weighting factors given in ICRP Publication 26 (ICRP 1977), even though these factors are based on lifetime incidence of effects, while any time may be specified for the analysis.
- **Committed Effective Dose Equivalent** - The committed effective dose equivalent received in 50 years from the start of exposure.

3.1.3 Dose Assessment Mode: Calendar Year Doses

This assessment mode is intended to provide information in support of recordkeeping requirements of DOE Order 5480.11. For each intake defined for a given worker, the following doses are calculated. The code calculates the organ dose equivalent and effective dose equivalents on a calendar year basis. The dose in the first year may, therefore, be for a time period less than a full year. Before this assessment mode can be activated, the user must describe the intake by providing a quantitative estimate of the intake activity. The intake can be estimated by the user or the intake assessment mode can be used to provide a quantitative estimate based on bioassay measurement data.

3.1.4 Bioassay Projection Mode

This assessment mode is intended to provide estimates of the activity in specific organs (total body, lungs, and thyroid) and the activity excreted (fecal or urinary) at specified times following the intake. For tritium intakes, the concentration in urine is reported. The results can be compared with known bioassay data (or with anticipated future bioassay analyses). Results are reported in activity units specified by the user.

3.2 EXPOSURE SCENARIO OPTIONS

Options are available to the user to accommodate a range of potential internal exposure scenarios. It is intended that in most cases, the user will be able to define and run a complete internal exposure evaluation run in a single interactive session. However, for complicated exposure cases (those, for example, involving concurrent acute and chronic intakes), it may be necessary to evaluate the exposure as if it consisted of multiple concurrent exposures. CINDY provides the user with the following options for specifying an internal exposure case to be run:

- **Intake Mode(s)** - Intake (defined at a specific time) may consist of any combination of the following intake modes: inhalation, ingestion, and direct intake (absorption or injection). The user is required to specify the fraction of the total intake attributed to each intake mode.

- **Multiple Intakes** - If previous intakes have occurred, and are specified, the code considers the contribution of the previous intakes to the expected bioassay compartment values. [*** Multiple Intake option is not implemented in Version 1.0 of CINDY. ***]
- **Exposure Duration** - Intakes can be either, but not both, acute or chronic. For acute intakes, the initial deposition of the radionuclide at a body location is assumed to be instantaneous. For a chronic intake, the deposition is assumed to be constant and continuous over the specified time period. The code does not allow acute and chronic exposures to be evaluated for the same intake; however, it does allow the user to divide the intake into two concurrent intakes and specify input parameters for each one individually. For chronic intakes, the code will compute bioassay compartment and dose values beyond the termination of the chronic intake period. For example, a chronic intake could be defined for a 1-year exposure period, followed by several years in which no additional activity is taken in.
- **Contaminant Types** - The CINDY code allows the user to model an intake composed of radionuclides in different physical and chemical forms. For example, an intake may consist of a mixture of inhalation class-W and class-Y material at a specified ratio; or may consist of ingestion of a material with an insoluble and a soluble fraction (with appropriate uptake fractions, f_1 , defined for each). Intake mixtures can also consist of components that differ in particle size, or in specific biokinetic characteristics for which customized model parameter adjustments are made.

3.3 BIOKINETIC MODELING OPTIONS

Several models are included in CINDY to describe the biokinetic processes for intake, translocation, metabolism, and elimination of radionuclides. These models represent the deposition and translocation of the radionuclide in the respiratory tract, GI tract, systemic organs, and excretion compartments. The biokinetic models are maintained in a model library which accesses the specific models selected for a given analysis. Table 3.3 shows the biokinetic models currently maintained in the CINDY model library. These models, with the exception of the direct uptake model, the Jones model, and the Dunford and Johnson tritium model, are those recommended by the ICRP in Publications 30 (ICRP 1979-1980), 48 (ICRP 1986), and 54 (ICRP 1988). A complete description of these models, as implemented in the code, is provided in Section 4.0. (In the future, additional models that meet DOE criteria could be added to the library.)

TABLE 3.3. CINDY Model Library

Respiratory Tract Models

- ICRP 30 lung model

Gastrointestinal Tract Models

- ICRP 30 GI-tract model

Direct Uptake Model

- Multicompartment presystemic deposition model

Systemic Organ Models

- General ICRP model (as described in ICRP 30 and updates)
- Alkaline earth model
- Iodine model
- Radium/radon model
- Tritium (ICRP; Dunford and Johnson)
- Carbon model
- Tellurium/iodine model

Excretion Model

- ICRP 54 excretion functions model
- ICRP 30 default systemic retention model (when excretion functions are not provided)
- Jones plutonium excretion model
- Durbin plutonium excretion model
- Tritium excretion model

Models in the CINDY model library are initially set up to run using default values for model parameters based on ICRP recommendations. However, the user is provided the opportunity to customize the generalized model to achieve better agreement with observed bioassay measurement results or known biokinetic characteristics of the individual or exposure situation. Tabular comparisons of observed bioassay values to those predicted by the model and a goodness-of-fit indication are provided by CINDY to assist the user in evaluating the appropriateness of the selected model and intake assumptions. Each run of the CINDY code creates an output file that includes all model parameter values used in the analysis. This file can be reviewed to check that the analysis was performed as desired, and it also serves as a permanent

record that can be reviewed in the future should questions arise regarding reported results.

To maintain control over the model library, model parameter changes cannot be stored as a redefined model in the model library; however, the user can store the modified model parameters in a subject model library file that can be retrieved for later use.

3.4 RADIONUCLIDES

The CINDY radionuclide library contains about 250 radionuclides with half-lives 10 minutes and longer. Radiations emitted from daughter radionuclides with half-lives less than 10 minutes are included in the specific effective energy factors for the parent radionuclide for dose assessment purposes. With the exception of the tellurium-iodine model, daughter radionuclides are assumed to behave metabolically like the parent radionuclide as recommended by ICRP (1979).

The combining of SEE factors [as defined for Equation (2.1)] for cases involving short-lived daughters is performed as follows:

$$\text{SEE}(\text{parent} + \text{daughters}) = \text{SEE}(\text{parent}) + \sum_n B_n \text{SEE}(\text{daughter})_n \quad (3.21)$$

where $\text{SEE}(\text{parent} + \text{daughters})$ = effective SEE for the parent plus short-lived daughters,

$\text{SEE}(\text{parent})$ = SEE for the parent radionuclide,

$\text{SEE}(\text{daughter})_n$ = SEE for the short-lived daughter radionuclide n ,

B_n = number of disintegrations of short-lived daughter radionuclide n , per disintegration of the parent.

Special consideration is given to the selection of SEE factors for bone. The ICRP has made determinations for each radionuclide as a "volume seeker" or a "surface seeker," or that no determination is necessary (the radionuclide does not accumulate significantly in the bone). The source library for SEE factors (see Section 5.0) contains SEE factors for each radionuclide as both a bone

and a surface seeker. The values used in the CINDY library are selected from the source library to correspond with the ICRP determination. For radionuclides that have no determination but are to be included as contributing to a parent radionuclide decay energy in the bone, it is necessary to select one set of SEE factors. The criteria for selection are based on the half-life of the daughter as recommended by ICRP (1979). Radionuclides with half-lives less than 15 days are treated as surface seekers, and those with half-lives greater than 15 days are treated as volume seekers.

3.5 SITE SET-UP

Each DOE site (or other user facility) has radionuclides and analysis requirements specific to that site. When the CINDY code is installed for use at a site, the user may take advantage of "site set-up" features that will result in a more efficient operation of the code. For example, during site set-up of the code, the user creates a site-specific radionuclide directory containing those radionuclides of interest at the user's site. Data for these radionuclides are maintained in readily accessible files. The use of the abbreviated radionuclide data file improves code operating speed and simplifies user input.

Site set-up enables users to customize the operation of CINDY for their particular application requirements. For example, the user may specify that input bioassay data will be specified in radiological units of nCi, or that doses are to be reported in Sv. The user may select and retain conventions for the following items:

- radionuclide list
- radionuclides of concern
- radiological working units
- radionuclide daughter handling
- operating mode
- subject identification
- intake information
- reference excretion volume and mass
- dose integration period
- dose reporting limit

- bioassay projection endpoint
- option of user-selected versus computer-selected bioassay projection report times
- user-specified report times
- run title
- printer definition
- selection of output reports
- error tolerances
- screen colors
- edit mode

The selected site-specific options may be saved for automatic use by the CINDY code on subsequent analyses. Site-specific set-up options are considered important to enable CINDY to fit into currently existing bioassay programs with minimal problems. Significant effort has been devoted to incorporating special features and needs for the different dosimetry programs that will use the code. Details of site set-up features are provided in Part 2 (User's Guide) of the CINDY documentation.

4.0 DESCRIPTION OF BIOKINETIC MODELS

The dose evaluations performed with the CINDY code require estimates of the dose equivalents in a number of target organs. As described in Section 2.0 the dose in a target organ is based on the activity of the radionuclide in a given source organ. For each type of radiation i , the dose equivalent H_i in target organ T from radionuclide j in source organ S is the product of two factors:

- the total number of nuclear transformations of radionuclide j in organ S over the period of interest following intake
- the energy absorbed per gram in target organ T , suitably modified for the quality factor, from radiation of type i per transformation of radionuclide j in source organ S .

The number of nuclear transformations of the radionuclide in the body is a critical factor in the dose estimate. The calculation of the number of nuclear transformations is accomplished by mathematical solution of biokinetic models that describe the distribution, translocation, retention, and excretion of the radionuclide of interest in the various organs and tissues of interest. Because of the complexity of the model equations, a consistent set of nomenclature has been developed for this report. The nomenclature is described in the next section, followed by descriptions of the mathematical models and algorithms used in the CINDY program. These models are derived from the recommendations of the ICRP (ICRP 1979) and other sources, as indicated.

4.1 NOMENCLATURE CONVENTIONS

The equations describing dosimetry and metabolism involve many parameters with multiple dimensions requiring a complex system of nomenclature. The nomenclature conventions used in this report are designed to be as consistent as possible with original equation presentations of ICRP, NCRP, and other sources. None of the past conventions are entirely sufficient to meet the needs of the equations in this document. This has resulted in extension of the past conventions and generation of some new conventions. The nomenclature conventions used in this report are described in the following sections,

with those related to dosimetry presented first, followed by those for metabolism.

4.1.1 Dosimetry Nomenclature

The primary output from the dosimetry analysis of the CINDY program is an estimate of radiation dose. The dose may be to specific organs of the body, or an effective dose equivalent may be provided. Following the practice of ICRP reports, the letter "H" is used to represent dose equivalent. Subscripts are added to identify specific types of dose equivalent. When the dose equivalent is referenced to a specific tissue, the subscript "T" is added. For example, H_T represents a dose equivalent to tissue T. This representation gives no information on the time period over which the dose is delivered and is a general representation of dose to a tissue. When the time period is to be identified with the dose, another subscript is added. For example, the ICRP (1979) uses a subscript of 50 to represent dose delivered over a 50-year period. Then, $H_{50,T}$ represents the dose to tissue T delivered over 50 years following the start of exposure. (This term is given the specific name "Committed Dose Equivalent" by the ICRP and is also used without the "T" subscript.) When the dose period is an undefined time period, a general subscript "t" is used: $H_{t,T}$.

An additional dosimetric term defined by ICRP (1987) is the "effective dose equivalent," which is represented by a subscript E. Because this dose term is evaluated as a sum over contributions from several tissues (see Section 5.0), there is no need for the tissue subscript. However, the time period index is needed because time is not fixed. As an example of the effective dose equivalent nomenclature as used in this report, the dose over a period of 1 year would be represented by $H_{1,E}$.

4.1.2 Metabolism Nomenclature

Several conventions are established for parameters used in defining the metabolic models of the CINDY program. The general approach taken is to define necessary compartments (or boxes) within each major physiological model of the body. The major models include the three intake modes (respiratory tract, gastrointestinal tract, and direct intake), the transfer compartment (systemic fluids or blood), systemic organs, and models related to excretion.

The parameters of particular interest are those used to describe initial deposition in compartments of the intake models, and transfer rates between compartments and to elimination (excretion).

Each major model has specific compartments that are used to describe the retention of activity as a function of time. The nomenclature conventions include a primary letter descriptor identifying the major model plus secondary descriptors identifying compartments within the major model. The conventions used for the model descriptors are given in Table 4.1. These conventions maintain the conventions used in ICRP publications describing respiratory tract and gastrointestinal tract models.

Use of the descriptors depends on the type of parameter being defined. Initial deposition into compartments of one of the intake models is defined using the letter D and subscripts necessary to define unambiguously the term in question. The conventions are as given in Table 4.2. Note that the ICRP usage for initial deposition into the three major portions of the respiratory tract is retained. No deposition fractions need be defined for the gastrointestinal tract because all material taken in (or transferred from the respiratory tract) is assumed to go directly to the stomach. The deposition fractions for the direct intake model use a subscript "A" (for "absorption") to distinguish the parameters from those for the respiratory system.

The activity of a radionuclide in a given compartment is represented by the letter "Y" with subscripts to define the compartment and radionuclide. Following the ICRP conventions for the respiratory and gastrointestinal tracts, the compartment subscripts are those defined in Table 4.1 for secondary descriptors (except that lower case is used for the GI-tract compartments). The general subscript "n" is used to represent radionuclides. No subscript is needed to indicate the time at which the activity is evaluated because the activity is always taken to represent a time-dependent variable. As an example of the nomenclature usage for activity, the term $Y_{b,n}$ represents the activity of radionuclide n in respiratory compartment b . The term $Y_{si,n}$ represents the activity of radionuclide n in small intestines, and the term $Y_{S,n}$ represents the activity of radionuclide n in source tissue S .

TABLE 4.1. Descriptors for Major Metabolic Models

<u>Model</u>	<u>Primary Descriptor</u>	<u>Secondary Descriptors</u>
Respiratory tract	R	a-j
Nasal passage	1	a,b
Tracheo-bronchial	2	c,d
Pulmonary parenchyma	3	e-h
Lung lymph nodes	-	i,j
Gastrointestinal tract	G	
Stomach		s
Small intestine		si
Upper large intestine		uli
Lower large intestine		lli
Direct intake	A	
Compartment 1		1
Compartment 2		2
Compartment 3		3
Compartment 4		4
Transfer Compartment	B	
Systemic Organs	O	m
Excretion - urinary	U	u
" - fecal	F	f
Target tissues	T	
Source tissues	S	
Jones excretion model	J	j
Compartment 1		1
Compartment 2		2
Compartment 3		3
Compartment 4		4
Durbin excretion model	P	j
Compartment 1		1
Compartment 2		2
Compartment 3		3
Compartment 4		4
Compartment 5		5
Dunford and Johnson tritium model		
Bound tritium-1	H1	
Bound tritium-2	H2	
Body water (tritium)	W	

TABLE 4.1. (contd)

<u>Model</u>	<u>Primary Descriptor</u>	<u>Secondary Descriptors</u>
Alkaline earth model		
Cortical bone	Co	1,2
Cancellous bone	Ca	1,2
Bone surface	Bs	
Iodine Model		
Thyroid	Th	
Organic iodine	I	

TABLE 4.2. Deposition Fraction Nomenclature

<u>Model and Compartment</u>	<u>Representation</u>
Respiratory tract	D _R
Nasal passage	D ₁
Tracheo-bronchial	D ₂
Pulmonary	D ₃
Gastrointestinal	(not needed)
Direct deposition	D _A
Compartment 1	D _{A1}
Compartment 2	D _{A2}
Compartment 3	D _{A3}
Compartment 4	D _{A4}

One of the important output parameters for the metabolic models is the total number of nuclear transformations occurring for each radionuclide over a defined time period. This parameter is used directly in the dosimetry analysis to estimate radiation dose for the time period. The number of transformations is represented by the letter "U" with subscripts to indicate 1) the time period over which the transformations are accumulated, 2) the compartment or tissue in which the transformations occur, and 3) the radionuclide of interest. The tissue subscript notation is the same as that defined in Table 4.1 and illustrated for the activity term Y. The time subscript is either a numeric value indicating the total accumulation period following the start of exposure, or a general index "t". The general index "n" is used for the radionuclide subscript. For example, the number of transformations to be

used in evaluation of the 50-year dose equivalent to a systemic tissue "0" from radionuclide "n" would be represented as $U_{50,0,n}$.

Transfer of activity between compartments is based on transfer rate constants that are dependent on source compartment and destination compartment. The transfer rate nomenclature does not include a radionuclide index because a generic index of "n" is assumed for all rates that are dependent on radionuclide or element. Two subscripts are used with the general letter "k" which is often used in the literature to describe rate constants. (In the CINDY report the Greek letter lambda [λ] is used only for the radiological decay rate constant.) The compartment subscripts are the same as those defined in Table 4.1 and as used for other parameters. For example, the transfer rate constant for movement of material from the tracheo-bronchial compartment "d" to the stomach is represented as $k_{d,s}$. While this representation is somewhat more cumbersome than the ICRP usage of λ , the proposed method is relatively free of ambiguity, especially for cases where the transfer between compartments can be in both directions (i.e., recirculation). For some compartments, one additional transfer rate constant is defined that represents the total transfer rate out of the compartment: the letter "K" is used for this parameter with a single subscript for the compartment from which the material is leaving. This representation is useful when more than one transfer route out of the compartment is defined. For example, the total transfer rate out of the systemic fluids is represented by K_p .

4.2 GENERALIZED MODEL CONFIGURATION

The biokinetic model implemented by CINDY consists of a group of linked models, representing the respiratory tract, the GI tract, direct uptake, systemic organs, and systemic excretion, as illustrated in Figure 4.1. The models are linked together via a transfer compartment that is taken to represent the systemic circulation. The separation of the generalized biokinetic model into component models allows the flexibility for adding additional model options to the code in the future. For example, a future version of CINDY could provide the option for evaluating internal exposures using either the current respiratory tract model recommended by the ICRP or the forthcoming revised ICRP lung model.

The following sections present the models currently implemented in the CINDY code. Exceptions to the generalized model configuration indicated in Figure 4.1 are noted for specific models. For example, the Jones excretion model for plutonium bypasses the transfer compartment.

4.3 RESPIRATORY TRACT

The respiratory tract model of the ICRP Task Group on Lung Dynamics, as presented in ICRP 30 (1979), is illustrated in Figure 4.2. Compartments a and b represent the nasal passage region; compartments c and d the trachea and bronchial tree region; compartments e-h the pulmonary region; and compartments i and j the lymph nodes. Table 4.3 (taken from ICRP 30) gives regional deposition fractions for a 1- μ m Activity Median Aerodynamic Diameter (AMAD) particulate and compartment fractions and retention half-times for three

FIGURE 4.1. Generalized Biokinetic Model Configuration

FIGURE 4.2. ICRP 30 Respiratory Tract Model

TABLE 4.3. Deposition Fractions and Clearance Half-times^(a) ($t_{1/2}$) for the Lung Model

Region	D_i (b)	Compartment	Class D		Class W		Class Y	
			F_i	$t_{1/2}$	F_i	$t_{1/2}$	F_i	$t_{1/2}$
Naso-Pharyngeal	0.3	a	0.5	0.01	0.1	0.01	0.01	0.01
		b	0.5	0.001	0.9	0.40	0.99	0.40
Tracheo-Bronchial	0.08	c	0.95	0.01	0.5	0.01	0.01	0.01
		d	0.05	0.2	0.5	0.2	0.99	0.2
Pulmonary	0.25	e	0.8	0.5	0.15	50	0.05	500
		f	0	0	0.4	1.0	0.4	1.0
		g	0	0	0.4	50	0.4	500
		h	0.2	0.5	0.05	50	0.15	500
Lymph		i	1.0	0.5	1.0	50	0.9	1000
		j	0	0	0	0	0.1	∞

(a) From ICRP 54 (1988) in days.

(b) For a 1- μ m-Activity Median Aerodynamic Diameter (AMAD) aerosol.

transportability classes. The model is described in more detail in ICRP 30 (ICRP 1979). Equations describing the activity in each compartment are:

$$\frac{dY_{an}}{dt} = I(t) D_1 F_a - k_{a,B} Y_{an} + \Delta_{an} \quad (4.1)$$

$$\frac{dY_{bn}}{dt} = I(t) D_1 F_b - k_{b,G} Y_{bn} + \Delta_{bn} \quad (4.2)$$

$$\frac{dY_{cn}}{dt} = I(t) D_2 F_c - k_{c,B} Y_{cn} + \Delta_{cn} \quad (4.3)$$

$$\frac{dY_{dn}}{dt} = I(t) D_2 F_d + k_{f,d} Y_{fn} + k_{g,d} Y_{gn} - k_{d,G} Y_{dn} + \Delta_{dn} \quad (4.4)$$

$$\frac{dY_{en}}{dt} = I(t) D_3 F_e - k_{e,B} Y_{en} + \Delta_{en} \quad (4.5)$$

$$\frac{dY_{fn}}{dt} = I(t) D_e F_f - k_{f,d} Y_{fn} + \Delta_{fn} \quad (4.6)$$

$$\frac{dY_{gn}}{dt} = I(t) D_3 F_g - k_{g,d} Y_{gn} + \Delta_{gn} \quad (4.7)$$

$$\frac{dY_{hn}}{dt} = I(t) D_3 F_h - (k_{h,i} + k_{h,j}) Y_{hn} + \Delta_{hn} \quad (4.8)$$

$$\frac{dY_{in}}{dt} = F_i k_{h,i} Y_{hn} - k_{i,B} Y_{in} + \Delta_{in} \quad (4.9)$$

$$\frac{dY_{jn}}{dt} = F_j k_{h,j} Y_{jn} + \Delta_{jn} \quad (4.10)$$

where Y_{in} = the quantity of radionuclide n in compartment i as a function of time, in Bq.

$I(t)$ = the intake rate of radionuclide n into the body via compartment i .

D_i = the deposition fraction of inhaled radionuclides into the major physiological regions, i , of the lung, dependent on the particle size. The deposition fractions used correspond to a set of equations fit to the curves in Figure 5.1 of ICRP 30, Part 1 (ICRP 1979a). Values of D_i for $1\text{-}\mu\text{m}$ particulates are given in Table 4.3.

F_i = the fraction of deposited material assumed to be in each of the lung compartments (subscripts a-j), dependent on the translocation class of the inhaled material. Values of F_i are given in Table 4.3.

$k_{i,j}$ = the rate constant describing the transfer of material out of compartment i and into a compartment j , day^{-1} .

Δ_{ij} = the net instantaneous rate of radiological ingrowth (or decay) for radionuclide j in a compartment i .

The equations given above are those formulated by the ICRP (1979). These equations are implemented in the CINDY code in a slightly modified manner in order to keep track of the amount of material transferred from the pulmonary region (compartments f and g) and cleared via the trachea-bronchial region to the GI tract. The modification involves definition of an additional compartment "m" for accumulation of the transferred material. The equations as implemented for compartments d, f, g, and m are as follows:

$$\frac{dY_{dn}}{dt} = I(t) D_2 F_d - k_{d,G} Y_{dn} + \Delta_{dn} \quad (4.11)$$

$$\frac{dY_{fn}}{dt} = I(t) D_3 F_f - k_{f,m} Y_{fn} + \Delta_{fn} \quad (4.12)$$

$$\frac{dY_{gn}}{dt} = I(t) D_3 F_g - k_{g,m} Y_{gn} + \Delta_{gn} \quad (4.13)$$

$$\frac{dY_{mn}}{dt} = k_{f,m} Y_{fn} + k_{g,m} Y_{gn} - k_{m,G} Y_{mn} + \Delta_{mn} \quad (4.14)$$

where terms are as previously defined. The transfer rate constant from compartment m to the GI tract is set equal to the rate constant from compartment d to the GI tract.

Another modification to the original ICRP (1979) compartment model is a split of compartment h into two compartments with h1 representing the material that ultimately clears to compartment i and h2 representing the material that clears to compartment j. The revised equations are as follows:

$$\frac{dY_{h1n}}{dt} = I(t) D_3 F_h F_i - k_{h1,i} Y_{h1n} + \Delta_{h1n} \quad (4.15)$$

$$\frac{dY_{h2n}}{dt} = I(t) D_3 F_h F_j - k_{h2,G} Y_{h2n} + \Delta_{h2n} \quad (4.16)$$

$$\frac{dY_{in}}{dt} = k_{h1,i} Y_{h1n} - k_{i,B} Y_{in} + \Delta_{in} \quad (4.17)$$

$$\frac{dY_{jn}}{dt} = k_{h2,j} Y_{h2n} + \Delta_{jn} \quad (4.18)$$

Note that this revised implementation is not a change in the model; the results of the analysis are the same with the activity in the initial compartment "h" being equal to the sum of the activities in the new compartments "h1" and "h2".

The term Δ_{in} is developed using a recursive application of the Bateman equations (Bateman 1910). It is used with the standard assumption that daughters produced in vivo can be described with the same metabolic parameters as the parent radionuclide. While this assumption is in general not valid, data in most cases do not exist from which the parameters for in vivo produced daughters can be estimated. Parameters can be estimated for the daughters not produced in vivo, but in general the daughters are transported

to different organs than the parent. Even if the parent and daughter go to the same organ, the parameters describing the retention of the daughter taken up by the organ rather than produced in the organ are not necessarily the same.

The evaluation of Δ_{in} can best be described using an example decay chain, as illustrated in Figure 4.3. Five radioactive chain members are illustrated with radionuclide 2 decaying by two modes to give two possible decay products, both of which subsequently decay to the fifth chain member. The decay chain is described by parameters defined for each radionuclide: radiological half-life and branching ratios. These parameters are defined in a data library accessed by the CINDY code as illustrated in Table 4.4 for the example decay chain. The data for each radionuclide is oriented toward the source (parent) radionuclide rather than the normal convention in which the decay leads (daughters). For each radionuclide there are at most two possible parent radionuclides (e.g., radionuclide 5 may be produced from radionuclides

FIGURE 4.3. Example Decay Chain

TABLE 4.4. Chain Decay Parameters

Radionuclide	Half-life	Parent 1 Data		Parent 2 Data	
		Index	Fraction	Index	Fraction
R1	T1	none		none	
R2	T2	1	1.0	none	
R3	T3	2	f2,3	none	
R4	T4	2	f2,4	none	
R5	T5	3	1.0	4	1.0

3 or 4). The index (Table 4.4) gives the position of the parent in the decay chain (see Figure 4.3). The fraction is the fraction of the parent that decays to the daughter radionuclide of interest. These data are used in a decay processor to evaluate the instantaneous rate of change (Δ_{in}) of each chain member at the time of interest. The processor in effect reconstructs the Bateman equation to include the contribution from each parent to each radionuclide with consideration given to multiple branching within the chain. (The decay equations used by the processor are described in Section 4.8.2.) When there is only one member of the chain (a parent without daughters), the term Δ_{in} is exactly equal to the radiological decay constant multiplied by the activity present, $\lambda_n Y_{in}$.

FIGURE 4.4. ICRP 30 GI Tract Model

4.4 GASTROINTESTINAL TRACT

The GI tract model, as described in ICRP 30 (1979), is implemented in the CINDY code. The model is illustrated in Figure 4.4 with equations for each compartment as described below:

$$\frac{dY_{s,n}}{dt} = k_{b,G} Y_{2j} + k_{d,G} Y_{dn} + k_{m,g} Y_{mn} + I(t) - k_{s,si} Y_{sn} + \Delta_{sn} \quad (4.19)$$

$$\frac{dY_{si,n}}{dt} = \delta_f k_{s,si} Y_{sn} - \left[\frac{\delta_f f_1 k_{si,uli}}{1 - f_1} \right] + k_{si,uli} Y_{si,n} + \Delta_{si,n} \quad (4.20)$$

$$\frac{dY_{uli,n}}{dt} = k_{si,uli} Y_{si,n} - k_{uli,lli} Y_{uli,n} + \Delta_{uli,n} \quad (4.21)$$

$$\frac{dY_{lli,n}}{dt} = k_{uli,lli} Y_{uli,n} - k_{lli,F} Y_{lli,n} + \Delta_{lli,n} \quad (4.22)$$

and where δ_f = a Kronecker delta function, where $\delta_f = 1$ if f_1 is not equal to 1.0, and where $\delta_f = 0$ if $f_1 = 1.0$, and

f_1 = the fractional uptake from the GI tract to the transfer compartment and the other symbols are as defined in Section 4.1.

4.5 DIRECT UPTAKE MODEL

Intake of activity may occur through a wound or following absorption of activity on the skin. These modes are referred to as injection or direct uptake. A four-compartment model is used to describe the delay following intake and entry into the transfer compartment, as illustrated in Figure 4.5. The equation for the uptake compartments is as follows:

$$\frac{dY_{Ai,n}}{dt} = I(t) D_{Ai} - K_{Ai} Y_{Ai,n} + \Delta_{Ai,n} \text{ where } i = 1,4 \quad (4.23)$$

Terms are as previously defined, with I representing the total activity intake rate and D_{Ai} the fraction of the intake being deposited in each of the direct intake compartments. Because direct intakes may be from wounds, skin absorption, or injections, CINDY does not contain values for any of the parameters for the direct intake model; the user must supply all values. When the intake is acute, the intake is defined as a total activity and the value for I is set to zero and initial values of $Y_{Ai,n}$ are set accordingly. For chronic intakes

FIGURE 4.5. Direct Uptake Compartment Model

(e.g., absorption of material through the skin) the intake is a rate for the given time period. In all cases, the total intake is divided among the four compartments by the deposition fractions D_{Ai} ($i = 1,4$). Material leaving the direct intake compartments goes directly to the transfer compartment for most models in the CINDY code. However, for the Durbin and Jones plutonium excretion models, the material goes directly to the excretion function compartments (strictly a mathematical representation).

4.6 SYSTEMIC DEPOSITION AND RETENTION MODEL

The systemic deposition and retention model implemented by CINDY follows the recommendations of ICRP Publication 30 (1979). For most radionuclides, a general systemic compartment model is used. In the general systemic compartment model, each organ or tissue of deposition is assumed to consist of from one to four compartments, and from each of these the radionuclide is removed at a given rate. For simplicity, it is assumed in the general model that no feedback to the transfer compartment occurs either from routes of elimination

or from organ compartments. Where the ICRP has recommended the use of models that do incorporate feedback (e.g., alkaline earth elements and iodine), special models have been implemented. The general systemic model as well as the special systemic compartment models implemented by CINDY are presented in this section.

4.6.1 General Systemic Compartment Model

The general systemic compartment model is implemented for most radio-nuclides. The model follows the recommendations of the ICRP for uptake deposition and retention and is illustrated in Figure 4.6. Equations governing the material in the transfer compartment and systemic compartments are as follows:

Transfer Compartment

$$\begin{aligned} \frac{dY_{Bn}}{dt} = & k_{a,B} Y_{an} + k_{c,B} Y_{cn} + k_{e,B} Y_{en} + k_{i,B} Y_{in} \\ & + \frac{\delta_f f_1 k_{si,uli}}{1 - f_1} Y_{si,n} + (1 - \delta_f) k_{s,si} Y_{s,n} \\ & + \sum_{i=1}^4 k_{Ai,B} Y_{Ai,n} - K_B Y_B + \Delta_{Bn} \end{aligned} \quad (4.24)$$

Organ Compartments

$$\frac{dY_{Omn}}{dt} = f_m k_{B,0} Y_B - k_{Omn} Y_{Omn} - \Delta_{Omn} \quad \text{where } m = 1,5 \quad (4.25)$$

where Y_{Omn} = activity of radionuclide n in subcompartment m of systemic organ 0 , pCi,

f_m = fraction of total deposition in systemic organ 0 that is deposited in subcompartment m , dimensionless.

The above equation is evaluated for each systemic organ 0 which may have up to 5 subcompartments m . The fractional intake factor, f_m , represents the fraction of the total intake by the organ that is deposited (mathematically speaking) in the subcompartment m .

FIGURE 4.6. General Systemic Compartment Model

4.6.2 Alkaline Earth Model

The ICRP alkaline earth model (1973; 1979-1982) is used in CINDY to describe the retention of alkaline earth elements (calcium, strontium, barium, and radium). The original form of the model (ICRP 1973) used a power function to describe retention in the mineral bone. This form is difficult to evaluate numerically for chronic exposures and has been replaced in CINDY with Johnson's (1981) adaptation of the alkaline earth model that approximates the power function with a series of exponential terms. This model is illustrated in Figure 4.7.

Because the alkaline earth model addresses retention in systemic organs, the equations describing transfer from the respiratory system and the gastrointestinal tract are as described above. The differential equations

FIGURE 4.7. Alkaline Earth Model

describing the transfer compartment and systemic organs for the alkaline earth model are given below. A main difference between the alkaline earth model and the general model is the inclusion of transfer from the organ compartments back to the transfer compartment. These transfers are indicated in Figure 4.7 and the Equations (4.26-4.32).

Transfer compartment

$$\begin{aligned} \frac{dY_B}{dt} = & k_{a,B} Y_{an} + k_{c,B} Y_{c,n} + k_{e,B} Y_{en} + k_{i,B} Y_{in} \\ & + \frac{\delta_f f_1 k_{si,uli}}{1 - f_1} Y_{si,n} + (1 - \delta_f) k_{s,si} Y_{s,n} \end{aligned} \quad (4.26)$$

$$\begin{aligned}
& + \sum_{i=1}^4 k_{Ai} Y_{Ai,n} \\
& + k_{cal,B} Y_{cal,n} + k_{col,n} Y_{col,n} + k_{Bs,B} Y_{BSn} + \sum_0 \sum_m k_{Om,B} Y_{Omn} \\
& - (k_{B,u} + k_{B,f} + k_{B,cal} + k_{B,col} + k_{B,Bs} + \sum_{0,M} k_{B,O}) Y_B + \Delta_B
\end{aligned}$$

Cancellous bone compartments

$$\frac{dY_{cal,n}}{dt} = k_{B,cal} Y_B + k_{ca2,cal} Y_{ca2,n} \quad (4.27)$$

$$- (k_{cal,B} + k_{cal,ca2}) Y_{cal,n} + \Delta_{cal,n}$$

$$\frac{dY_{ca2,n}}{dt} = k_{cal,ca2} Y_{cal,n} - k_{ca2,cal} Y_{ca2,n} + \Delta_{ca2,n} \quad (4.28)$$

Cortical bone compartments

$$\frac{dY_{col}}{dt} = k_{B,col} Y_B - k_{co2,col} Y_{co2,n} \quad (4.29)$$

$$- (k_{col,B} + k_{col,co2}) Y_{col,n} + \Delta_{col,n}$$

$$\frac{dY_{co2}}{dt} = k_{col,co2} Y_{col,n} - k_{co2,col} Y_{co2,n} + \Delta_{co2,n} \quad (4.30)$$

Bone surface compartment

$$\frac{dY_{BSn}}{dt} = k_{B,Bs} Y_B - k_{Bs,B} Y_{BSn} - \Delta_{BSn} \quad (4.31)$$

Other soft tissue compartment

$$\frac{dY_{Omn}}{dt} = k_{B,O} Y_B - k_{OmB,B} Y_{Omn} - \Delta_{Omn} \quad (4.32)$$

Equation (4.32) is evaluated for all systemic organs, O , and subcompartments, m , as are important for radionuclide n .

4.6.3 Iodine Model

The biokinetic behavior of radioiodine is described by the model given in ICRP Publication 54 (ICRP 1988), as shown in Figure 4.8. Of the iodine reaching the transfer compartment (blood), 70% is assumed to be excreted via urine and the remainder is transferred to the thyroid as inorganic iodine. The iodine in the thyroid is lost from the thyroid as organic iodine and is assumed to be uniformly distributed among all other organs of the body (other than the thyroid). Part (10%) of the organic iodine is assumed to be excreted via feces, and the remainder (90%) is assumed to be returned to the transfer compartment. The biological half-times for the various transfers are given in Table 4.5.

FIGURE 4.8. The Iodine Model

TABLE 4.5. Iodine Model Biological Half-times

<u>Compartment</u>	<u>Half-time (days)</u>
Transfer compartment	0.25
Thyroid	12
Organic iodine	80

The equations for the iodine model are given in Equations (4.33)-(4.35).

Transfer compartment (B)

$$\begin{aligned} \frac{dY_{Bn}}{dt} = & k_{a,B} Y_{an} + k_{c,B} Y_{cn} + k_{e,B} Y_{en} + k_{i,B} Y_{in} \\ & + k_{s,B} + 0.9 K_I - K_B Y_{Bn} \\ & + \sum_{i=1}^4 k_{Ai} Y_{Ai,n} + \Delta_{Bn} \end{aligned} \quad (4.33)$$

Thyroid (Th)

$$\frac{dY_{Thn}}{dt} = 0.3 K_B Y_{Bn} - k_{Th,I} Y_{Thn} + \Delta_{Thn} \quad (4.34)$$

Organic iodine (I)

$$\frac{dT_{In}}{dt} = k_{Th,I} Y_{Thn} - K_I Y_{In} + \Delta_{In} \quad (4.35)$$

4.6.4 Tellurium Iodine Model

Metabolism of radioiodine produced by decay of tellurium isotopes is described using the iodine model (see Section 4.6.3). The iodine produced is assumed to be instantaneously translocated to the iodine inorganic transfer compartment. The metabolism of tellurium is described by the general model. The coupled model is shown schematically in Figure 4.9.

FIGURE 4.9. Tellurium/Iodine Model

The equations for the tellurium/iodine model are essentially the same as those for the general model and the iodine model. An exception is the equations for the transfer compartment for the inorganic iodine which includes the production of iodine as a decay product of tellurium from all body tissues (m) in which tellurium is present:

$$\frac{dY_{Bn}}{dt} = 0.9 k_I Y_{In} - k_B Y_{Bn} + \sum_m \Delta_{mn} + \Delta_{Bn} \quad (4.36)$$

where m is the index for tissues that produce iodine by decay of tellurium and n is the iodine index only.

4.6.5 Tritium Models

Tritium may be encountered in the work environment in the elemental form (HT or T₂) or as water vapor (HTO). Models are included in the CINDY code to describe metabolism and excretion of both forms of tritium. A general compartmental description of the tritium models is given in Figure 4.10, which indicates intake of tritium in both forms. Inhalation of elemental tritium is

* Bound HTO Compartments are used only in the Dunford Model

FIGURE 4.10. Tritium Metabolic Models

assumed to involve oxidation of the tritium to water in the gut (indicated in Figure 4.10 during transfer from blood to body water). Therefore, metabolic models for tritium as water are used for intake of both forms of tritium. Two models are available in the CINDY code to describe tritium metabolism in the form of water (HTO): the ICRP model (ICRP 1979) and the Dunford and Johnson model (Dunford and Johnson 1987).

The models included in CINDY are for intake of tritium in elemental form and as tritiated water. The models may not be appropriate for ingestion of tritium in foods where the tritium may exist in organic form. However, for typical occupational exposure situations, ingestion of contaminated foods is not likely to be encountered. The direct intake mode (wound or absorption) is not allowed for tritium. However, the ingestion mode can be used to simulate direct intake exposures of HTO.

4.6.5.1 Tritium as Water Vapor

The ICRP model (ICRP 1979) for metabolism of tritium in the form of water assumes tritium (inhaled or ingested) to be instantaneously absorbed and mixed within the body water. The retention of tritium in body water is described as a single exponential with a half-time of 10 days. The differential equation for the activity of tritium in body water as a function of time is given as follows:

Tritium in body water, ICRP model

$$\frac{dY_{Wn}}{dt} = I(t) - K_W Y_{Wn} + D_{Wn} \quad (4.37)$$

where Y_{Wn} = activity of tritium (radionuclide n) in body water, pCi

$I(t)$ = intake rate of tritium into the body, pCi/d

K_W = removal rate constant for tritium from body water, d⁻¹

D_{Wn} = net decay rate of tritium, pCi/d.

The Dunford and Johnson model for tritium metabolism is similar to the ICRP model, except that two additional compartments are included to account for conversion and elimination of bound tritium. The differential equations for activity of tritium in each compartment of the Dunford and Johnson tritium model are as follows:

Tritium in body water, Dunford and Johnson model

$$\begin{aligned} \frac{dY_{Wn}}{dt} = & k_{B,W} Y_{Bn} + k_{H1,W} Y_{H1} + k_{H2,W} Y_{H2} \\ & - k_{W,H1} Y_{Wn} - k_{W,H2} Y_{Wn} - k_{W,u} Y_{Wn} + \Delta_{Wn} \end{aligned} \quad (4.38)$$

Bound tritium compartments

$$\frac{dY_{H1}}{dt} = k_{W,H1} Y_{Wn} - k_{H1,W} Y_{H1} + \Delta_{H1n} \quad (4.39)$$

$$\frac{dY_{H2}}{dt} = k_{W,H2} Y_{Wn} - k_{H2,W} Y_{H2} + \Delta_{H2n} \quad (4.40)$$

4.6.5.2 Elemental Tritium

The published ICRP model for estimation of dose from elemental tritium considers only exposure from the tritium contained in the lungs as a gas during breathing. When the ICRP model is selected for elemental tritium, an additional dose component is included in CINDY that considers absorption of a small amount of tritium gas into the blood with subsequent oxidation in the body (by bacteria in the GI tract). This oxidized tritium is then treated as HTO (see Figure 4.10). The equations for elemental tritium metabolism after oxidation occurs are the same for tritium as water, except that an additional equation must be defined for tritium in the lungs and blood. The differential equations for the activity in the lungs and blood during the exposure period are given as follows:

Tritium in lungs (L)

$$\frac{dY_{Ln}}{dt} = I(t) + k_{B,L} Y_{Bn} - K_L Y_{Ln} + \Delta_{Ln} \quad (4.41)$$

Tritium in blood (B)

$$\frac{dY_B}{dt} = k_{L,B} Y_L - k_{B,W} Y_{Bn} - k_{B,L} Y_{Bn} + \Delta_{Bn} \quad (4.42)$$

Treatment of the tritium in the body following oxidation is described by the equations for the specific metabolic model used for tritium (ICRP or Dunford and Johnson) as given in Section 4.6.5.1. Values for the transfer rate constants for the tritium models are given in Table 4.6.

4.6.6 Carbon Model

The ICRP (1981) considers carbon intake in the form of organic compounds and labelled gases such as carbon monoxide and carbon dioxide: other forms of carbon are not considered. For inhalation of carbon, the absorbed activity is assumed to be instantaneously and completely translocated to the systemic

TABLE 4.6. Parameter Values for Tritium Models

<u>Transfer Path</u>	<u>Rate Constant, d⁻¹</u>	<u>Parameter Symbol</u>
Lungs to air	7680	$k_{L,air}$
Lungs to blood	13.01	$k_{L,B}$
Blood to lungs	60	$k_{B,L}$
Blood to body water	1.851	$k_{B,W}$
Body water to excretion	0.069	k_W, f_{WU}
Body water to bound HTO-1	0.00011	$k_{W,H1}$
Body water to bound HTO-2	0.0011	$k_{W,H2}$
Bound HTO-1 to body water	0.002	$k_{H1,W}$
Bound HTO-2 to body water	0.02	$k_{H2,W}$

circulation without changing chemical form. All of the inhaled activity is assumed to be absorbed for organic compounds and carbon dioxide. For carbon monoxide 40% of the activity is assumed to be absorbed and 60% is exhaled. Organic labelled compounds taken in by ingestion are assumed to be instantaneously uniformly distributed throughout all organs of the body and are retained with a biological half-life of 40 days.

The model for carbon implemented in CINDY considers only the organic form of carbon, at this time. The model is illustrated in Figure 4.11. This implementation is the same as the recommended ICRP models except that the transfer compartment is used for all intakes, including ingestion of organic labelled compounds.

4.6.7 Radium-226 Model

Radium isotopes are evaluated in CINDY using the alkaline earth model. A special case is implemented for decay of Ra-226 through the noble gas Rn-222. In accordance with recommendations of ICRP (1979a), radon is assumed to diffuse entirely out of soft tissues or before decaying and to be retained at 30% in mineral bone tissues. Daughter products of radon in the bone compartments are assumed to remain in the compartments. The following equations define the implementation of this assumption regarding radon production.

FIGURE 4.11. Carbon Model

Soft tissue compartment

set $\Delta_{omn} = 0.0$, where n is the radon-222 index,

Bone compartments

set $\lambda'_{cn} = 0.3 \Delta_{cn}$, where c is the bone compartment index (ca1, ca2, co1, co2, or BS) and n is the radon-222 index. The value for λ'_{cn} is used in place of λ_{cn} in the alkaline earth model equations.

4.7 EXCRETION FUNCTIONS

Since the general systemic retention model simplifies the process of recycling of material among various compartments of the body, the derivation of an excretion function directly from the retention model may not be appropriate and can in some cases lead to significant errors in evaluating intake from excreta data. For this reason, the ICRP has prescribed specific uptake excretion functions for several important radionuclides and has presented these in its Publication 54 (ICRP 1988). These excretion functions are incorporated into the CINDY program's systemic excretion function model. Where specific excretion functions are not provided in ICRP 54, systemic

excretion is calculated by differentiation of the systemic compartment retention equations. The equations for excretion rate from the general model are as follows:

Excretion rate to feces

$$E_{Fn} = \frac{dY_{Fn}}{dt} = k_{l1i,f} Y_{l1i,n} + f_{fn} \sum_{i=1}^m k_{i,f} Y_{in} \quad (4.43)$$

Excretion rate to urine

$$E_{Un} = \frac{dY_{Un}}{dt} = k_{Bu} Y_B + f_{un} \sum_{i=1}^m k_{i,u} Y_{in} \quad (4.44)$$

where E_{Fn} = fecal excretion rate for radionuclide n, in pCi/d

E_{Un} = urinary excretion rate for radionuclide n, in pCi/d

Y_{Fn} = cumulative activity of radionuclide n excreted in feces, in pCi

Y_{Un} = cumulative activity of radionuclide n excreted in urine, in pCi

Y_{in} = activity of radionuclide n in systemic retention compartment i, in pCi

Y_{Bn} = activity of radionuclide n in transfer compartment, in pCi

f_{un} = fraction of radionuclide n excreted via urine

f_{fn} = fraction of radionuclide n excreted via feces

f_t = fraction of material taken up by the body that is not assigned to a specific systemic organ

$k_{B,u}$ = transfer rate constant from the transfer compartment to urine, in d^{-1}

$k_{i,f}$ = transfer rate constant from systemic retention compartment i to feces, in d^{-1}

$k_{i,u}$ = transfer rate constant from systemic retention compartment i to urine, in d^{-1}

$k_{l1i,f}$ = transfer rate constant from lower large intestine to feces, in d^{-1} .

Other terms are as previously defined. The material represented by the fraction f_t is assumed to be excreted in the urine.

4.7.1 Jones Plutonium Excretion Model

One special excretion model used in CINDY is the Jones model (Jones 1985; Strong and Jones 1989), which describes time dependence of plutonium urinary excretion. This model is used with the standard respiratory tract, gastrointestinal tract, and direct intake models currently employed in CINDY. A schematic diagram of the Jones model is shown in Figure 4.12. There are four compartments that describe the excretion based on the amount of plutonium taken into the body. The Jones model was initially developed to describe the excretion rate of plutonium following an acute intake via injection. Because the CINDY program includes evaluation of chronic intakes and because daughter products are also considered, the basic Jones model has been extended and described in a differential form for application using the numerical solver. The equation giving the urinary excretion rate following an acute injection of unit activity is as follows:

FIGURE 4.12. Jones Plutonium Excretion Model

$$E_u = \sum_{j=1}^4 F_{Jj} \exp(-k_{Jj} t) \quad (4.45)$$

where E_u = urinary excretion rate of plutonium at time t , in pCi/d

F_{Jj} = fraction of injected activity that excretes according to exponential term j , in pCi/d per pCi injected

k_{Jj} = rate constant for decrease of excretion for exponential term j , in d^{-1} .

The parameter values (F_{Jj} and k_{Jj}) are given in Table 4.7. Note that the fractions have units of inverse days and represent conversion of uptake (activity) to excretion rate (activity/time). The differential equations for each pseudo compartment are as indicated below. The material leaving the intake models (respiratory, GI, or direct) is modeled as going directly into the Jones model excretion compartments. The amount of material excreted to feces is set equal to the urinary excretion plus the amount from initial passage of material through the GI tract. In these equations the parameter E represents a rate (as opposed to the activity as the parameter Y represents in other equations). The differential equations then describe the change in excretion rate with time.

TABLE 4.7. Jones Model Transfer Parameters

Compartment	Rate Constant, d^{-1}	Fraction of Excretion by Compartment, d^{-1}
1	5.58×10^{-1}	4.75×10^{-3}
2	4.42×10^{-2}	2.39×10^{-4}
3	3.80×10^{-3}	8.55×10^{-5}
4	2.84×10^{-5}	1.42×10^{-5}

Jones compartment j

Initial rate for acute intakes:

$$E_{Jj,n} = I_n F_{Jj} \quad (4.46)$$

Change in excretion rate:

$$\begin{aligned} \frac{dE_{Jj,n}}{dt} = & [K_a Y_{a,n} + K_c Y_{c,n} + K_e Y_{e,n} + K_i Y_{i,n}] F_{Jj} \\ & + \left[\frac{\delta_f f_{1,n} k_{si,uli}}{1 - f_{1,n}} Y_{si,n} + (1 - \delta_f) k_{s,B} Y_{s,n} \right] F_{Jj} \\ & + \sum_{i=1}^4 k_{Ai,Jj} Y_{Ain} \\ & - k_{Jj,U} E_{Jj,n} - \Delta_{Jj,n} \end{aligned} \quad (4.47)$$

Excretion rate to urine

$$E_u = \sum_{j=1}^4 E_{Jj,n} \quad (4.48)$$

Excretion rate to feces

$$E_u = \sum_{j=1}^4 E_{Jj,n} + k_{11i,F} Y_{11i} \quad (4.49)$$

4.7.2 Durbin Plutonium Excretion Model

The user has the option to select the Durbin plutonium excretion model (ICRP 1988) to describe time dependence of plutonium excretion. The model consists of five exponential terms with constants given in Table 4.8. Implementation of the model parallels that of the Jones model, in which the parameter evaluated is actually the excretion rate rather than the activity retained. This approach is used so the excretion rate for chronic intakes can be evaluated within the numerical framework of the CINDY code. The equation

TABLE 4.8. Parameter Values for Durbin Plutonium Excretion Model

Excretion Compartment	Urine Excretion		Fecal Excretion	
	Fraction	Rate Constant, 1/d	Fraction	Rate Constant, 1/d
1	4.1×10^{-3}	5.78×10^{-1}	6.0×10^{-3}	3.47×10^{-1}
2	1.2×10^{-3}	1.26×10^{-1}	1.6×10^{-3}	1.05×10^{-1}
3	1.3×10^{-4}	1.65×10^{-2}	1.2×10^{-4}	1.24×10^{-2}
4	3.0×10^{-5}	2.31×10^{-3}	2.0×10^{-5}	1.82×10^{-3}
5	1.2×10^{-5}	1.73×10^{-4}	1.2×10^{-5}	1.73×10^{-4}

giving the urinary excretion rate following an acute injection of unit activity is as follows:

$$E_{u,t} = \sum_{j=1}^5 F_{pj} \exp(-k_{pj}t) \quad (4.50)$$

where E_u = urinary excretion rate of plutonium at time t , in pCi/d

F_{pj} = fraction of injected activity that excretes according to exponential term j , in pCi/d per pCi injected

k_{pj} = rate constant for decrease of excretion for exponential term j , d^{-1} .

The model fractions have units of inverse days (as in the Jones model) and represent conversion of uptake (activity) to excretion rate (activity/time). The material leaving the intake models (respiratory, GI, or direct) is modeled as going directly into the Durbin model excretion compartments. In the differential equations that follow, the parameter E represents a rate (as opposed to an activity as the parameter Y is used in other equations). The differential equations then describe the change in excretion rate with time.

Durbin model compartment j

Initial rate for acute injection:

$$E_{pj,n} = I_n F_{pj} \quad (4.51)$$

Change in excretion rate (all intakes):

$$\begin{aligned} \frac{dE_{pj,n}}{dt} = & [k_a Y_{a,n} + k_c Y_{c,n} + k_e Y_{e,n} + k_i Y_{i,n}] F_{pj} \\ & + \frac{\delta_f f_{1,n} k_{si,B}}{1 - f_{1,n}} \left[Y_{si,n} + (1 - \delta_f) k_{s,B} Y_{s,n} F_{pj} \right] \\ & - k_{pj,U} E_{pj,n} - \delta_{pj,m} \end{aligned} \quad (4.52)$$

The equations for the excretion rates to feces and urine are as follows:

Excretion to feces

$$E_f = \sum_{j=1}^5 E_{pj,n} + k_{11i,F} Y_{11i} \quad (4.53)$$

Excretion to urine

$$E_u = \sum_{j=1}^5 E_{pj,n} \quad (4.54)$$

4.7.3 Iodine Excretion Model

The model for iodine metabolism and excretion differs slightly from the general metabolic model. The differences in metabolism have been described in Section 4.6.3. The excretion of iodine is assumed to occur from the transfer compartment (B) via urine and from the organic iodine compartment (I) via feces. No excretion from the GI tract occurs because all iodine is assumed to be absorbed in the GI tract and transferred to the transfer compartment. The equations for excretion of iodine are as follows:

Excretion to urine

$$E_{un} = \frac{dY_{un}}{dt} = 0.7 K_B Y_{Bn} \quad (4.55)$$

Excretion to feces

$$E_{fn} = \frac{dY_{fn}}{dt} = 0.1 K_I Y_{In} \quad (4.56)$$

where Y_{un} = total amount of iodine excreted via urine, in pCi

Y_{fn} = total amount of iodine excreted via feces, in pCi

E_{un} = instantaneous iodine excretion rate via urine, in pCi/d

E_{fn} = instantaneous iodine excretion rate via feces, in pCi/d.

Other terms are as defined for the iodine metabolic model in Section 4.6.3.

4.7.4 Excretion Model for Tritium

The tritium in the body water is assumed to be excreted with a half-time of 10 days (ICRP 1988). The concentration of tritium in the urine is evaluated for dilution in the total volume of body water, taken to be 42 liters. The concentration in urine is then given by

$$C_u(t) = 1/42,000 \exp(-0.693 t / 10) \quad (4.57)$$

where $C_u(t)$ is the tritium concentration in urine at time t following an acute intake, in pCi/mL, and 10 days is the excretion half-time for tritium. The CINDY code is programmed to evaluate the urine concentration from the instantaneous estimate of body water activity. While the above equation applies to an acute intake of tritium, the CINDY implementation can be used to describe any intake history (and the ICRP or Dunford and Johnson tritium metabolism models). The total activity of tritium in the body water is determined by the metabolic model selected, and the excretion rate at any time is evaluated as follows:

$$E_u = K_W f_{Wu} Y_W \quad (4.58)$$

where E_{un} = excretion rate of tritium in urine, in pCi/d

f_{wu} = fraction of tritium in body water that is eliminated via urine

K_w = tritium elimination rate constant from body water, in d^{-1}

Y_{wn} = total activity of tritium in body water, in pCi.

The factor f_{wu} is included to allow for loss of tritium through the skin and via exhalation.

4.7.5 Alkaline Earth Excretion Model

Special models are used in the CINDY program to describe retention and excretion of alkaline earth radionuclides (calcium, strontium, barium, and radium). The alkaline earth model has been described in Section 4.6.2 and is illustrated in Figure 4.7. As the figure indicates, all excretion is evaluated based on the activity in the transfer compartment. The differential equations for excretion of alkaline earth radionuclides are as follows:

Excretion to urine

$$\frac{dY_{un}}{dt} = f_u K_{B,u} Y_{Bn} \quad (4.59)$$

Excretion to feces

$$\frac{dY_{fn}}{dt} = f_f K_{B,f} Y_{Bn} \quad (4.60)$$

4.8 DATA FOR SOLUTION OF THE BIOKINETIC MODELS

Three types of data are required to evaluate the biokinetic models contained in CINDY. The first type is the metabolic data describing the movement and distribution of each radionuclide among the various tissues of the body. The second type describes the radiological decay and transformation of radionuclides including chain decay and branching. The third type describes the dosimetry of radionuclide decay and provides data needed to convert the tissue activity to dose.

4.8.1 Metabolic Data

Values for the fractional uptake of materials, their transfer coefficients from compartment to compartment, and their elimination rates are all contained in a standard computer library. The data in this library are generally adapted directly from ICRP 30 (1979-1982).

The actinide metabolic data have been updated to account for the revised recommendations of the ICRP in Publication 30, Part 4 (1989). This update includes new f_1 factors, as well as the half-time data and fractional uptake data for specific organs.

The CINDY program requires values for the urinary and fecal excretion fractions (f_{un} and f_{fn}) for each radionuclide. Values are provided in ICRP publications for many radionuclides, but for some radionuclides values have been taken from work of Johnson and coworkers. Values used in the CINDY program are given in Table 4.9 (found at the end of this chapter).

4.8.2 Decay Data

Some radionuclides decay through a number of unstable daughters before reaching a stable (or very long-lived) end state. These decay chains are important in that the decay energies of the daughter products contribute to the total dose received from intake of the parent.

To simplify calculations and thus decrease execution time, daughters are handled either implicitly or explicitly, depending on whether or not they are always assumed to be in equilibrium with their parent. Implicit and explicit daughters are defined as follows:

- **Implicit Daughters.** Radionuclides with half-lives short compared to that of the parent (or 30 minutes or less) are assumed to be in equilibrium with the parent radionuclide and are referred to as "implicit daughters." Short-lived radionuclides are of little importance in terms of internal dose, except where they are members of longer decay chains. In CINDY, the decay energies associated with these short-lived daughters are assigned to the parent. This assignment includes correction of the SEE factors during the building of site-specific libraries during site set-up. (See Section 3.4.) The appropriate branching ratios have been considered.

- **Explicit Daughters.** Daughters with half-lives greater than 10 minutes and that may not be in equilibrium with their parents are referred to as explicit daughters. The CINDY software tracks explicit daughters independently throughout all calculations.

The data on radionuclide half-lives, decay chains, and various fractional branching ratios within chains used in the CINDY code are taken from ICRP Publication 38 (ICRP 1983). To reduce program size and thus execution speed, radionuclide chain size has been reduced to one parent, two explicit daughters and any number of implicit daughters. In a few cases radionuclides with half-lives greater than 30 minutes are considered as implicit daughters. Radionuclide decay and daughter ingrowth chain organization, branching ratios, and explicit/implicit daughter classification are shown in Table 4.10 at the end of this chapter.

The CINDY program includes a generalized chain decay processor that can give the activity of any member of a decay chain as a function of time from any initializing condition. The chain processor operates on a recursive application of the Bateman equations (Bateman 1910), modified to include branching. This implementation of the Bateman equations provides a simple means of solving the differential equations describing chain decay. The general form of the decay equation for the j -th member of a decay chain is as follows:

$$Q_j(t) = \sum_{m=1}^j C_{j,m} e^{-\lambda_m t} \quad (4.61)$$

where $Q_j(t)$ = quantity of chain member j at time t , in atoms

λ_m = decay constant of radionuclide m , in d^{-1}

$C_{j,m}$ = coefficient for term m of chain member j , in atoms.

The amount of each radionuclide is expressed in units proportional to the number of atoms present. The units are related to the activity as

$$Q_j(t) = \frac{k Y_j}{\lambda_j} \quad (4.62)$$

where k is the proportionality constant, equal for all radionuclides ($k = 1$ when activity is given in Bq and λ_j in inverse seconds).

Evaluation of the coefficients is performed by starting with the first member and proceeding downward through the chain. The number of coefficients needed for a given chain member is equal to the position of the member in the chain. For example, the third chain member requires three coefficients. The coefficient for the first chain member is just the amount present at the start of the decay period:

$$C_{1,1} = Q_1(0) \quad (4.63)$$

The coefficients for other chain members are evaluated using the following formulas and previously evaluated coefficients:

$$C_{j,m(m=1 \text{ to } j-1)} = \frac{\left[\sum_{i=m}^{j-1} f_{i,j} \lambda_i C_{i,m} \right]}{(\lambda_j - \lambda_m)} \quad (4.64)$$

and

$$C_{j,j} = Q_j(0) - \sum_{i=1}^{j-1} C_{j,i} \quad (4.65)$$

where $f_{i,j}$ is the fraction of radionuclide i decays that result in production of radionuclide j , in dimensionless, units; other terms are as previously defined. This generic representation of the Bateman equations allows decay and branching from any chain member to any member lower in the chain. In practice, it is necessary to include only terms in the equation for which the branching fractions ($f_{i,j}$) are greater than zero. The subroutine that

implements the decay calculation in the CINDY code includes logic to include only those branches that are defined to be present.

The decay term used in the metabolic equations, Δ_{in} , is evaluated as follows

$$\Delta_{in} = \frac{[Q_n(t_0 + \Delta_t) - Q_n(t_0)] \lambda_n}{\Delta t} \quad (4.66)$$

where Δ_{in} = instantaneous increase in activity of radionuclide n in compartment i at time t, in pCi/d

$Q_n(t_0 + \Delta_t)$ = amount (atoms) of radionuclide n present at a short time, Δ_t , after the initial time, t_0 , in pCi/d

$Q(t_0)$ = initial amount of radionuclide n present, in pCi/d

λ_n = decay constant, in pCi

Δ_t = time increment used to evaluate the instantaneous change in activity, d.

The time increment is set equal to the smaller of either 1 day, or one-tenth of the half-life of the shortest-lived member of the decay chain. The decay constant, λ_n , converts from atom units to activity units.

For radionuclides with no significant daughter radionuclides, the decay term is evaluated as follows:

$$\Delta_{in} = \lambda_n Y_{in} \quad (4.67)$$

4.8.3 Dosimetric Data

As described in Section 2.0, calculation of dose from integrated retentions requires specific effective energy data for each radionuclide and each radiation type. The parameters are also defined for each target and source organ considered in the biokinetic models. The factors for specific effective energy are from a tape of SEE factors provided by ORNL^(a) during the developmental phase of the GENII computer program (Napier et al. 1988).

(a) Personal communication from Keith Eckerman of Oak Ridge National Laboratory, Oak Ridge, Tennessee, to Bruce Napier of Pacific Northwest Laboratory.

TABLE 4.9. Urinary and Fecal Excretion Fractions

<u>Element</u>	<u>Urinary Fraction</u>	<u>Fecal Fraction</u>	<u>Source of Data Values</u>
Hydrogen	0.47	0.0	Johnson and Carver (1981)
Beryllium	1.0	0.0	Johnson and Carver (1981)
Carbon	0.5	0.0	Johnson and Carver (1981)
Fluorine	0.95	0.05	Johnson and Carver (1981)
Sodium	0.75	0.02	Johnson and Carver (1981)
Silicon	1.0	0.0	Johnson and Carver (1981)
Phosphorus	0.9	0.1	ICRP Publication 54 (1988)
Sulfur	0.8	0.14	Johnson and Carver (1981)
Chlorine	0.95	0.03	Johnson and Carver (1981)
Arsenic	0.05	0.8	Johnson and Carver (1981)
Potassium	0.85	0.11	Johnson and Carver (1981)
Calcium	0.68	0.32	Johnson and Carver (1981)
Scandium	0.9	0.1	Johnson and Carver (1981)
Chromium	0.5	0.5	Johnson and Carver (1981)
Manganese	0.08	0.92	Johnson and Carver (1981)
Iron	0.16	0.84	Johnson and Carver (1981)
Cobalt	0.7	0.3	ICRP Publication 54 (1988)
Nickel	0.5	0.0	Johnson and Carver (1981)
Copper	0.03	0.97	Johnson and Carver (1981)
Zinc	0.077	0.7	Johnson and Carver (1981)
Gallium	0.1	0.1	Johnson and Carver (1981)
Germanium	1.0	0.0	Johnson and Carver (1981)
Selenium	0.35	0.14	Johnson and Carver (1981)

TABLE 4.9. (contd)

<u>Element</u>	<u>Urinary Fraction</u>	<u>Fecal Fraction</u>	<u>Source of Data Values</u>
Bromine	0.93	.009	Johnson and Carver (1981)
Rubidium	0.86	0.14	Johnson and Carver (1981)
Strontium	0.80	0.20	ICRP Publication 54 (1988)
Yttrium	1.0	0.0	Johnson and Carver (1981)
Zirconium	1.0	0.0	Johnson and Carver (1981)
Niobium	1.0	0.0	Johnson and Carver (1981)
Molybdenum	0.63	0.1	Johnson and Carver (1981)
Technetium	0.67	0.33	Johnson and Carver (1981)
Ruthenium	0.8	0.2	ICRP Publication 54 (1988)
Rhodium	0.5	0.5	Johnson and Carver (1981)
Palladium	0.5	0.5	Johnson and Carver (1981)
Silver	0.1	0.8	Johnson and Carver (1981)
Cadmium	0.8	0.2	Johnson and Carver (1981)
Indium	0.1	0.1	Johnson and Carver (1981)
Tin	0.10	0.	Johnson and Carver (1981)
Antimony	1.0	0.0	Johnson and Carver (1981)
Tellurium	1.0	0.0	Johnson and Carver (1981)
Iodine	-	-	(Determined by iodine model)
Cesium	0.8	0.2	ICRP Publication 54 (1988)
Barium	0.1	0.9	Johnson and Carver (1981)
Lanthanum	1.0	0.0	Johnson and Carver (1981)
Cerium	0.1	0.9	ICRP Publication 54 (1988)
Praseodymium	1.0	0.0	Johnson and Carver (1981)

TABLE 4.9. (contd)

<u>Element</u>	<u>Urinary Fraction</u>	<u>Fecal Fraction</u>	<u>Source of Data Values</u>
Neodymium	0.5	0.5	Johnson and Carver (1981)
Promethium	0.5	0.5	Johnson and Carver (1981)
Samarium	0.5	0.5	Johnson and Carver (1981)
Europium	0.5	0.5	Johnson and Carver (1981)
Gadolinium	0.5	0.5	Johnson and Carver (1981)
Terbium	0.5	0.5	Johnson and Carver (1981)
Dyprosium	1.0	0.0	Johnson and Carver (1981)
Holmium	0.1	0.9	Johnson and Carver (1981)
Erbium	1.0	0.0	Johnson and Carver (1981)
Ytterbium	0.5	0.5	Johnson and Carver (1981)
Hafnium	1.0	0.0	Johnson and Carver (1981)
Tantalum	1.0	0.0	Johnson and Carver (1981)
Tungsten	0.6	0.1	Johnson and Carver (1981)
Rhenium	0.67	0.33	Johnson and Carver (1981)
Osmium	0.5	0.5	Set to iridium values
Iridium	0.5	0.5	Johnson and Carver (1981)
Gold	1.0	0.0	Johnson and Carver (1981)
Mercury	1.0	0.0	Johnson and Carver (1981)
Thallium	0.67	0.33	Johnson and Carver (1981)
Lead	0.1	0.67	Johnson and Carver (1981)
Bismuth	0.9	0.1	Johnson and Carver (1981)
Polonium	0.05	0.95	Johnson and Carver (1981)
Francium	0.9	0.05	Set to cesium values

TABLE 4.9. (contd)

<u>Element</u>	<u>Urinary Fraction</u>	<u>Fecal Fraction</u>	<u>Source of Data Values</u>
Radium	0.05	0.95	ICRP Publication 54 (1988)
Actinium	1.0	0.0	Johnson and Carver (1981)
Thorium	1.0	0.0	ICRP Publication 54 (1988)
Protactinium	0.5	0.5	Johnson and Carver (1981)
Uranium	1.0	0.0	ICRP Publication 54 (1988)
Neptunium	0.5	0.5	Johnson and Carver (1981)
Plutonium	0.5	0.5	Johnson and Carver (1981)
Americium	0.5	0.5	Johnson and Carver (1981)
Curium	0.5	0.5	Johnson and Carver (1981)
Californium	0.5	0.5	Johnson and Carver (1981)

TABLE 4.10. Radionuclide Decay and Daughter Ingrowth Chain Organization
in the CINDY Radionuclide Master Library^(a)

<u>Designation</u>	<u>Explicit Daughters^(b)</u>				<u>Implicit Daughters^(c)</u>		
	<u>CINDY Position Index^(d)</u>	<u>Chain Radio- nuclide</u>	<u>Half- life^(d)</u>	<u>Primary Precursor/ Branching Ratio^(e)</u>	<u>Alternate Precursor/ Branching Ratio^(f)</u>	<u>Radio- nuclide</u>	<u>Precursor/ Branching Ratio^(g)</u>
H3	1	H 3	4.52E+3				
C14	1	C 14	2.09E+6				
N13	1	N 13	6.92E-3				
F18	1	F 18	7.62E-2				
Na22	1	NA22	9.50E+2				
Na24	1	NA24	6.25E-1				
Si31	1	S131	1.09E-1				
P32	1	P 32	1.43E+1				
K40	1	K 40	4.67E11				
Sc46	1	SC46	8.38E+1				
Cr51	1	CR51	2.77E+1				
Mn54	1	MN54	3.13E+2				
Fe55	1	FE55	9.86E+2				
Fe59	1	FE59	4.45E+1				
Co57	1	CO57	2.71E+2				

TABLE 4.10. (contd)

Designation	Explicit Daughters ^(b)				Implicit Daughters ^(c)		
	CINDY Position Index ^(d)	Chain Radio-nuclide	Half-life ^(d)	Primary Precursor/ Branching Ratio ^(e)	Alternate Precursor/ Branching Ratio ^(f)	Radio-nuclide	Precursor/ Branching Ratio ^(g)
Co58	1	C058	7.08E+1				
Co60	1	C060	1.92E+3				
Zn65	1	ZN65	2.44E+2				
Se75	1	SE75	1.20E+2				
Sr89	1	SR89	5.05E+1				
Sr90/Y90	1	SR90	1.04E+4				
	2	Y 90	2.67E+0	1 1.0000	0 0.0000		
Y91m	1	Y 91M	3.45E-2				
	2	Y 91	5.85E+1	1 1.0000	0 0.0000		
Y92	1	Y 92	1.48E-1				
Zr95	1	ZR95	6.40E+1				
	2	NB95M	3.61E+0	1 0.0080	0 0.0000		
	3	NB95	3.51E+1	2 0.9450	1 0.9922		
Zr97	1	ZR97	7.04E-1				
Nb95	1	NB95	3.51E+1				
Mo99	1	M099	2.75E+0				
	2	TC99M	2.51E-1	1 0.8860	0 0.0000		
	3	TC99	7.77E+7	2 1.0000	1 0.1140		

TABLE 4.10. (contd)

Designation	Explicit Daughters ^(b)				Implicit Daughters ^(c)		
	CINDY Position Index ^(d)	Chain Radio-nuclide	Half-life ^(d)	Primary Precursor/ Branching Ratio ^(e)	Alternate Precursor/ Branching Ratio ^(f)	Radio-nuclide	Precursor/ Branching Ratio ^(g)
Tc99m	1	TC99M	2.51E-1				
	2	TC99	7.77E+7	1 1.0000	0 0.0000		
Tc99	1	TC99	7.77E+7				
Ru103	1	RU103	3.94E+1				
	2	PD103	1.70E+1	0 0.0000	0 0.0000		
	3	RH103M	3.90E-2	1 0.9974	2 0.9997		
Ru105	1	RU105	1.85E-1				
	2	RH105	1.47E+0	1 1.0000	0 0.0000	RH105	1 1.0000
Ru106	1	RU106	3.68E+2				
						RH106	1 1.0000
Ag110m	1	AG110M	2.50E+2				
Cd109	1	CD109	4.64E+2				
Sn113	1	SN113	1.15E+2				
	2	IN113M	6.91E-2	1 1.0000	0 0.0000		
Sb122	1	SB122	2.70E+0				
Sb124	1	SB124	6.02E+1				
Sb125	1	SB125	1.01E+3				
	2	TE125M	5.80E+1	1 0.2310	0 0.0000		

TABLE 4.10. (contd)

Designation	Explicit Daughters ^(b)				Implicit Daughters ^(c)		
	CINDY Position Index ^(d)	Chain Radio-nuclide	Half-life ^(d)	Primary Precursor/ Branching Ratio ^(e)	Alternate Precursor/ Branching Ratio ^(f)	Radio-nuclide	Precursor/ Branching Ratio ^(g)
Te129	1	TE129	4.83E-2				
	2	I 129	5.73E+9	1 1.0000	0 0.0000		
Te132	1	TE132	3.26E+0				
	2	I 132	9.58E-2	1 1.0000	0 0.0000		
I125	1	I 125	6.01E+1				
I129	1	I 129	5.73E+9				
I130	1	I 130	5.15E-1				
I131	1	I 131	8.04E+0				
	2	XE131M	1.18E+1	1 0.0109	0 0.0000		
I132	1	I 132	9.58E-2				
I133	1	I 133	8.67E-1				
	2	XE133M	2.19E+0	1 0.0288	0 0.0000		
	3	XE133	5.25E+0	2 1.0000	1 0.9712		
I135	1	I 135	2.75E-1				
Cs134	1	CS134	7.53E+2				
Cs136	1	CS136	1.31E+1				
Cs137	1	CS137	1.10E+4				

TABLE 4.10. (contd)

Designation	Explicit Daughters ^(b)				Implicit Daughters ^(c)		
	CINDY Position Index ^(d)	Chain Radio-nuclide	Half-life ^(d)	Primary Precursor/ Branching Ratio ^(e)	Alternate Precursor/ Branching Ratio ^(f)	Radio-nuclide	Precursor/ Branching Ratio ^(g)
Cs139	1	CS139	6.53E-3				
Ba140						BA137M	1 0.9460
	1	BA140	1.28E+1				
	2	LA140	1.68E+0	1 1.0000	0 0.0000		
La140							
	1	LA140	1.68E+0				
La142							
	1	LA142	6.42E-2				
Ce141							
	1	CE141	3.25E+1				
Ce144							
	1	CE144	2.84E+2				
	2	PR144M	5.00E-3	1 0.0143	0 0.0000		
	3	PR144	1.20E-2	2 1.0000	1 0.9857		
Pr144							
	1	PR144	1.20E-2				
Pm147							
	1	PM147	9.58E+2				
Eu152							
	1	EU152	4.87E+3				
Eu154							
	1	EU154	3.21E+3				
Eu155							
	1	EU155	1.81E+3				
Gd153							
	1	GD153	2.42E+2				
W187							
	1	W 187	9.96E-1				

TABLE 4.10. (contd)

Designation	Explicit Daughters ^(b)				Implicit Daughters ^(c)		
	CINDY Position Index ^(d)	Chain Radio-nuclide	Half-life ^(d)	Primary Precursor/ Branching Ratio ^(e)	Alternate Precursor/ Branching Ratio ^(f)	Radio-nuclide	Precursor/ Branching Ratio ^(g)
Os185	1	OS185	9.40E+1				
Hg203	1	HG203	4.66E+1				
Pb210	1	PB210	8.12E+3				
	2	BI210	5.01E+0	1 1.0000	0 0.0000		
	3	PO210	1.38E+2	2 1.0000	0 0.0000		
Po210	1	PO210	1.38E+2				
Rn222	1	RN222	3.82E+0				
						P0218	1 1.0000
						PB214	1 1.0000
						BI214	1 1.0000
						P0214	1 1.0000
	2	PB210	8.12E+3	1 1.0000	0 0.0000		
						BI210	2 1.0000
						P0210	2 1.0000
	1	RA226	5.84E+5				
	2	RN222	3.82E+0	1 1.0000	0 0.0000		
Ra226						P0218	2 1.0000
						PB214	2 1.0000
						BI214	2 1.0000
						P0214	2 1.0000
	3	PB210	8.12E+3	2 1.0000	0 0.0000		
						BI210	3 1.0000
						P0210	3 1.0000

TABLE 4.10. (contd)

Designation	Explicit Daughters ^(b)				Implicit Daughters ^(c)		
	CINDY Position Index ^(d)	Chain Radio-nuclide	Half-life ^(d)	Primary Precursor/ Branching Ratio ^(e)	Alternate Precursor/ Branching Ratio ^(f)	Radio-nuclide	Precursor/ Branching Ratio ^(g)
Ra228	1	RA228	2.10E+3				
	2	RA224	3.62E+0				
						RN220	1 1.0000
						P0216	1 1.0000
						PB212	1 1.0000
						BI212	1 1.0000
						P0212	1 0.6407
						TL208	1 0.3593
Ac227	1	AC227	7.95E+3				
	2	TH227	1.87E+1	1 0.9862		FR223	1 0.0138
	3	RA223	1.14E+1	2 1.0000			
						RN219	3 1.0000
						P0215	3 1.0000
						PB211	3 1.0000
						BI211	3 1.0000
						P0211	3 0.0028
						TL207	3 0.9972
Th228	1	TH228	6.98E+2				
	2	RA224	3.62E+0	1 1.0000	0 0.0000		
						RN220	2 1.0000
						P0216	2 1.0000
						PB212	2 1.0000
						BI212	2 1.0000
						P0212	2 0.6407
						TL208	2 0.3593

TABLE 4.10. (contd)

Designation	Explicit Daughters ^(b)				Implicit Daughters ^(c)		
	CINDY Position Index ^(d)	Chain Radio-nuclide	Half-life ^(d)	Primary Precursor/ Branching Ratio ^(e)	Alternate Precursor/ Branching Ratio ^(f)	Radio-nuclide	Precursor/ Branching Ratio ^(g)
Th229	1	TH229	2.68E+6			RA225	1 1.0000
						AC225	1 1.0000
						FR221	1 1.0000
						AT217	1 1.0000
						BI213	1 1.0000
						P0213	1 0.9784
						TL209	1 0.0216
						PB209	1 1.0000
Th230	1	TH230	2.81E+7				
Th232	1	TH232	5.13E12				
	2	RA228	2.10E+3	1 1.0000	0 0.0000	AC228	2 1.0000
	3	TH228	6.98E+2	2 1.0000	0 0.0000	RA224	3 1.0000
						RN220	3 1.0000
						P0216	3 1.0000
						PB212	3 1.0000
						8I212	3 1.0000
						P0212	3 0.6407
						TL208	3 0.3593
Th234	1	TH234	2.41E+1			PA234M	1 0.9980
						PA234	1 0.0016
Pa231	1	PA231	1.36E+7				
	2	AC227	7.95E+3	1 1.0000	0 0.0000	FR223	2 0.0138

TABLE 4.10. (contd)

Designation	CINDY Position Index ^(d)	Explicit Daughters ^(b)			Implicit Daughters ^(c)		
		Chain Radio-nuclide	Half-life ^(d)	Primary Precursor/ Branching Ratio ^(e)	Alternate Precursor/ Branching Ratio ^(f)	Radio-nuclide	Precursor/ Branching Ratio ^(g)
Pa231 (contd)	3	TH227	1.87E+1	2 0.9862		RA223	3 1.0000
						RN219	3 1.0000
						PO215	3 1.0000
						PB211	3 1.0000
						BI211	3 1.0000
						PO211	3 0.0028
						TL207	3 0.9972
U232	1	U 232	2.36E+4				
	2	TH228	6.98E+2	1 1.0000	0 0.0000		
	3	RA224	3.62E+0	2 1.0000	0 0.0000		
						RN220	3 1.0000
						PO216	3 1.0000
						PB212	3 1.0000
						BI212	3 1.0000
						PO212	3 0.6407
						TL208	3 0.3593
U233	1	U 233	5.58E+7				
U234	1	U 234	8.93E+7				
U235	1	U 235	2.57E11				
U236	1	U 236	8.55E+9				

TABLE 4.10. (contd)

Designation	Explicit Daughters ^(b)				Implicit Daughters ^(c)		
	CINOY Position Index ^(d)	Chain Radio-nuclide	Half-life ^(d)	Primary Precursor/ Branching Ratio ^(e)	Alternate Precursor/ Branching Ratio ^(f)	Radio-nuclide	Precursor/ Branching Ratio ^(g)
U238	1	U 238	1.63E12				
	2	TH234	2.41E+1	1 1.0000	0 0.0000		
						PA234M	2 0.9980
						PA234	2 0.0016
Np237	1	NP237	7.81E+8				
	2	PA233	2.70E+1	1 1.0000	0 0.0000		
Np239	1	NP239	2.36E+0				
	2	PU239	8.81E+6	1 1.0000	2 0.9976		
Pu238	1	PU238	3.20E+4				
Pu239	1	PU239	8.79E+6				
Pu240	1	PU240	2.39E+6				
Pu241	1	PU241	5.26E+3				
	2	AM241	1.58E+5	1 1.0000	0 0.0000		
Am241	1	AM241	1.58E+5				
Cm242	1	CM242	1.63E+2				
	2	PU238	3.20E+4	1 1.000			
Cm244	1	CM244	6.61E+3				
Cf252	1	CF252	9.63E+2				

-
- (a) The radionuclide master library contains all radiological decay and daughter ingrowth data used by CINDY. In this library radionuclides are organized into chains controlled by integer indices.
 - (b) Daughters that may not be in equilibrium with their parents are tracked independently throughout the system.
 - (c) Short-lived daughters that are always assumed to be in equilibrium with their parents. The decay energies associated with these short-lived daughters have been assigned to the parent.
 - (d) Explicit daughter chain position index is an indicator of relative position in the decay chain (where 1 is highest position). This index is used to identify and control decay calculations for radionuclides in the chain.
 - (e) Chain position index of primary precursor in decay chain (as designated in the first column of this table), followed by the branching ratio.
 - (f) Chain position index of alternate precursor in decay chain (as defined in the first column of this table), followed by the branching ratio.
 - (g) Explicit daughter chain position index of precursor in decay chain (as designated in the first column of this table), followed by the branching ratio.

5.0 DESCRIPTION OF DOSE CALCULATIONS

As described in Section 2.0, once the integrated retentions of the radionuclides in the source organs have been calculated, the dose to each target organ is calculated for each radiation of type i from radionuclide j :

$$H(T + S)_i = U_S (1.6 \times 10^{-13}) \text{ SEE}(T + S)_i (10^3) \quad (5.1)$$

where U_S = the number of transformations of radionuclide j in source organ S over the period of integration following intake of the radionuclide

1.6×10^{-13} = the number of joules in 1 MeV

$\text{SEE}(T + S)_i$ = the specific effective energy for radiation type i , suitably modified by quality factor, absorbed in T from each transformation in S , in MeV g^{-1} per transformation

10^3 = the conversion factor from g^{-1} to kg^{-1} .

In general, for the intake of any mixture of radionuclides, i.e., parent with daughters, the dose in target organ T from radioactivity in several different sources S is given by

$$H = 1.6 \times 10^{-10} \sum_s \sum_j [U_{S_i} \sum \text{SEE}(T + S_i)_j] \quad (5.2)$$

The factors for specific effective energy are from a tape of SEE factors from Oak Ridge National Laboratory.^(a) For purposes of tabulating SEE values, the body is divided into a set of identified source and target regions with the remaining tissue assigned as "other." This region is largely muscle. The breast dose is based on the SEE values for "muscle" as a target.

The SEE value for "other" as a source is computed from an energy balance as

(a) Personal communication from Keith Eckerman of Oak Ridge National Laboratory, Oak Ridge, Tennessee.

$$\text{SEE}(T + \text{other}) = \frac{M_{TB} \text{ SEE}(T + TB) - \sum_S M_S \text{ SEE}(T + S)}{M_{\text{other}}} \quad (5.3)$$

where M_{TB} and M_S are the masses of the total body and source organs. The summation extends over all explicitly identified organs (source regions) in the metabolic model. The mass of the "other" tissue is

$$M_{\text{other}} = M_{TB} - \sum_S M_S. \quad (5.4)$$

5.1 DOSE TO ORGANS FROM MATERIAL IN THE TRANSFER COMPARTMENT

The evaluation of dose to organs includes consideration of activity in the transfer compartment. The transfer compartment is physically represented as the blood and is assumed to be distributed uniformly throughout all body organs and tissues, except for the contents of the bladder and GI tract. The evaluation of dose to specific organs from the activity in the transfer compartment involves redistribution of the transfer compartment transformations to other organs. The redistribution is performed on the basis of the mass of the specific organs as defined in ICRP (1979) for "Target Organs". These organ masses represent the location of the blood in the organ. The masses for "Source" and "Target" organs are the same for all organs except for the GI tract compartments which reflect differences between organ contents and organ wall tissues (ICRP 1979, Part I, page 17). The distribution factor is defined as follows.

$$R_{B0} = M_0 / M_{\text{Total Body}} \quad (5.5)$$

where R_{B0} = fraction of total transformation in the transfer compartment that occur in organ 0

M_0 = mass of organ or tissue 0, g,

$M_{\text{Total Body}}$ = mass of the total body, 70,000 g.

The number of transformation in the organs is then evaluated as follows.

$$U_{On} = U_{Bn} R_{BO} \quad (5.6)$$

where U_{On} = number of transformation of radionuclide n occurring in organ O ,

U_{Bn} = number of transformation of radionuclide n calculated to occur in the transfer compartment.

5.2 DOSE TO ORGANS FROM MATERIAL IN THE "OTHER" COMPARTMENT

The metabolic retention data for several radionuclides include a general organ designated as "other". For example, cesium has two entries under "other", having 10% and 90% uptake and retention half times of 2 and 110 days, respectively. The total activity distributed to "other" is then 100%, or uniform distribution throughout the body. In the evaluation of dose, the CINDY program evaluates the total number of transformations occurring in this "other" organ. These transformations are assumed to occur uniformly throughout the body in all organs except those specifically named in the metabolic data library. The redistribution is performed by a mass fraction method, similar to the method for redistribution of transformation in the transfer compartment. The redistribution factors are evaluated as follows.

$$R_{O0} = M_O / (M_{\text{Total Body}} - M_{\text{Named}}) \quad (5.7)$$

where R_{O0} = fraction of "other" compartment transformation that are assigned to occur in organ O ,

M_{Named} = total mass of all organs and tissues specifically named in the metabolic data set, g.

The number of transformations occurring in an organ or tissue from redistribution of "other" compartment transformations is evaluated using Equation 5.6 with R_{O0} in place of R_{BO} and U_{On} in place of U_{Bn} . The transformations not reassigned are assumed to occur in the remainder of the "other" tissues, which have a mass given as follows.

$$M_{\text{Remainder}} = M_{\text{Total Body}} - M_{\text{Named}} - \sum M_O \quad (5.8)$$

where $M_{\text{Remainder}}$ = mass of remaining tissues, g, and other terms are as previously defined. The organs included in the summation of Equation 5.8 include organs not named in the metabolic data library, but which are included in the dose calculation. These include lungs, GI compartments (wall tissue), gonads, breast, red marrow, thyroid, and bone surface. The fraction of the transformations assigned to the remaining tissue is as follows.

$$U_{\text{Remainder}} = U_{\text{Other}} M_{\text{Remainder}} / M_{\text{Other}} \quad (5.9)$$

where $U_{\text{Remainder}}$ = number of transformations occurring in the remaining organs and tissues, and other terms are as previously defined.

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APPENDIX A

TERMS USED

APPENDIX A

TERMS USED

Absorbed dose - The total energy absorbed per unit mass by an organ or tissue.

Activity median aerodynamic diameter (AMAD) - The aerodynamic diameter for a lognormal distribution of diameters, where half the activity present is associated with particles less than, and half of the activity is associated with particles greater than, the stated diameter.

Aerodynamic diameter - The diameter of a unit density sphere (1 g/cm^3) with the same terminal settling velocity in air as that of the aerosol particle.

Annual limit on intake (ALI) - The activity of a radionuclide which taken alone would irradiate a person, represented by Reference Man, to the limit set by ICRP for each year of occupational exposure.

Bioassay - The measurement of activity in naturally excreted products or in specific portions of the body.

Committed dose equivalent - The total dose equivalent averaged throughout a tissue in a specified time period after intake of a radionuclide into the body.

Committed effective dose equivalent - The sum of the committed dose equivalents to individual tissues resulting from an intake of a radionuclide multiplied by the appropriate weighting factors.

Derived air concentration (DAC) - The ALI (of a radionuclide) divided by the volume of air inhaled by Reference Man in a working year (2400 m^3).

Dose equivalent - The product of absorbed dose, the quality factor Q , and the product of any other modifying factors N (currently = 1).

GI - gastrointestinal.

Intake - The quantity of material introduced into the body by inhalation, by ingestion, or through the skin or a wound.

Quality factor - The principal modifying factor (which depends on the collision stopping power for charged particles) that is employed to derive dose equivalent from absorbed dose.

Recycling model - A compartmental model in which material can re-enter a compartment.

Reference Man - A hypothetical person with the anatomical and physiological characteristics defined by the ICRP Task Group on Reference Man (ICRP Publication 23, ICRP 1975).

SEE - Specific effective energy.

Sievert - The name for the SI unit of dose equivalent ($1 \text{ Sv} = 1 \text{ Joule/kg}$).

Stochastic effect - An effect for which the probability of occurrence is a function of the dose without threshold.

Translocation - The movement of material (deposited in the respiratory tract) by dissolution and absorption into blood.

Weighting factor - The ratio of the stochastic risk arising from exposure of a tissue to the total risk when the whole body is uniformly irradiated.

APPENDIX B

METABOLIC DATA

APPENDIX B

METABOLIC DATA

J. R. Johnson's metabolic data library (Johnson and Carver 1981; Johnson and Myers 1981) has been modified and expanded for use with the internal dosimetry programs in the CINDY Software Package. The adult metabolic data are taken from ICRP 30 (1979a, 1980, 1981b) with minor exceptions. The library contains adult and infant data on uptake by blood, f_1 values for each inhalation class, and distribution and retention in organs, as well as fraction of excretion via urine and feces. See Section 4.8.1 for additional information on metabolic data. Values of metabolic parameters describing transfer, retention, and excretion of radionuclides in the body are presented in Tables B.1 (general model radionuclides) and B.2 (alkaline earth radionuclides).

TABLE B.1. Metabolic Data in the CINDY Library

Element	Compartment Data				Excretion Fractions	
	Name	Part (a)	Fraction	Half-time days	Urine	Feces
Hydrogen	Other	1	1.0	10.0	0.47	0.0
Beryllium	Bone	1	0.40	1500.0	1.0	0.0
	Other	1	0.16	15.0	1.0	0.0
		2	0.04	1500.0	1.0	0.0
Carbon (organic)	Other	1	1.0	40.0	0.5	0.0
Fluorine	Bone	1	1.0	100.0	0.95	0.05
Sodium	Bone	1	0.3	10.0	0.75	0.02
		2	0.003	500.0	0.75	0.02
	Other	1	0.7	15.0	0.75	0.02
Silicon	Other	1	0.4	5.0	1.0	0.0
		2	0.6	100.0	1.0	0.0
Phosphorus	Bone	1	0.3	1500.0	0.8	0.2
	Other	1	0.15	2.0	0.8	0.2
		2	0.4	19.0	0.8	0.2
Sulfur	Other	1	0.15	20.0	0.80	0.14
		2	0.05	2000.0	0.80	0.14
Chlorine	Other	1	1.0	10.0	0.95	0.03
Potassium	Other	1	1.0	30.0	0.85	0.11
Scandium	Bone	1	0.04	5.0	0.1	0.9
		2	0.36	1500.0	0.1	0.9
	Liver	1	0.03	5.0	0.1	0.9
		2	0.27	1500.0	0.1	0.9
	Spleen	1	0.01	5.0	0.1	0.9
		1	0.09	1500.0	0.1	0.9
	Other	1	0.02	5.0	0.1	0.9
		2	0.18	1500.0	0.1	0.9
Chromium	Bone	1	0.05	1000.0	0.5	0.5
	Other	1	0.4	6.0	0.5	0.5
		2	0.25	80.0	0.5	0.5

TABLE B.1. (contd)

Element	Compartment Data				Excretion Fractions	
	Name	Part (a)	Fraction	Half-time days	Urine	Feces
Manganese	Bone	1	0.35	40.0	0.08	0.92
	Liver	1	0.1	4.0	0.08	0.92
		2	0.15	40.0	0.08	0.92
	Other	1	0.2	4.0	0.08	0.92
		2	0.2	40.0	0.08	0.92
Iron	Liver	1	0.08	2000.0	0.16	0.84
	Spleen	1	0.013	2000.0	0.16	0.84
	Other	1	0.907	2000.0	0.16	0.84
Cobalt	Liver	1	0.03	6.0	0.7	0.3
		2	0.01	60.0	0.7	0.3
		3	0.01	800.0	0.7	0.3
	Other	1	0.27	6.0	0.7	0.3
		2	0.09	60.0	0.7	0.3
		3	0.09	800.0	0.7	0.3
Nickel	Kidneys	1	0.02	0.2	0.50	0.0
	Other	1	0.30	1200.0	0.50	0.0
Copper	Liver	1	0.1	40.0	0.03	0.97
	Brain	1	0.1	40.0	0.03	0.97
	Pancreas	1	0.006	40.0	0.03	0.97
	Other	1	0.797	40.0	0.03	0.97
Zinc	Bone	1	0.2	400.0	0.077	0.7
	Other	1	0.24	20.0	0.077	0.7
		2	0.56	400.0	0.077	0.7
Gallium	Bone	1	0.09	1.0	0.1	0.1
		2	0.21	50.0	0.1	0.1
	Liver	1	0.027	1.0	0.1	0.1
		2	0.063	50.0	0.1	0.1
	Spleen	1	0.003	1.0	0.1	0.1
		2	0.007	50.0	0.1	0.1
	Other	1	0.18	1.0	0.1	0.1
		2	0.42	50.0	0.1	0.1
Germanium	Kidneys	1	0.5	0.02	1.0	0.0
	Other	1	0.5	1.0	1.0	0.0

TABLE B.1. (contd)

Element	Compartment Data				Excretion Fractions	
	Name	Part (a)	Fraction	Half-time days	Urine	Feces
Arsenic	Liver	1	0.028	1.0	0.05	0.8
		2	0.042	10.0	0.05	0.8
	Kidneys	1	0.006	1.0	0.05	0.8
		2	0.009	10.0	0.05	0.8
	Spleen	1	0.002	1.0	0.05	0.8
		2	0.003	10.0	0.05	0.8
	Other	1	0.22	1.0	0.05	0.8
		2	0.34	10.0	0.05	0.8
Selenium	Liver	1	0.015	3.0	0.35	0.14
		2	0.060	30.0	0.35	0.14
		3	0.075	150.0	0.35	0.14
	Kidneys	1	0.005	3.0	0.35	0.14
		2	0.02	30.0	0.35	0.14
		3	0.025	150.0	0.35	0.14
	Spleen	1	0.001	3.0	0.35	0.14
		2	0.004	30.0	0.35	0.14
		3	0.005	150.0	0.35	0.14
	Other	1	0.079	3.0	0.35	0.14
		2	0.31	30.0	0.35	0.14
		3	0.39	150.0	0.35	0.14
Bromine	Other	1	1.0	10.0	0.93	0.009
Rubidium	Bone	1	0.25	44.0	0.86	0.14
	Other	1	0.75	44.0	0.86	0.14
Yttrium	Bone	1	0.5	8000.0	0.1	0.9
	Liver	1	0.15	8000.0	0.1	0.9
	Other	1	0.10	8000.0	0.1	0.9
Zirconium	Bone	1	0.5	8000.0	1.0	0.0
	Other	1	0.5	7.0	1.0	0.0
Niobium	Bone	1	0.35	6.0	1.0	0.0
		2	0.35	200.0	1.0	0.0
	Kidneys	1	0.009	6.0	1.0	0.0
		2	0.009	200.0	1.0	0.0
	Spleen	1	0.005	6.0	1.0	0.0
		2	0.005	200.0	1.0	0.0
	Other	1	0.13	6.0	1.0	0.0
		2	0.13	200.0	1.0	0.0

TABLE B.1. (contd)

Element	Compartment Data				Excretion Fractions	
	Name	Part (a)	Fraction	Half-time days	Urine	Feces
Molybdenum	Bone	1	0.015	1.0	0.63	0.1
		2	0.14	50.0	0.63	0.1
	Liver	1	0.03	1.0	0.63	0.1
		2	0.27	50.0	0.63	0.1
	Kidneys	1	0.005	1.0	0.63	0.1
		2	0.045	50.0	0.63	0.1
	Other	1	0.05	1.0	0.63	0.1
		2	0.45	50.0	0.63	0.1
Technetium	S Wall	1	0.075	1.6	0.67	0.33
		2	0.02	3.7	0.67	0.33
		3	0.005	22.0	0.67	0.33
	Kidneys	1	0.05	1.6	0.67	0.33
		2	0.02	3.7	0.67	0.33
		3	0.005	22.0	0.67	0.33
	Thyroid	1	0.04	0.5	0.67	0.33
		2	0.0007	100.0	0.67	0.33
	Other	1	0.64	1.6	0.67	0.33
		2	0.17	3.7	0.67	0.33
		3	0.04	22.0	0.67	0.33
Ruthenium	Other	1	0.35	8.0	0.8	0.2
		2	0.30	35.0	0.8	0.2
		3	0.2	1000.0	0.8	0.2
Rhodium	Other	1	0.35	8.0	0.5	0.5
		2	0.30	35.0	0.5	0.5
		3	0.2	1000.0	0.5	0.5
Palladium	Liver	1	0.45	15.0	0.5	0.5
	Kidneys	1	0.15	15.0	0.5	0.5
	Bone	1	0.07	15.0	0.5	0.5
	Other	1	0.03	15.0	0.5	0.5
Silver	Liver	1	0.08	3.5	0.1	0.8
		2	0.72	50.0	0.1	0.8
	Other	1	0.02	3.5	0.1	0.8
		2	0.18	50.0	0.1	0.8
Cadmium	Liver	1	0.3	9000.0	0.8	0.2
	Kidneys	1	0.3	9000.0	0.8	0.2
	Other	1	0.4	9000.0	0.8	0.2

TABLE B.1. (contd)

Element	Compartment Data				Excretion Fractions	
	Name	Part (a)	Fraction	Half-time days	Urine	Feces
Indium	R Marrow	1	0.3	8000.0	0.1	0.1
	Liver	1	0.2	8000.0	0.1	0.1
	Kidneys	1	0.07	8000.0	0.1	0.1
	Spleen	1	0.01	8000.0	0.1	0.1
Tin	Bone	1	0.07	4.0	0.1	0.0
		2	0.07	25.0	0.1	0.0
		3	0.21	400.0	0.1	0.0
	Other	1	0.03	4.0	0.1	0.0
		2	0.03	25.0	0.1	0.0
		3	0.09	400.0	0.1	0.0
Antimony	Bone	1	0.19	5.0	1.0	0.0
		2	0.01	100.0	1.0	0.0
	Liver	1	0.095	5.0	1.0	0.0
		2	0.005	100.0	1.0	0.0
	Other	1	0.475	5.0	1.0	0.0
		2	0.025	100.0	1.0	0.0
Tellurium	Bone	1	0.25	5000.0	1.0	0.0
	Other	2	0.25	20.0	1.0	0.0
Cesium	Other	1	0.1	2.0	0.8	0.2
		2	0.9	110.0	0.8	0.2
Lanthanum	Bone	1	0.2	3500.0	0.1	0.9
	Liver	2	0.6	3500.0	0.1	0.9
	Other	1	0.20	3500.0	0.1	0.9
Cerium	Bone	1	0.2	3500.0	0.1	0.9
	Liver	1	0.6	3500.0	0.1	0.9
	Spleen	1	0.05	3500.0	0.1	0.9
	Other	1	0.15	3500.0	0.1	0.9
Praseodymium	Bone	1	0.25	3500.0	0.1	0.9
	Liver	1	0.6	3500.0	0.1	0.9
	Kidneys	1	0.05	10.0	0.1	0.9
Neodymium	Bone	1	0.45	3500.0	0.5	0.5
	Liver	1	0.45	3500.0	0.5	0.5
Promethium	Bone	1	0.45	3500.0	0.5	0.5
	Liver	1	0.45	3500.0	0.5	0.5
Samarium	Bone	1	0.45	3500.0	0.5	0.5
	Liver	1	0.45	3500.0	0.5	0.5

TABLE B.1. (contd)

Element	Compartment Data				Excretion Fractions	
	Name	Part (a)	Fraction	Half-time days	Urine	Feces
Europium	Bone	1	0.4	3500.0	0.5	0.5
	Kidneys	1	0.06	10.0	0.5	0.5
	Liver	1	0.4	3500.0	0.5	0.5
Gadolinium	Bone	1	0.45	3500.0	0.5	0.5
	Kidneys	1	0.03	10.0	0.5	0.5
	Liver	1	0.3	3500.0	0.5	0.5
Terbium	Bone	1	0.5	3500.0	0.5	0.5
	Kidneys	1	0.05	10.0	0.5	0.5
	Liver	1	0.25	3500.0	0.5	0.5
Dysprosium	Bone	1	0.6	3500.0	1.0	0.0
	Liver	1	0.1	3500.0	1.0	0.0
	Kidneys	1	0.02	10.0	1.0	0.0
Holmium	Bone	1	0.4	3500.0	0.1	0.9
	Liver	1	0.4	3500.0	0.1	0.9
	Pancreas	1	0.05	3500.0	0.1	0.9
Erbium	Bone	1	0.6	3500.0	1.0	0.0
	Liver	1	0.05	3500.0	1.0	0.0
	Other	1	0.1	3500.0	1.0	0.0
Ytterbium	Bone	1	0.50	3500.0	0.5	0.5
	Kidneys	1	0.02	10.0	0.5	0.5
	Spleen	1	0.005	3500.0	0.5	0.5
	Liver	1	0.03	3500.0	0.5	0.5
Hafnium	Bone	1	0.5	8000.0	1.0	0.0
	Other	1	0.5	7.0	1.0	0.0
Tantalum	Bone	1	0.3	100.0	1.0	0.0
	Kidneys	1	0.03	4.0	1.0	0.0
		2	0.03	100.0	1.0	0.0
	Other	1	0.32	4.0	1.0	0.0
		2	0.32	100.0	1.0	0.0
Tungsten	Bone	1	0.005	5.0	0.6	0.1
		2	0.0025	100.0	0.6	0.1
		3	0.018	1000.0	0.6	0.1
	Kidneys	1	0.007	5.0	0.6	0.1
		2	0.003	100.0	0.6	0.1
	Liver	1	0.007	5.0	0.6	0.1
		2	0.003	100.0	0.6	0.1

TABLE B.1. (contd)

Element	Compartment Data				Excretion Fractions	
	Name	Part (a)	Fraction	Half-time days	Urine	Feces
Tungsten (contd)	Spleen	1	0.0035	5.0	0.6	0.1
		2	0.0015	100.0	0.6	0.1
Rhenium	Thyroid S Wall	1	0.04	0.5	0.67	0.33
		1	0.075	1.6	0.67	0.33
		2	0.02	3.7	0.67	0.33
		3	0.005	22.0	0.67	0.33
	Liver	1	0.0225	1.6	0.67	0.33
		2	0.006	3.7	0.67	0.33
		3	0.0015	22.0	0.67	0.33
	Other	1	0.62	1.6	0.67	0.33
		2	0.17	3.7	0.67	0.33
		3	0.04	22.0	0.67	0.33
Osmium	Liver	1	0.04	8.0	0.5	0.5
		2	0.16	200.0	0.5	0.5
	Kidneys	1	0.0075	8.0	0.5	0.5
		2	0.033	200.0	0.5	0.5
	Spleen	1	0.004	8.0	0.5	0.5
		2	0.016	200.0	0.5	0.5
	Other	1	0.1	8.0	0.5	0.5
		2	0.44	200.0	0.5	0.5
Iridium	Liver	1	0.04	8.0	0.5	0.5
		2	0.16	200.0	0.5	0.5
	Kidneys	1	0.0075	8.0	0.5	0.5
		2	0.033	200.0	0.5	0.5
	Spleen	1	0.004	8.0	0.5	0.5
		2	0.016	200.0	0.5	0.5
	Other	1	0.1	8.0	0.5	0.5
		2	0.44	200.0	0.5	0.5
Gold	Other	1	1.0	3.0	1.0	0.0
Mercury	Brain	1	0.19	80.0	1.0	0.0
		2	0.01	10000.0	1.0	0.0
	Kidneys	1	0.076	80.0	1.0	0.0
		2	0.004	10000.0	1.0	0.0
	Other	1	0.68	80.0	1.0	0.0
		2	0.036	10000.0	1.0	0.0
Thallium	Kidneys	1	0.03	10.0	0.67	0.33
	Other	1	0.97	10.0	0.67	0.33

TABLE B.1. (contd)

Element	Compartment Data				Excretion Fractions	
	Name	Part (a)	Fraction	Half-time days	Urine	Feces
Lead	Bone	1	0.33	12.0	0.1	0.67
		2	0.11	180.0	0.1	0.67
		3	0.11	10000.0	0.1	0.67
	Liver	1	0.2	12.0	0.1	0.67
		2	0.045	180.0	0.1	0.67
		3	0.005	10000.0	0.1	0.67
	Kidneys	1	0.016	12.0	0.1	0.67
		2	0.0036	180.0	0.1	0.67
		2	0.0004	10000.0	0.1	0.67
	Other	1	0.14	12.0	0.1	0.67
		2	0.032	180.0	0.1	0.67
		3	0.0036	12000.0	0.1	0.67
Bismuth	Kidneys	1	0.24	0.6	0.9	0.1
		2	0.16	5.0	0.9	0.1
	Other	1	0.18	0.6	0.9	0.1
		2	0.12	5.0	0.9	0.1
Polonium	Liver	1	0.1	50.0	0.05	0.95
	Kidneys	1	0.1	50.0	0.05	0.95
	Spleen	1	0.1	50.0	0.05	0.95
	Other	1	0.7	50.0	0.05	0.95
Francium	Other	1	0.1	2.0	0.8	0.2
		2	0.9	110.0	0.8	0.2
Actinium	Bone	1	0.45	36500.0	0.1	0.9
	Liver	1	0.45	15000.0	0.1	0.9
	Testes	1	0.00035	36500.0	0.1	0.9
	Ovaries	1	0.00011	36500.0	0.1	0.9
Thorium	Bone	1	0.7	8000.0	1.0	0.0
	Liver	1	0.04	700.0	1.0	0.0
	Other	1	0.16	700.0	1.0	0.0
Protactinium	Bone	1	0.4	36500.0	0.5	0.5
		1	0.11	10.0	0.5	0.5
	Liver	2	0.05	60.0	0.5	0.5
		1	0.004	10.0	0.5	0.5
		2	0.016	60.0	0.5	0.5

TABLE B.1. (contd)

Element	Compartment Data				Excretion Fractions	
	Name	Part (a)	Fraction	Half-time days	Urine	Feces
Uranium	Bone	1	0.2	20.0	1.0	0.0
		2	0.023	5000.0	1.0	0.0
	Kidneys	1	0.12	6.0	1.0	0.0
		2	0.00052	1500.0	1.0	0.0
	Other	1	0.12	6.0	1.0	0.0
		2	0.00052	1500.0	1.0	0.0
Neptunium	Bone	1	0.75	36500.0	0.5	0.5
	Liver	1	0.15	15000.0	0.5	0.5
	Testes	1	0.00035	36500.0	0.5	0.5
	Ovaries	1	0.00011	36500.0	0.5	0.5
Plutonium	Bone	1	0.45	18250.0	0.5	0.5
	Liver	1	0.45	7300.0	0.5	0.5
	Testes	1	0.00035	36500.0	0.5	0.5
	Ovaries	1	0.00011	36500.0	0.5	0.5
Americium	Bone	1	0.45	18250.0	0.5	0.5
	Liver	1	0.45	7300.0	0.5	0.5
	Testes	1	0.00035	36500.0	0.5	0.5
	Ovaries	1	0.00011	36500.0	0.5	0.5
Curium	Bone	1	0.45	18250.0	0.5	0.5
	Liver	1	0.45	7300.0	0.5	0.5
	Testes	1	0.00035	36500.0	0.5	0.5
	Ovaries	1	0.00011	36500.0	0.5	0.5
Californium	Bone	1	0.65	18250.0	0.5	0.5
	Liver	1	0.25	7300.0	0.5	0.5
	Testes	1	0.00035	36500.0	0.5	0.5
	Ovaries	1	0.00011	36500.0	0.5	0.5

(a) Systemic organs may have up to 4 mathematical subcompartments. The index given here is the subcompartment index defined for the organ.

TABLE B.2. Alkaline Earth Element Metabolic Data

Element	Compartment	Part (a)	Rate Constant, days ⁻¹		Excretion Fractions	
			Into	From	Urine	Feces
Calcium	Bone Cancellous	Ca1	0.426	0.001120		
		Ca2	0.000605	0.000852		
	Bone Cortical	Co1	0.543	0.00439		
		Co2	0.00366	0.000189		
	Bone Surface	Bs	10.5	0.883		
	Other	O	11.1	1.54		
	Transfer	B	-	0.919	0.68	0.32
Strontium	Bone Cancellous	Ca1	0.378	0.00479		
		Ca2	0.00725	0.00105		
	Bone Cortical	Co1	0.516	0.00214		
		Co2	0.00136	0.000149		
	Bone Surface	Bs	2.66	0.403		
	Other	O	17.6	1.29		
	Transfer	B	-	3.44	0.8	0.2
Barium	Bone Cancellous	Ca1	0.776	0.00109		
		Ca2	0.000396	0.000863		
	Bone Cortical	Co1	1.21	0.00483		
		Co2	0.00318	0.000219		
	Bone Surface	Bs	2.95	0.265		
	Other	O	18.4	0.927		
	Transfer	B	-	30.9	0.10	0.90
Radium	Bone Cancellous	Ca1	0.241	0.000462		
		Ca2	0.00009	0.000251		
	Bone Cortical	Co1	0.430	0.00188		
		Co2	0.000991	0.000121		
	Bone Surface	Bs	7.83	0.221		
	Other	O	16.2	1.08		
	Transfer	B	-	26.9	0.05	0.95

(a) Cancellous bone (Ca1 and Ca2) and cortical bone (Co1 and Co2) are described by two subcompartments as indicated in Figure 4.7. See also Section 4.1.2 on nomenclature conventions.

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APPENDIX C

SOLVING ORDINARY DIFFERENTIAL EQUATIONS

APPENDIX C

SOLVING ORDINARY DIFFERENTIAL EQUATIONS

[Note: This Appendix is taken from Napier et al. 1988.]

The CINDY package is written in standard FORTRAN 77 using a Lahey compiler. Most routines are simple algebraic solutions, and no special logic is employed. The exception is the INTDF code, which calculates internal dose factors and uses a general purpose solver for ordinary differential equations. The solver used is from the ODEPACK collection developed at Lawrence Livermore National Laboratory (Hindmarsh 1983). The specific portion of ODEPACK used is called LSODES.

The LSODES package solves explicit systems of stiff differential equations. Stiffness is related to the rate constants of the equations and may require large numbers of iterations for some solution techniques. LSODES uses a backwards differentiation formulation, based on the multistep methods first implemented by Gear (1971). The following description was adapted from a publication by Hindmarsh (1983).

When solving a stiff system of size N, of the general form

$$\dot{y} \equiv dy/dt = f(t,y) \quad (C.1)$$

the LSODES package makes use of the Jacobian matrix of partial derivatives:

$$J = \delta f / \delta y \quad (C.2)$$

For stiff problems, LSODES uses the Backward Difference Formula (BDF)

$$y_n = \sum_{i=1}^q \alpha_i y_{n-i} + h \beta_0 \dot{y}_n \quad (C.3)$$

$$= a_n + h \beta_0 f(t_n, y_n) \quad (C.4)$$

where again q is the order (here $1 \leq q \leq 5$), and $\beta_0 > 0$. Stiffness makes functional iteration fail to converge for the step sizes of interest because of strong dependencies in f upon y . Therefore, LSODES uses a modified Newton iteration

$$-P [y_{n(m+1)} - y_{n(m)}] = y_{n(m)} - a_n - h \beta_0 f(t_n, y_{n(m)}) \quad (C.5)$$

where P is an $N \times N$ matrix approximating the Jacobian of the algebraic system to be solved:

$$P \approx I - h \beta_0 J, \quad J = \delta f / \delta y \quad (C.6)$$

where I here denotes the $N \times N$ identity matrix. Again, a prediction $y_{n(0)}$ is formed from an analogous explicit formula. This iteration differs from a true Newton method in that J is evaluated only periodically. In fact, J is evaluated only at predicted values $y_{n(0)}$ and only on those steps where a new value appears necessary, on the basis of a convergence failure or other indication. The same value of P (or its LU decomposition, if used) is used over all iterations in any one step, and typically also over several time steps, until a reevaluation of J and P is called for. (In the case of the LSODES solver, P is sometimes updated and LU-decomposed without a reevaluation of J .) Again, h and q are both varied to meet local error tolerance requirements.

In applying the BDF method to large stiff problems, it is important to note that a numerical solution of the linear system

$$Px = r \quad (C.7)$$

where x is the correction vector and r is the residual vector, can very often easily take advantage of a sparse structure in P . This is accomplished either through suitable structured LU decompositions, or through iterative linear system methods that use a given matrix structure. The use of structure is especially important in solving ODE systems that come from time-dependent partial differential equation (PDE) systems by the method of lines, whereby spatial variables are discretized, leaving ODEs in time.

The LSODES package solves explicit systems $\dot{y} = f$, but treats the Jacobian matrix J as a general sparse matrix in the stiff case. In LSODES, linear systems are solved using parts of the Yale Sparse Matrix Package (YSMP) (Eisenstat et al. 1977a and 1977b). Recall that the systems to be solved have the form

$$Px = r, \quad P = I - h\theta_0 J \quad (C.8)$$

where x is a correction vector, h is the step size, and θ_0 is a scalar depending on the current method order. The solution of these systems involves several phases:

1. Determination of sparsity structure. This is inferred from calls to the f routine.
2. Determination of pivot order. Diagonal pivot locations are chosen, and the choice is based on maintaining maximum sparsity. This is done by YSMP (ODRV module) (Eisenstat et al. 1977a). The ordering algorithm (minimum degree algorithm) operates only on a symmetric sparsity structure, and in LSODES the structure used for this is that of $J + J^T$.
3. Symbolic LU factorization of the matrix P . This is based only on sparsity and the pivot order, and uses the module in YSMP designed for nonsymmetric matrices with compressed pointer storage (CDRV module) (Eisenstat et al. 1977b).
4. Construction of J . This is done internally by difference quotients. The number of f evaluations needed is kept to a minimum by a column grouping technique due to Curtis, Powell, and Reid (1974). J is stored internally in an appropriate packed form. Evaluations of J are done only occasionally, as explained below.
5. Construction of $P = I - h\theta_0 J$. LSODES does not force a reevaluation of J whenever the existing P is deemed unsuitable for the corrector iterations. Instead, when the value of J contained in the stored value of P is likely to be usable (and P is not, only because $h\theta_0$ has changed significantly), then a new matrix P is constructed from the old one, with careful attention to roundoff error. This cuts down greatly on the total number of J evaluations.
6. Numerical LU factorization of P . This is done by YSMP (CDRV module) in sparse form, and the array containing P is saved in the process. Because of the absence of partial pivoting for numerical stability, this operation can conceivably fail. However, this has only rarely been observed in practice, and if it does occur (with

a current value of J), the step size h gets reduced and the difficulty disappears.

7. Solution of $Px = r$. This is done by YSMP (CDRV module) using the existing sparse factorization of P . Because a modified Newton iteration is used, many values of r (i.e., many linear systems) can arise for the same P , and the separation of the various phases takes advantage of that fact.

The first three phases and part of the fourth (column grouping for difference quotients) are normally done only at the start of the problem. However, the user can specify that the sparsity structure is to be redetermined in the middle of the problem, and then these operations are repeated.

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