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User Instructions for the Computer Codes of the Toolkit for Integrated Impact Assessments (TIIA), Version 1

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Abstract

Exposure estimation modeling is a central component of risk assessments. It is used for examining effects of past-practice discharges to the environment, estimating the consequences of accidental releases of hazardous materials, and determining if and how chemicals may be used in an environmental setting (for pesticide registration, for example). Ecological exposure models exhibit an array of complexity, ranging from relatively simplistic single-species, single-chemical, single-environmental-compartment models to more sophisticated multi-species, multi-chemical, multi-compartment models. Regulators and stakeholders occasionally require complex models to accommodate complex ecological or environmental conditions that are thought to be inadequately represented by simple or generalized models.

A number of existing ecological exposure models accommodate one or more aspects of complex ecosystems and exposure pathways. Historically, a single multimedia modeling system capable of addressing inorganic, organic, and radionuclide contaminants in both aquatic and terrestrial systems has not been available. Lack of such a system produces a potentially significant stumbling block to analyses of complex environmental systems, such as the U.S. Department of Energy's Hanford Site, where all three classes of contaminants have been introduced to the environment since nuclear operations began on the site in 1943.

The Toolkit for Integrated Impact Assessments (TIIA) is a suite of computer tools created as a multimedia modeling system to simulate the impacts of contaminants present in an ecosystem; including dose to humans and ecological impacts. This document describes the mathematical models implemented in this suite of codes and provides detailed user instructions for running the models.

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1.0 Introduction and Background

1.1 Background

Exposure estimation modeling is a central component of risk assessments. It is used for examining effects of past-practice discharges to the environment, estimating the consequences of accidental releases of hazardous materials, and determining if and how chemicals may be used in an environmental setting (for pesticide registration, for example). Ecological exposure models exhibit an array of complexity, ranging from relatively simplistic single-species, single-chemical, single-environmental-compartment models (such as in EPA, 1999) to more sophisticated multi-species, multi chemical. multi-compartment models (such as in Gobas, et al, 1988; Freeman et. al, 2004; Zakikhani et. al, 2006). Regulators and stakeholders occasionally require complex models to accommodate complex ecological or environmental conditions that are thought to be inadequately represented by simple or generalized models.

A number of existing ecological exposure models are able to accommodate one or more aspects of complex ecosystems and exposure pathways. The Wildlife Contaminants Exposure Model, which was developed by the Canadian Wildlife Service through a cooperative agreement with the National Center for Environmental Assessment of the U.S. Environmental Protection Agency's Office of Research and Development, estimates wildlife exposure to organic and inorganic contaminants through inhalation and ingestion of food, water and soil. The model addresses 24 species of birds, 17 mammals, 5 reptiles, and 3 amphibians from North American environments (Freeman et. al, 2004).

The Terrestrial Wildlife Exposure Model, which is a component of the U.S. Army Corps of Engineers' Army Risk Assessment Modeling System (ARAMS), addresses ingestion of food, soil, and surface water for 26 species of birds, 21 mammals, and 8 reptiles representing North American fauna (CH2MHILL 2001). Limitations of this model include its taxonomic coverage, limited exposure pathways, and lack of mechanistic components to address aquatic ecosystems (Zakikhani et. al, 2006). Aquatic species in ARAMS are addressed by a combination of databases (Environmental Residue Effects Database, biota/sediment accumulation factor database) and single-compartment models (such as the Theoretical Bioaccumulation Potential Model) that estimate tissue concentrations using measured sediment concentrations and the biota/sediment accumulation factor database (Zakikhani et. al, 2006). However, ARAMS does include a component module that accommodates species with home ranges that encompass spatially varying environmental concentrations of contaminants (the Spatially Explicit Exposure Model Von Stackelberg et. al, 2005).

A number of models address biological accumulation in aquatic food webs, including AQUAWEB (Arnot and Gobas, 2004], the EcoFate Model (Gobas et. al, 1998), and other unnamed models [Thomann 1989, Thomann et al., 1992; Thomann et. al, 1995). AQUAWEB and EcoFate are limited to organic chemicals, as is the Thomann (1989) and Thomann et al. (1992) models, while the Thomann et al. (1995) model addresses only metals in sediment. These models address exposure of aquatic species through ingestion and gill uptake pathways from water and/or sediment compartments, and include at least two components of a larger food web.

A number of ecological exposure and bioaccumulation models have been developed to address radionuclide transport in the environment. Most of these models have the human food supply as their primary output, including milk, meat, and eggs (for example, GENII (Napier, et. al, 2002) and ERMYN

(Wu, 2003)). Most rely upon transfer factors or coefficients to convert abiotic media concentrations into specific tissue concentrations for common species of interest, such as cattle, sheep, and pigs (Ng et. al, 1982, for example), although coefficients for less common wild foods such as seals and walrus have been developed to support specific components of society ((Layton et. al, 1997) for example). These models primarily address exposure and accumulation within a single receptor from radionuclides where the model uses only one or two environmental compartments. The GENII code provides a more complete analytical framework, including problematic radionuclides such as tritium and ^{14}C occurring in multiple abiotic compartments and a limited food chain capability.

Accumulation of contaminants in plants has been addressed through a variety of methods, including simple use of transfer factors/coefficients for specific species and contaminants ((Baes et. al, 1984 and Sheppard, 1985, for example) to complex multimedia models with uptake from leaves, stems, and roots for organic compounds (Trapp et. al, 1990 for example). RESRAD accommodates plant uptake from radionuclides in soils as well as in air (Yu et. al, 2002).

1.2 Document Purpose

Historically, a single, multimedia modeling system capable of addressing inorganic, organic, and radionuclide contaminants in both aquatic and terrestrial systems has not been available. Lack of such a system produces a potentially significant stumbling block to analyses of complex environmental systems, such as the U.S. Department of Energy's Hanford Site, where all three classes of contaminants have been introduced to the environment since nuclear operations began on the site in 1943 (Gephart, 2003).

The Toolkit for Integrated Impact Assessments (TIIA) is a suite of computer tools created as a multimedia modeling system to simulate the impacts of contaminants present in a ecosystem; including dose to humans and ecological impacts. This document describes the mathematical models implemented in this suite of codes and provides detailed user instructions for running the models.

1.3 Overview of the TIIA Codes

The TIIA system of codes includes computer programs, electronic data libraries, and data formatting processors (or data translators). The relationships among code modules that make up the TIIA are illustrated in Figure 1.1. The toolkit consists of two major modules (ECEM and HUMAN), two supporting modules (SOIL and RIPSAC), and a suite of 10 utility codes. Codes in the TIIA communicate through shared data files. One advantage of this structure is that measured data can be utilized for many inputs in place of simulated data, allowing customization of the problem to match the level of knowledge specific to the individual analysis. An overview of the computer codes described in this document is provided in Table 1.1.

The ECEM module (in the center of the diagram) calculates impacts to ecological species and concentrations in food products used for human consumption. The HUMAN module (in the center of the diagram) calculates impacts to humans from environmental exposures and consumption of contaminated foods. The two supporting modules appearing in the center of the diagram (SOIL and RIPSAC) calculate environmental accumulation of analytes in soil given concentrations of those analytes in groundwater and/or surface water.

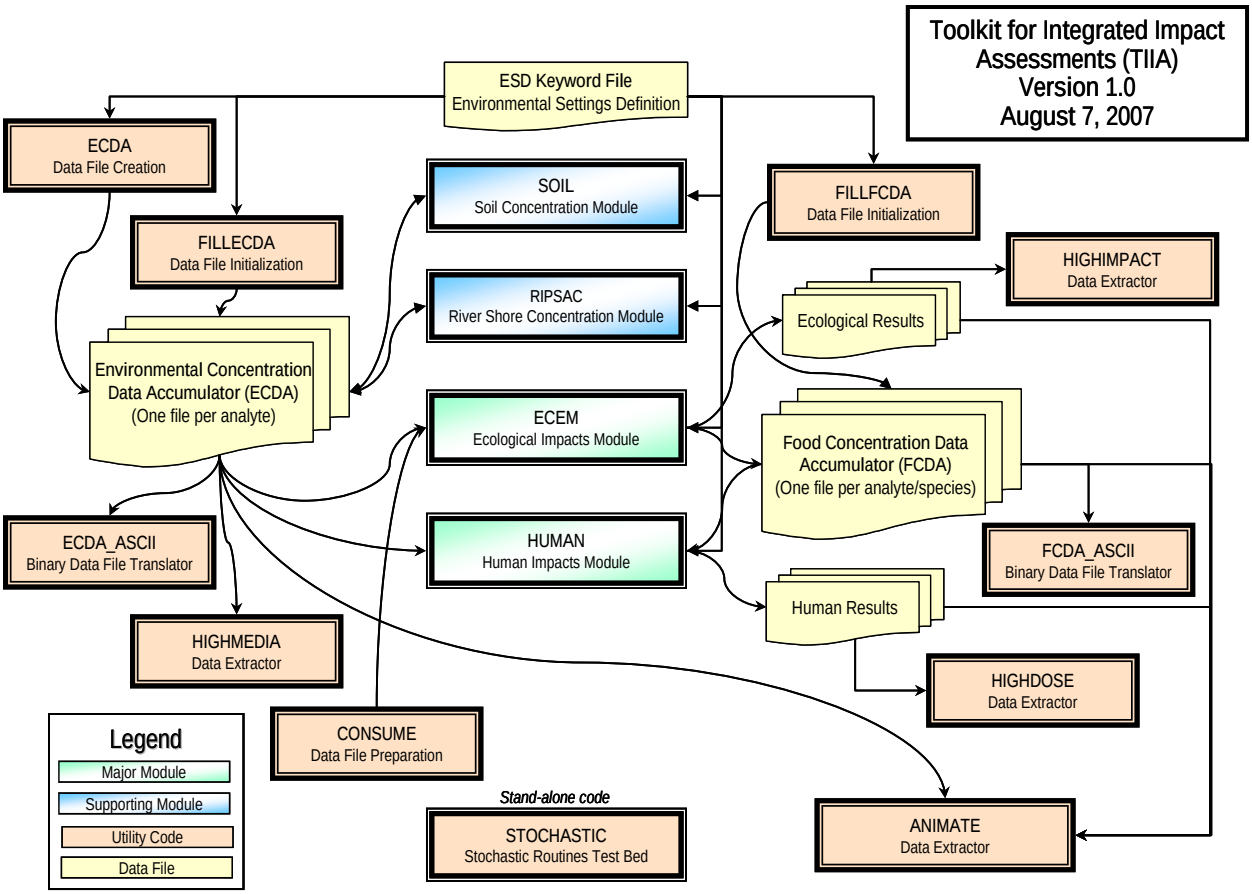

Figure 1.1 Module Information Flow for the TIIA Rev. 1 Impacts Codes

Table 1.1 Overview of TIIA Computer Codes

Code Name	Purpose
Environmental Concentrations in Abiotic Media	
SOIL	This program calculates the concentrations of analytes in near-surface soil given concentrations in irrigation water and deposition from the atmosphere. The model includes the effects of air deposition, precipitation and evaporation, irrigation with contaminated water, leaching from soil due to precipitation and irrigation, and radioactive decay.
RIPSAC	This program calculates the concentrations of analytes in seep water and soil given concentrations of analytes in groundwater and surface water. The algorithms apply only in the region along the edge of a body of water where there is significant interaction between groundwater and surface water.
Ecological and Human Impacts	
ECEM	This program calculates contaminant body burdens in ecological species and the dose or impact to those species. It also calculates contaminant concentrations in aquatic foods, terrestrial crops, and animal products for use in the HUMAN code.

Code Name	Purpose
HUMAN	This program calculates the dose or impact to humans from long-term contamination in the environment. Exposures can be due to contaminant concentrations in surface soil from irrigation, air from resuspension and volatilization, aquatic foods, terrestrial crops, and animal products.
Utility Functions - Stochastic Values Generation	
STOCHASTIC	This program can generate sample data sets and summary statistics for any stochastic variable. It also serves as a test bed for the stochastic routines common to the other codes.
Utility Functions - Environmental Concentration Data Files	
ECDA	This program creates the binary environmental concentration data accumulator (ECDA) files and initializes the contents for each medium.
ECDA_ASCII	This program converts a user-specified number of records in an ECDA file from binary storage mode to ASCII storage mode to allow visual inspection.
FILLECDA	This program allows user-specified values of concentration data to be inserted into an existing ECDA file.
HIGHMEDIA	This program allows extraction of the largest media value in an ECDA file for a suite of user-specified locations and years.
Utility Functions - Food Concentration Data Files	
FCDA_ASCII	This program converts a user-specified number of records in an FCDA (food concentration data) file from binary storage mode to ASCII storage mode to allow visual inspection.
FILLFCDA	This program allows user-specified values of concentration data to be inserted into an existing FCDA file.
Utility Functions - Impacts-Related	
ANIMATE	This program extracts data from the ECDA or outputs from ECEM or HUMAN and prepares data files for performing animations in the Tecplot© plotting program.
CONSUME	This program reformats species data contained in a spreadsheet into keyword data for use in the ECEM code.
HIGHDOSE	This program generates a summary table of the ecological species with the highest impacts for a suite of user-specified solutions.
HIGHIMPACT	This program extracts the highest impact (from a suite of possible impacts) for each year for a user-specified set of impact locations.

The TIIA codes can analyze exposures in aquatic systems, riparian systems (along the shoreline of a body of water) and upland systems. Impacts can be assessed for multiple analytes at multiple locations and multiple times in a single run of the codes. These codes implement chronic exposure models intended for use in situations where the environmental contamination conditions are static or only slowly varying (a value does not change significantly over one calendar year). These models are not appropriate for estimating risks from short-term accidental releases. The codes can handle three classes of contaminants: radioactive; non-radioactive and carcinogenic contaminants; and non-radioactive, hazardous, non-carcinogenic contaminants.

The TIIA codes are designed to accept multiple realizations of concentration of contaminants in the environment. They allow definition of stochastic exposure parameters, which combine with the

uncertainty in the input media concentrations to provide a full range of uncertainty on the final dose or risk to the exposed individual organism. The general approach to handling uncertainty in the TIIA is a Monte Carlo approach. Conceptually, a value is generated for every stochastic parameter in the code (the entire sequence of modules from inventory through transport and impacts), and then the simulation is executed to obtain an output value or result. This process is often called one *realization*. The entire process is then repeated, obtaining another result that is different from the first but as equally likely to occur as the first result. After repeating this process a number of times, one has a set of equally likely consequences that represent the statistical distribution of all outcomes. Several specialized sampling techniques have been developed to reduce the number of realizations required in a Monte Carlo analysis to obtain a satisfactory description of the output distribution. One of the techniques, called Latin Hypercube Sampling (Iman and Conover 1982), has proven successful for mass transport applications in groundwater systems. The general Monte Carlo approach still applies, and the specific values of the input parameters are chosen from the same statistical distributions; however, the sampling scheme spreads the values in a way that reduces sampling variability while also supporting a correlation structure between input variables.

1.4 General Rules for Reading Keyword Descriptions

Many of the programs described in this document are controlled by data files containing text entries called keyword records. A keyword record is typically constructed from an identifying "keyword" name (such as "ANALYTE") and data associated with the keyword (such as the names of analytes used in a simulation run). A description of the general syntax for keyword language is provided in Section 18.0. In the keyword descriptions of this document, some data are optional for a particular problem definition and some are required. For simplicity of interpretation, the following additional rules apply to the *keyword descriptions* that you will see in this document:

- Data that are required are enclosed in square brackets. For example, if AB were required, it would be denoted by [AB].
- If only one of the three items AB, BC, CD were required, it would be written as [AB|BC|CD]. The vertical bars indicate that the user must select one of the items in the list.
- Optional items are enclosed in normal brackets. For example, if DE were an optional entry, it would be denoted by {DE}.
- The {} or [] brackets or | vertical bars are NOT entered when constructing the actual keyword record: the keyword syntax specifications in this document use them only to indicate whether an item for the keyword is {optional} or [required] or a [required|choice].
- The keyword name can contain one or more characters; however, only the first eight characters are used (for example, REALIZAT has the same effect as REALIZATION).
- In some instances, numerical values or quote strings are associated with a modifier. This association is indicated by using the equal (=) symbol. The = symbol is not required but may be used when the keyword is constructed. When a numerical value or quote string is associated with a modifier, it must be entered on the input line directly after the modifier. Quote strings must be enclosed in double quotation marks. For example:

```
FILE C_ECDA  ANALYTE="U"  NAME="/home/CPO/ecda/U_CPO.dat"  CREATE
```

- Although keyword examples are indented in this document for the purpose of display, actual keyword records always start in column 1. Continuation records, which are treated as a continuation of a keyword record, appear further indented in the examples. For example:

```
SITES "300_RLWS" "300_RRLWS" "300_VTS" "300-121"
```

2.0 Shared Data Files

As shown in Figure 1.1, the TIIA codes consist of a number of component models that are executed independently. Some information, such as the start time and stop time of a simulated problem, are needed by more than one component of the systems code. The environmental settings definition (ESD) keyword file contains this common information. Generally, if information is needed by more than one module of the suite of codes, it will be entered in the ESD keyword file.

2.1 ESD Keyword File

The ESD keyword file is read by a number of different programs. Data required by one program may not be used in another program; thus, specifications of data being optional or required are not made in this section.

2.1.1 ANALYTE Keyword in the ESD Keyword File

The ANALYTE keyword is used to define the analytes to be used in the simulation. The following is this keyword's syntax:

```
ANALYTE ID="quote 1" TYPE="quote 2" NAME="quote 3"
HENRY=N1 DFIMM=N2 DFSED=N3 GAMMA=N4 HALFLIFE=N5 MOLDIFF=N6 COMPUTE
```

A separate ANALYTE keyword must be entered for every analyte to be included in the simulation.

Table 2.1 describes the modifiers for the ANALYTE keyword.

Table 2.1 Modifiers for the ANALYTE Keyword in the ESD File

Modifier	Description
COMPUTE	This modifier must be present for the ECDA program to create the associated binary concentration file. No file is created if this modifier is not present. Only the ECDA program uses this modifier.
DFIMM	The numerical entry associated with the DFIMM modifier is the immersion dose factor for radioactive analytes. This value has units of mrad/yr per μCi/m^3. Entry of this modifier is optional. If it is not present, the value of DFIMM defaults to zero. This value is used only in the ECEM code.
DFSED	The numerical entry associated with the DFSED modifier is the sediment external dose factor for radioactive analytes. This value has units of Sv-m^3/s-Bq. Entry of this modifier is optional. If it is not present, the value of DFSED defaults to zero. This value is used only in the ECEM code.
GAMMA	The numerical entry associated with the GAMMA modifier is the gamma decay energy for radioactive analytes. This value has units of MeV/nt. Entry of this modifier is optional. If it is not present, the value of GAMMA defaults to zero. This value is used only in the ECEM code.

Modifier	Description
HALFLIFE	The numerical entry associated with the HALFLIFE modifier is the half-life of the analyte. This value has units of years. Entry of this modifier is necessary when defining a radioactive analyte but should be omitted for nonradioactive analytes. If it is not present, the value of HALFLIFE defaults to infinity (decay constant value of zero).
HENRY	The numerical entry associated with the HENRY modifier is the Henry's law coefficient for organic analytes. This value has units of Pa-m^3/mol. Entry of this modifier is optional. If it is not present, the value of HENRY defaults to zero.
ID	The quote string associated with the ID modifier is an analyte identification string up to six characters in length. It is expected that common chemical formulae or acronyms would be used for the analyte identification string. The analyte identification string is case sensitive, and spaces or hyphens change the definition. All data in the analyte identification strings must satisfy the following conventions: • Only the first entry in the analyte identification string is capitalized. • No embedded spaces or hyphens are used, even for radionuclides. For example, *Np237* should be used for the nuclide neptunium-237 rather than *Np 237* or *Np-237* • Individual elements are defined using the standard element abbreviation. For example, use *U* for uranium. • The analyte identification string is also used as a directory name, so naming conventions in Windows or Linux must also be considered when assigning the identification string.
MOLDIFF	The numerical entry associated with the MOLDIFF modifier is the molecular diffusivity of the analyte. This value has units of cm^2/s and is used only in the ecological modules. Entry of this modifier is optional. If it is not present, the value of MOLDIFF defaults to zero.
NAME	The quote string associated with the NAME modifier is an analyte name or description up to 72 characters in length.
TYPE	The quote string associated with the TYPE modifier string is a two-character analyte type indicator. The following are the valid entries for this string: • NR – if the analyte is a radioactive element or an inorganic compound containing a radionuclide • NS – if the analyte is a stable (nonradioactive) element or inorganic compound • OR – if the analyte is an organic compound containing a radionuclide • OS – if the analyte is an organic compound containing a stable (nonradioactive) elemental analyte or compound

The following ANALYTE keywords select the analytes carbon tetrachloride, strontium-90 and carbon-14 for analysis.

```
ANALYTE ID="CCl4"   NAME="Carbon Tetrachloride" TYPE="NS"  COMPUTE
   HENRY  = 2.99E+03   MOLDIFF=5.0E-08  HALFLIFE = 0.0
ANALYTE ID="Sr90"  NAME="Strontium-90"  TYPE="NR"  COMPUTE
   HALFLIFE=28.78  DFIMM=1.703575E-03 DFSED=3.72E-21  GAMMA=0.0
   MOLDIFF=1.05E-05  HENRY=0.0
```

```
ANALYTE ID="C14"  NAME="Carbon-14"  TYPE="NR" AIR="NOBLE"      COMPUTE
   HALFLIFE=5.715E+03  DFIMM=5.122392E-05 DFSED=7.200000E-23  GAMMA=0.0
   MOLDIFF=1.05E-05  HENRY=0.0
```

2.1.2 DEBUG Keyword in the ESD Keyword File

The DEBUG keyword initiates output of optional data when the ECDA utility code is executed. The following is this keyword's syntax:

```
DEBUG ECDA
```

2.1.3 DILUTE Keyword in the ESD Keyword File

The DILUTE keyword is used to enter the definition of a statistical distribution for stochastic water dilution variables used in the riparian zone water mixing model. The following is this keyword's syntax:

```
DILUTE [ID="quote1"] [Dist_Index Parameters] {TRUNCATE U1 U2}
   {LABEL="quote2"}  [UNITS="quote3"]
```

The quote string associated with the ID modifier is a unique character string of up to 20 characters that will be used to identify this stochastic variable for subsequent uses. It is case sensitive, and embedded spaces are significant. The quote string associated with the optional modifier LABEL contains a description for the stochastic variable that can be up to 64 characters long. An entry for quote2 is not required, although it is used for labeling purposes if present. However, if the modifier LABEL is present, the associated quote string must be entered as well. The quote string associated with the UNITS modifier contains a units descriptor for the data. The strings "none" or "unitless" should be used if the variable is unitless. Section 19.0 contains further information about generating stochastic values, including use of the TRUNCATE option.

More than one DILUTE keyword may be entered. The set of DILUTE keywords is used to generate a library of stochastic values that can be accessed by any TIIA code. At this time only the RIPSAC code uses these values. The name of the library file is defined using the DILUTE modifier on the FILE keyword (Section 5.3.6).

A dilution factor that is triangular on the triple (0.2, 0.5, 0.99) could use the following keyword entry:

```
DILUTE ID="ID#1" 6 0.2 0.5 0.99 LABEL="Example dilution factor"
   UNITS="none"
```

2.1.4 ECHO Keyword in the ESD Keyword File

The ECHO keyword is used to initiate output of summary information by the ECDA utility code when processing the statistical distributions defined by KDSOIL and DILUTE keywords. The following is this keyword's syntax:

```
ECHO {KDSOIL} {DILUTE} {INFILT}
```

If the KDSOIL modifier is present, then variable definitions and summary statistics on generated values will be written to the report file for every distribution specified on a KDSOIL keyword. If the DILUTE modifier is present, then variable definitions and summary statistics on generated values will be written to the report file for every distribution specified on a DILUTE keyword. If the INFILT modifier is present,

then variable definitions and summary statistics on generated values will be written to the report file for every distribution specified on a INFILTRATION keyword containing the DEFINE modifier. Example uses of this keyword are the following:

```
ECHO KDSOIL
ECHO DILUTE
ECHO DILUTE KDSOIL INFILT
```

2.1.5 END Keyword in the ESD Keyword File

The END keyword signifies the end of all keyword data. It should be the last keyword in the keyword file. Any data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

2.1.6 FILE Keyword in the ESD Keyword File

The FILE keyword is used to enter the names of many of the files used in a simulation run. The following is this keyword's syntax:

```
FILE [NAME="quote1"] {ANALYTE="quote2"} {SEED=N1}
   [ HEADER | KDSOIL | DILUTE | INFILT | C_ECDA | I_ECDA ] {CREATE}
```

The file names must be entered with complete path information. Every file definition requires the entry of a separate FILE keyword. One FILE keyword is required for every analyte for which concentrations are to be generated. The modifiers for this keyword are described in Table 2.2.

Table 2.2 Modifiers for the FILE Keyword in the ESD File

Modifier	Description
ANALYTE	If the file name is associated with the C_ECDA modifier, the ANALYTE keyword must also be entered. The quote string associated with the ANALYTE modifier contains the ID for the analyte associated with the ECDA concentration data file (see the ANALYTE keyword in Section 5.3.1).
CREATE	This modifier is only used by the ECDA utility program. If this modifier is present, the file will be created during execution of the ECDA utility code. If the CREATE modifier is not present, no file creation actions occur for the file.
C_ECDA	This modifier indicates that the FILE keyword is defining an ECDA file. Data for each analyte are contained in separate files. The ANALYTE modifier is used to associate an analyte with this file (see the ANALYTE keyword in Section 5.3.1).
DILUTE	This modifier indicates that the FILE keyword is defining a file to contain stochastic realizations of all of the random variables defined using the DILUTE keyword.
HEADER	This modifier indicates that the FILE keyword is defining a header file for use by graphical post-processors that allow extraction of human-readable concentration data.
INFILT	This modifier indicates that the FILE keyword is defining a file to contain stochastic realizations of all of the random variables defined using the INFILTRATION keyword.
I_ECDA	This modifier indicates that the FILE keyword is defining a record index file for mapping into all ECDA concentration files.

Modifier	Description
KDSOIL	This modifier indicates that the FILE keyword is defining a file to contain stochastic realizations of all of the random variables defined using the KDSOIL keyword.
NAME	The quote string associated with the NAME modifier contains a file name (including path information) up to 200 characters in length.
SEED	If the file name is associated with the KDSOIL or DILUTE modifiers, the SEED modifier must also be entered. The numerical value associated with the SEED modifier is the value for the random number generator and must have an entry in the range 1 to 999999.

The following are example entries that define the concentration files for a suite of analytes:

```
FILE C_ECDA ANALYTE="H3" NAME="/test/ecda/H3_median.dat"  CREATE
FILE C_ECDA ANALYTE="C14" NAME="/test/ecda/C14_median.dat"  CREATE
FILE C_ECDA ANALYTE="I129" NAME="/test/ecda/I129_median.dat" CREATE
FILE C_ECDA ANALYTE="Tc99" NAME="/test/ecda/Tc99_median.dat" CREATE
```

If present, the CREATE flag causes the following actions by the ECDA code:

- Deletion of any existing file by that name and creation of a new file.
- If the file is associated with the HEADER, DILUTE, KDSOIL, C_ECDA or I_ECDA modifiers, new data are written to the file.

The following example entries define the files for soil-water Kd values, the water dilution factors for the river-shore module, and the groundwater infiltration rates for the soil module:

```
FILE KDSOIL NAME="KDSOIL.CSV" SEED=23232.0 CREATE
FILE DILUTE NAME="DILUTE.CSV" SEED=12345.0 CREATE
FILE INFILT NAME="infilt.dat"
```

The following example entries define the Header file and ECDA record number index files:

```
FILE HEADER NAME="/test/ecda/ECDA_median.hdr" CREATE
FILE I_ECDA  NAME="/test/ecda/ECDA_median.map"  CREATE
```

2.1.7 FILLECDA Keyword in the ESD Keyword File

The FILLECDA keyword tells the ECDA code which values to use for initialization when an ECDA file is created. The following is this keyword's syntax:

```
FILLECDA [GWAT|SWAT|AIRC|AIRD|PWAT|SEDI|SORP|SEEP|SODR|SOGW|SOSW]
   [FIXED=N1|RANDOM]
```

Multiple entries of this keyword are required to define values for the different media. The modifiers for this keyword are described in Table 2.3.

Table 2.3 Modifiers for the FILLECDA Keyword in the ESD File

Modifier	Description
AIRC	Presence of this optional modifier indicates that atmospheric concentrations will be initialized with the specified value.

Modifier	Description
AIRD	Presence of this optional modifier indicates that atmospheric deposition rates will be initialized with the specified value.
FIXED	The value N_1 associated with the FIXED modifier is the value to be used to initialize the specified media in the ECDA file. Concentrations are typically initialized to zero, or an invalid (-1.0) value.
GWAT	Presence of this optional modifier indicates that groundwater concentrations will be initialized with the specified value.
PWAT	Presence of this optional modifier indicates that river bottom pore water concentrations will be initialized with the specified value.
RANDOM	The RANDOM option is used only for testing purposes. When RANDOM is selected, the media concentrations are all filled with values from a uniform distribution on the (0,1) interval.
SEDI	Presence of this optional modifier indicates that sediment concentrations (on the river bottom) will be initialized with the specified value.
SEEP	Presence of this optional modifier indicates that seep water concentrations (on the land surface) will be initialized with the specified value.
SODR	Presence of this optional modifier indicates that upland soil concentrations from non-irrigated soils will be initialized with the specified value.
SOGW	Presence of this optional modifier indicates that upland soil concentrations using groundwater for irrigation will be initialized with the specified value.
SORP	Presence of this optional modifier indicates that riparian zone soil concentrations (on the land surface) will be initialized with the specified value.
SOSW	Presence of this optional modifier indicates that upland soil concentrations using surface water for irrigation will be initialized with the specified value.
SWAT	Presence of this optional modifier indicates that surface water concentrations will be initialized with the specified value.

The following example entries assign values to all 11 media for initialization of the ECDA files:

```
FILLECDA GWAT FIXED =  0.0
FILLECDA PWAT FIXED =  0.0
FILLECDA SWAT FIXED =  0.0
FILLECDA SEEP FIXED = -1.0
FILLECDA SEDI FIXED =  0.0
FILLECDA SORP FIXED = -1.0
FILLECDA SODR FIXED = -1.0
FILLECDA SOGW FIXED = -1.0
FILLECDA SOSW FIXED = -1.0
FILLECDA AIRC FIXED =  0.0
FILLECDA AIRD FIXED =  0.0
```

2.1.8 INFILTRATION Keyword in the ESD Keyword File

The INFILTRATION keyword defines the stochastic distribution for net natural infiltration rates through surface soil. The infiltration rates are tagged with an ID (called a CLASS) and they are assumed to be constant with time. If irrigation is used at one or more locations, then an infiltration rate must be

specified for each location. Multiple locations can use one infiltration rate by assigning that specific ID. Definition of infiltration rates use the following syntax:

```
INFILTRATION DEFINE [CLASS="quote 1"]  [UNIT="quote 2"]
   [Dist_Index Parameters]  {TRUNCATE U1 U2}  {"quote 3"}
```

The quote string associated with the CLASS modifier contains a user-specified ID for the infiltration class. The data for this class will be referenced by the ID. The quote string associated with the UNIT modifier must contain the data units. Units of mm/yr must be used. The quote string identified as quote3 contains a descriptive label for this infiltration class and must be the third quote string in the keyword entry.

The remaining entries for this syntax are used to define a statistical distribution for the infiltration rate. Additional information about these entries is provided in Section 19.1. Some example uses of this syntax are the following:

```
INFILTRATION DEFINE UNIT="mm/yr" CLASS="Hanford" 1 0.1 "Hanford Barrier"
INFILTRATION DEFINE UNIT="mm/yr" CLASS="Hs-dn" 1 55
```

2.1.9 IRRIGATE Keyword in the ESD Keyword File

The IRRIGATE keyword defines the irrigation rates to be used by the SOIL model. The following is this keyword's syntax:

```
IRRIGATE [SPRING=N1] [FALL=N2] [RATE=N3] [NET=N4] [START=N5]
   [THETAIRG=N6] [THETADRY=N7]
```

The modifiers for this keyword are defined in Table 2.4. The same irrigation period and water application rate applies to all locations in the model domain. No irrigation occurs before the start year. Once irrigation starts, it continues for every subsequent year in the simulation period.

Table 2.4 Modifiers for the IRRIGATE Keyword in the ESD File

Modifier	Description
FALL	The numerical entry associated with the FALL modifier is the last day of the year (in julian days) that irrigation occurs.
NET	The numerical entry associated with the NET modifier is the net fraction of irrigation that percolates below 15 cm in the soil.
RATE	The numerical entry associated with the RATE modifier is the irrigation rate that is applied. This value has units of cm/yr.
SPRING	The numerical entry associated with the SPRING modifier is the day of the year (in julian days) that irrigation begins in the spring.
START	The numerical entry associated with the START modifier is the calendar year that irrigation begins. The assumption is that no irrigation occurs before that date, and that once started, irrigation continues every year after that through the end of the simulation.
THETADRY	The numerical entry associated with the THETADRY modifier is the surface soil volumetric water content during the dry (non-irrigated) period. This value has units of mL/cm^3.

Modifier	Description
THETAIRG	The numerical entry associated with the THETAIRG modifier is the surface soil volumetric water content during the irrigation period. This value has units of mL/cm^3.

The following example begins yearly irrigation in 2004 at a rate of 75 cm per year with 20% of the water infiltrating below 15 cm in soil depth.

```
IRRIGATE SPRING=121 FALL=256 RATE=75.0 NET=0.20 START=2004 THETAIRG=0.5
   THETADRY=0.2
```

2.1.10 KDSOIL Keyword in the ESD Keyword File

The KDSOIL keyword is used to enter statistical distribution definitions for solid-aqueous distribution coefficients (K_d) to be used for calculating soil and sediment concentrations from water concentrations. The following is this keyword's syntax:

```
KDSOIL [ID="quote1"] [Dist_Index Parameters] {TRUNCATE U1 U2}
   {LABEL="quote2"}  [UNITS="quote3"]
```

- The quote string associated with the ID modifier is a unique character string of up to 20 characters that will be used to identify this stochastic variable for subsequent uses. It is case sensitive and embedded spaces are significant.
- The quote string associated with the optional modifier LABEL contains a description for the stochastic variable that can be up to 64 characters long. An entry for quote2 is not required, although it is used for labeling purposes if present. If the modifier LABEL is present the associated quote string must be entered as well.
- The quote string associated with the UNITS modifier contains a units descriptor for the data. The strings "none" or "unitless" should be used if the variable is unitless.
- Further information about defining statistical distributions is provided in Section 19.0.

More than one KDSOIL keyword may be entered. The set of KDSOIL keywords is used to generate a library of stochastic values that can be accessed by any TIIA code. The name of the library file is defined using the KDSOIL modifier on the FILE keyword (Section 5.3.6).

A K_d that is triangular on the triple (0.2, 0.5, 0.99) would use the following keyword entry:

```
KDSOIL ID="ID#1" 6 0.2 0.5 0.99 LABEL="Example Kd" UNITS= "L/g"
```

The data entered by this keyword are used in the river model MASS2, the riparian zone model RIPSAC, and the soil concentration model SOIL.

2.1.11 LOCATION Keyword in the ESD Keyword File

The LOCATION keyword identifies the locations where concentrations will be generated for use in the impacts modules. The following is this keyword's syntax:

```
LOCATION [ID="quote1"] [EASTING=N1] [NORTHING=N2] {AREA=N3}
   {POP=N4} {GWAT} {SWAT} {AIRC} {AIRD} {PWAT} {SEDI} {SORP}
   {SEEP} {SODR} {SOGW} {SOSW} [NAME="quote2"] [TYPE="quote3"]
   {APSD=N5} {POROSITY= N6} {FOC=N7} {VEGCOV=N8}
   {NECF=N9} {RHOS=N10} {SRH=N11} {TEMP=N12} {MSWIND=N13} {MZWIND=N14}
   {COXYGEN=N15} {MILE=N16} {IRG_SWAT="quote5"}
```

The modifiers and associated data for this keyword are described in Table 2.5.

Table 2.5 Modifiers for the LOCATION Keyword in the ESD File

Modifier	Description
AIRC	Presence of this optional modifier indicates that atmospheric concentrations will be stored in the ECDA files for this location.
AIRD	Presence of this optional modifier indicates that atmospheric deposition rates will be stored in the ECDA files for this location.
APSD	The numerical value associated with the APSD modifier is the aggregate particle size. This value has units of mm and is used only in the ECEM code. It is valid only for land locations.
AREA	The numerical value associated with the AREA modifier identifies the land surface area associated with the location. This value has units of m^2.
COXYGEN	The numerical value associated with the COXYGEN modifier is the concentration of oxygen in surface water. This value has units of g/L and is used only in the ECEM code. It is valid only for aquatic locations.
EASTING	The numerical value associated with the EASTING modifier is the easting coordinate for this location. These coordinates are used only for post-run plotting, thus any consistent coordinate system may be used.
FOC	The numerical value associated with the FOC modifier is the fraction of organic carbon content in the soil. This value is unitless and is used only in the ECEM code. It is valid only for land locations.
GWAT	Presence of this optional modifier indicates that groundwater concentrations will be stored in the ECDA files for this location. This option can be used only for upland or aquatic locations.
ID	The quote string associated with the ID modifier contains the ID for this location. This string is limited to 15 characters and must be unique. It is used to associate other data with a specific location.
IRG_SWAT	The quote string associated with the modifier indicates the source of surface water for use in computing soil concentrations. The quote string must contain the ID of a location where a surface water solution is computed.
MILE	The numerical value associated with the MILE modifier is the shoreline mile for the location. This value has units of miles and is used only for riparian or aquatic locations.
MSWIND	The numerical value associated with the MSWIND modifier is the mean annual wind speed. This value has units of m/s and is used only in the ECEM code. It is valid only for land locations.
MZWIND	The numerical value associated with the MZWIND modifier is the mixing zone wind speed. This value has units of m/s and is used only in the ECEM code. It is valid only for land locations.
NAME	The quote string associated with the NAME modifier is a name or description up to 72 characters in length for this location. This value is used for labeling purposes only.

Modifier	Description
NECF	The numerical value associated with the NECF modifier is the non-erodible elements correlation factor. This value is unitless and is used only in the ECEM code. It is valid only for land locations.
NORTHING	The numerical value associated with the NORTHING modifier is the northing coordinate for this location. These coordinates are used only for post-run plotting, thus any consistent coordinate system may be used.
POROSITY	The numerical value associated with the POROSITY modifier is the soil porosity. This value is unitless and is used only in the ECEM code. It is valid only for land locations.
POP	The numerical value associated with the POP modifier is the human population at this location. This value is used only in the HUMAN code for calculating population dose.
PWAT	Presence of this optional modifier indicates that river bottom pore water concentrations will be stored in the ECDA files for this location. This option can only be used for aquatic locations.
RHOS	The numerical value associated with the RHOS modifier is the soil density. This value has units of g/cm3 and is used in the ECEM and SOIL codes. It is valid only for land locations.
SEDI	Presence of this optional modifier indicates that sediment concentrations (on the river bottom) will be stored in the ECDA files for this location. This option can be used only for aquatic locations.
SEEP	Presence of this optional modifier indicates that seep water concentrations (on the land surface) will be stored in the ECDA files for this location. This option can be used only for upland or aquatic locations.
SODR	Presence of this optional modifier indicates that soil concentrations without irrigation will be stored in the ECDA files for this location. This option can be used only for upland locations.
SOGW	Presence of this optional modifier indicates that soil concentrations calculated by using groundwater for irrigation will be stored in the ECDA files for this location. This option can be used only for upland locations.
SORP	Presence of this optional modifier indicates that riparian zone soil concentrations (on the land surface) will be stored in the ECDA files for this location. This option can be used only for riparian locations.
SOSW	Presence of this optional modifier indicates that soil concentrations calculated by using surface water for irrigation will be stored in the ECDA files for this location. This option can be used only for upland locations.
SRH	The numerical value associated with the SRH modifier is the surface roughness height. This value has units of m and is used only in the ECEM code. It is valid only for land locations.
SWAT	Presence of this optional modifier indicates that surface water concentrations will be stored in the ECDA files for this location. This option can be used only for aquatic locations.
TEMP	The numerical value associated with the TEMP modifier is the temperature. This value has units of Kelvin and is used only in the ECEM model. It is valid only for land locations.

Modifier	Description
TYPE	The quote string associated with the TYPE modifier is the location type. The following are the valid entries for this string: UPLAND, RIPARIAN, or AQUATIC.
VEGCOV	The numerical value associated with the VEGCOV modifier is the fraction of vegetation cover at the location. This value is unitless and is used only in the ECEM model. It is valid only for land locations.

The following example keywords define three upland locations:

```
LOCATION ID="UH0001" NAME="UnsuitableForAgricul" EASTING=576022
   NORTHING=154367 GWAT SOGW SOSW SODR AIRC AIRD, TYPE = "UPLAND",
   APSD = 4.00E-02  POROSITY= 3.50E-01  FOC = 1.0E+00
   VEGCOV   = 5.00E-01  NECF    = 1.00E+00  RHOS   = 1.50E+00
   SRH  = 1.8E-02 TEMP     = 2.85E+02  MSWIND  = 3.44E+00
   MZWIND = 3.44E+00 IRG_SWAT ="QHP025"   AREA    = 1457376.1

LOCATION ID="UH0042" NAME="AgExclusionBuffer" EASTING=573022
   NORTHING=149867 GWAT SOGW SOSW SODR AIRC AIRD, TYPE = "UPLAND",
   APSD = 4.00E-02  POROSITY= 3.50E-01  FOC \\= 1.0E+00
   VEGCOV   = 5.00E-01  NECF    = 1.00E+00  RHOS   = 1.50E+00
   SRH  = 1.8E-02 TEMP     = 2.85E+02  MSWIND  = 3.44E+00
   MZWIND = 3.44E+00 IRG_SWAT ="QHP025"   AREA    =  562500.0

LOCATION ID="UH0015" NAME="Upland" EASTING=576022 NORTHING=152117
   GWAT SOGW SOSW SODR AIRC AIRD, TYPE = "UPLAND",
   APSD     = 4.00E-02  POROSITY= 3.50E-01  FOC    = 1.0E+00
   VEGCOV   = 5.00E-01  NECF    = 1.00E+00  RHOS   = 1.50E+00
   SRH  = 1.8E-02 TEMP     = 2.85E+02  MSWIND  = 3.44E+00
   MZWIND = 3.44E+00 IRG_SWAT ="QHP025"   AREA    =  562500.0
```

The following example keywords define three aquatic locations:

```
LOCATION ID="Q02I01" NAME="ISLAND 02,BLM" EASTING=574295.6
   NORTHING=155058.0 SWAT SEDI PWAT TYPE="AQUATIC"
   MILE=375.49 COXYGEN = 1.10E-02 AREA = 2.5E+03

LOCATION ID="Q06I04" NAME="ISLAND,06,LOCKE ISLAND,UPLANDS-DOE,SHORE-BLM"
   EASTING=577962.1 NORTHING=154231.9 SWAT SEDI PWAT TYPE="AQUATIC"
   MILE=373.09 COXYGEN = 1.10E-02 AREA = 2.5E+03

LOCATION ID="QTV008" NAME="Transect VERNITA-1 HRM 0.3" EASTING=559027
   NORTHING=146042 SWAT SEDI PWAT TYPE="AQUATIC"
   MILE=387.83 COXYGEN = 1.10E-02 AREA = 2.5E+03
```

The following example keywords define three riparian locations:

```
LOCATION ID="RFP021" NAME="RiparianGrantUpriver100BC" EASTING=564431.8
   NORTHING=145847.4 GWAT SEEP SORP AIRC AIRD TYPE="RIPARIAN"
   MILE=384.40 APSD    = 4.00E-02  COXYGEN = 1.10E-02
   POROSITY= 3.50E-01  FOC  = 1.0E+00   VEGCOV  = 5.00E-01
   NECF    = 1.00E+00  RHOS   = 1.50E+00  SRH   = 1.8E-02  TEMP = 2.85E+02
   MSWIND  = 3.44E+00 MZWIND  = 3.44E+00  AREA    = 9360
```

```
LOCATION ID="RFP022" NAME="RiparianGrant100BC" EASTING=564841.7
   NORTHING=145818.1 GWAT SEEP SORP AIRC AIRD TYPE="RIPARIAN"
   MILE=384.10 APSD    = 4.00E-02  COXYGEN = 1.10E-02
   POROSITY= 3.50E-01  FOC  = 1.0E+00   VEGCOV  = 5.00E-01
   NECF    = 1.00E+00  RHOS   = 1.50E+00  SRH  = 1.8E-02  TEMP = 2.85E+02
   MSWIND  = 3.44E+00 MZWIND  = 3.44E+00  AREA    = 9360

LOCATION ID="RFP031" NAME="RiparianGrantCoyoteRapids" EASTING=568198.5
   NORTHING=147140.3 GWAT SEEP SORP AIRC AIRD TYPE="RIPARIAN"
   MILE=381.70 APSD    = 4.00E-02  COXYGEN = 1.10E-02
   POROSITY= 3.50E-01  FOC  = 1.0E+00   VEGCOV  = 5.00E-01
   NECF    = 1.00E+00  RHOS  = 1.50E+00  SRH  = 1.8E-02  TEMP = 2.85E+02
   MSWIND  = 3.44E+00 MZWIND  = 3.44E+00  AREA    = 9360
```

2.1.12 PERIOD Keyword in the ESD Keyword File

The PERIOD keyword identifies the start and stop times for the entire simulation. The following is this keyword's syntax:

```
PERIOD [START=year1] [STOP=year2] [CLOSURE=year3]
```

The modifier START and the associated value $year_1$ identify the calendar year the simulation starts. The modifier STOP and the associated value $year_2$ identify the calendar year the simulation ends. Start and stop years should be entered as whole numbers with the stop year no smaller than the start year. The modifier CLOSURE and the associated value $year_3$ identify the year that site closure occurs (and all inventory actions have been completed). The year of site closure cannot be smaller than the start year. This keyword controls actions for other codes not included in the TIAA and the value can be set to the STOP year.

The following is an example PERIOD keyword that simulates from 1944 through 3050 with site closure also occurring at 3050:

```
PERIOD START=1944 STOP=3050 CLOSURE 3050
```

2.1.13 RADIUS Keyword in the ESD Keyword File

The RADIUS keyword is used to build a radius-dependent effective energy library. The ECEM code uses these radius-dependent energies for radiological dose calculations. The following is this keyword's syntax:

```
RADIUS [ID="quote 1"] value1 value2 … valuek
```

The first RADIUS keyword must always have ID="Radius", and the values are the radii for which the analyte data are given. The subsequent RADIUS keywords have an ID of an analyte name, and the values are the effective energies by radius for that analyte. The values with ID="Radius" are distances with units of cm. The values with the ID set to any specific analyte have units of kg-rad/ pCi/d. The following are example RADIUS keywords that provide effective energies for carbon-14, cesium-137, and chlorine-36:

```
RADIUS ID="Radius" 1.4E+0 2.0E+0 3.0E+0 5.0E+0 7.0E+0 1.0E+1 2.0E+1 3.0E+1
RADIUS ID="C14"    5.0E-2 5.0E-2 5.0E-2 5.0E-2 5.0E-2 5.0E-2 5.0E-2 5.0E-2
RADIUS ID="Cs137"  2.6E-1 2.7E-1 2.8E-1 3.2E-1 3.5E-1 3.9E-1 5.0E-1 5.8E-1
RADIUS ID="Cl36"   2.6E-1 2.6E-1 2.6E-1 2.6E-1 2.6E-1 2.6E-1 2.6E-1 2.6E-1
```

2.1.14 REALIZAT Keyword in the ESD Keyword File

The REALIZAT keyword identifies the number of realizations to be simulated. The following is this keyword's syntax:

```
REALIZAT N1
```

The number of realizations is given by the single numerical entry N_1. The valid number of realizations is 1 to 9999. Run times and disk storage requirements are directly proportional to the number of realizations. The following REALIZAT keyword requests 25 realizations:

```
REALIZAT 25
```

2.1.15 REPORT Keyword in the ESD Keyword File

The REPORT keyword defines the file that will contain diagnostic messages and log the progress for the current run of ESP. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The REPORT keyword must be the first keyword in the file. There can be comment lines before this keyword, but if it is not the first keyword, then the ESP program will error terminate. Programs other than ESP do not use the REPORT keyword in the ESD keyword file. The name of the report file is entered in a quote string, which must be enclosed in double quotation marks. File names up to 200 characters long are supported, and path information can be included. The following is an example REPORT keyword:

```
REPORT "/home/ANALYSIS/Initial2/ESD_Initial2.rpt"
```

2.1.16 SPECIES Keyword in the ESD Keyword File

The SPECIES keyword is used to enter definitions for ecological species to be simulated. The ECEM code uses species from this master list and passes computed information on to the HUMAN code. The following is this keyword's syntax:

```
SPECIES [ID="quote 1"] [TYPE="quote 2"] [NAME="quote 3"]
   {Modifier=N1} … {Modifier=N28} {EMERGENT}
```

A separate SPECIES keyword must be entered for every species being defined. Table 2.6 describes the modifiers associated with the SPECIES keyword.

Table 2.6 Modifiers for the SPECIES Keyword in the ESD File

Modifier	Description
ID	The quote string associated with the ID modifier is a unique species identification string up to six characters in length.
TYPE	The quote string associated with the TYPE modifier string is a two-character analyte type indicator. The following are the valid entries for this string: TA – if the species is a terrestrial animal TP – if the species is a terrestrial plant QA – if the species is an aquatic animal QP – if the species is an aquatic plant.

Modifier	Description
NAME	The quote string associated with the NAME modifier is a species name or description up to 72 characters in length.
AE	The numerical entry associated with the AE modifier is the assimilation efficiency of the species. This value is unitless. This modifier applies only to terrestrial plants and animals. If it is not present, the value of AE defaults to zero.
AWD	The numerical entry associated with the AWD modifier is the wet-to-dry weight ratio of the species. This value has units of g wet/g dry. This modifier applies only to aquatic plants and animals. If it is not present, the value of AWD defaults to zero.
DIFFHT	The numerical entry associated with the DIFFHT modifier is the diffusion height of the species. This value has units of meters. This modifier applies only to terrestrial plants and animals. If it is not present, the value of DIFFHT defaults to zero.
EMERGENT	There is no numerical entry associated with the EMERGENT modifier. Use of this modifier indicates that the species is an emergent plant. An emergent plant is one that has roots in water but grows in the air. This type of plant does not have rain splash of contaminated soil onto the leaves.
ETWATER	The numerical entry associated with the ETWATER modifier is the exposure time to water of the species. This value has units of hr/day. This modifier applies only to terrestrial plants and animals. If it is not present, the value of ETWATER defaults to zero.
FLIPID	The numerical entry associated with the FLIPID modifier is the fraction of the mass of the species that is lipid. This value has units of g lipid/g wet. This modifier applies only to aquatic plants and animals. If it is not present, the value of FLIPID defaults to zero.
FMR	The numerical entry associated with the FMR modifier is the free metabolic rate of predator species. This value has units of kcal/day. This modifier applies only to terrestrial animals. If it is not present, the value of FMR defaults to zero.
FOC	The numerical entry associated with the FOC modifier is the fraction organic carbon of the species. This value has units of g organic carbon/g dry weight. This modifier applies only to aquatic plants and animals. If it is not present, the value of FOC defaults to zero.
FPA	The numerical entry associated with the FPA modifier is the volume fraction of plant tissue that is air for the species. This value is unitless. This modifier applies only to terrestrial plants. If it is not present, the value of FPA defaults to zero.
FPL	The numerical entry associated with the FPL modifier is the volume fraction of plant tissue that is lipid for the species. This value is unitless. This modifier applies only to terrestrial plants. If it is not present, the value of FPL defaults to zero.
FPW	The numerical entry associated with the FPW modifier is the volume fraction of plant tissue that is water for the species. This value is unitless. This modifier applies only to terrestrial plants. If it is not present, the value of FPW defaults to zero.
FW	The numerical entry associated with the FW modifier is the water weight fraction of plant tissue for the species. This value is unitless. This modifier applies only to terrestrial plants. If it is not present, the value of FW defaults to zero.

Modifier	Description
FWATER	The numerical entry associated with the FWATER modifier is the fraction exposure to water for the species. This value is unitless. This modifier applies only to terrestrial plants and animals. If it is not present, the value of FWATER defaults to zero.
FDW	The numerical entry associated with the FDW modifier is the conversion from dry weight to wet weight for the species. This value has units of kg dry/kg wet. This modifier applies only to terrestrial animals. If it is not present, the value of FDW defaults to zero.
GE	The numerical entry associated with the GE modifier is the gross energy for the species. This value has units of kcal/kg wet weight. This modifier applies only to terrestrial plants and animals. If it is not present, the value of GE defaults to zero.
INHRATE	The numerical entry associated with the INHRATE modifier is the resting inhalation rate for the species. This value has units of m3/day. This modifier applies only to terrestrial animals. If it is not present, the value of INHRATE defaults to zero.
OCAR	The numerical entry associated with the OCAR modifier is the organic carbon assimilation rate for the species. This value has units of g organic carbon assimilated/g ingested. This modifier applies only to aquatic animals. If it is not present, the value of OCAR defaults to zero.
PCS	The numerical entry associated with the PCS modifier is the fraction of surface area in contact with soil for the species. This value has units of 1/day. This modifier applies only to terrestrial animals. If it is not present, the value of PCS defaults to zero.
PCW	The numerical entry associated with the PCW modifier is the fraction of surface area available to water soil for the species. This value is unitless. This modifier applies only to terrestrial animals. If it is not present, the value of PCW defaults to zero.
PSI	The numerical entry associated with the PSI modifier is the seasonality factor for the species. This value is unitless. This modifier applies only to terrestrial animals. If it is not present, the value of PSI defaults to zero.
RADIUS	The numerical entry associated with the RADIUS modifier is the radius of the species. This value has units of cm. This modifier applies to all ecological species. If it is not present, the value of RADIUS defaults to zero.
RHOP	The numerical entry associated with the RHOP modifier is the plant tissue density of the species. This value has units of kg/m^3. This modifier applies only to terrestrial plants. If it is not present, the value of RHOP defaults to zero.
SA	The numerical entry associated with the SA modifier is the surface area of the species. This value has units of cm^2. This modifier applies only to terrestrial animals. If it is not present, the value of SA defaults to zero.
SADHER	The numerical entry associated with the SADHER modifier is the skin adherence factor for the species. This value has units of mg/cm^2. This modifier applies only to terrestrial animals. If it is not present, the value of SADHER defaults to zero.
THETA	The numerical entry associated with the THETA modifier is the area use factor for the species. This value is unitless. This modifier applies only to terrestrial animals. If it is not present, the value of THETA defaults to zero.

Modifier	Description
WATERING	The numerical entry associated with the WATERING modifier is the water ingestion rate for the species. This value has units of liters/day. This modifier applies only to terrestrial animals. If it is not present, the value of WATERING defaults to zero.
WBMASS	The numerical entry associated with the WBMASS modifier is the wet body mass for the species. This value has units of grams. This modifier applies only to aquatic plants and animals. If it is not present, the value of WBMASS defaults to zero.
WEIGHT	The numerical entry associated with the WEIGHT modifier is the wet body weight for the species. This value has units of kg (wet). This modifier applies only to terrestrial plants and animals. If it is not present, the value of WEIGHT defaults to zero.

The following six examples illustrate the use of the SPECIES keyword for a variety of locations and species characteristics:

```
! Aquatic plant
SPECIES ID="QPERIP" TYPE="QP" NAME="periphyton" HABITAT="AQUATIC"
   AWD=10  FLIPID=0.0418   FOC=0.35  RADIUS=1.4   WBMASS=0.000035

! Aquatic animal
SPECIES ID="QCARPS" TYPE="QA" NAME="CARP  " HABITAT="AQUATIC"
   CAR=8.0000E-01   AWD=5.0000E+00 FLIPID=7.4000E-02 FOC=4.5000E-01
   BMASS=1.0500E+03 RADIUS=7.0000E+00

! Terrestrial animal - riparian location
SPECIES ID="RACOOT" TYPE="TA" NAME="American coot" HABITAT="RIPARIAN"
   AE=8.1000E-01   DIFFHT=2.0000E-01  ETWATER=2.0000E+01
   FMR=1.6309E+02  FWATER=5.0000E-01  FDW=0.4
   GE=1.9000E+03   INHRATE=6.1593E-01 PCS=2.5000E-01
   PCW=5.0000E-01     PSI=1.0000E+00      RADIUS=5.0000E+00
   SADHER=1.4500E+00  THETA=1.0000E+00   SA=7.8406E+02
   WATERING=4.6102E-02  WEIGHT=6.9200E-01

! Terrestrial animal - upland location
SPECIES ID="UBDGER" TYPE="TA" NAME="American badger" HABITAT="UPLAND"
   AE=8.1000E-01   DIFFHT=2.0000E-02  ETWATER=0.0000E+00
   FMR=8.2073E+02  FWATER=0.0000E+00  FDW=0.4
   GE=1.7000E+03   INHRATE=6.0032E+00 PCS=2.2000E-01
   PCW=0.0000E+00  PSI=1.0000E+00     RADIUS=1.0000E+01
   SADHER=1.4500E+00  THETA=1.0000E+00   SA=4.1972E+03
   WATERING=7.2063E-01  WEIGHT=9.0000E+00

! Terrestrial plant - riparian location
SPECIES ID="RCTWOD" TYPE="TP" NAME="black cottonwood" HABITAT="RIPARIAN"
   SURFACE=7.8050E+01 AE=3.4000E-01 DIFFHT=5.0000E+00 FPA=5.0000E-01
   FPL=1.0000E-02  FPW=4.0000E-01    FW=5.5000E-01 GE=3.2000E+03
   FWATER=0.0000E+00 RADIUS=3.0000E+01 RHOP=1.0000E+03
   WEIGHT=2.0000E+02 ETWATER=0.0000E+00

! Terrestrial plant - upland location
SPECIES ID="UFUNGI" TYPE="TP" NAME="fungi" HABITAT="UPLAND"
   SURFACE=1.0000E-03 AE=7.3000E-01 DIFFHT=5.0000E-02 FPA=5.0000E-01
   FPL=1.0000E-02  FPW=4.0000E-01    FW=9.1000E-01 GE=6.3000E+02
   FWATER=0.0000E+00 RADIUS=1.4000E+00 RHOP=1.0000E+03
```

```
WEIGHT=3.0000E-03 ETWATER=0.0000E+00
```

2.1.17 TIMES Keyword in the ESD Keyword File

The TIMES keyword identifies the times at which concentration data will be saved in the ECDA files to support the calculations by the impacts codes. The following is this keyword's syntax:

```
TIMES [T1] {T2} … {Tn}
```

The numerical entries T_1, T_2, …, T_n are the times (whole number calendar years) when concentration data are to be saved. The following example TIMES keyword requests concentration data for the three years 2020, 2075, and 3014:

```
TIMES 2020 2075 3014
```

2.1.18 TITLE Keyword in the ESD Keyword File

The TITLE keyword is used to define a single-line problem title for the ESD run. The problem title will be written to output files. If the title is not supplied, the program will error terminate. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 200 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the environmental settings control file."
```

2.1.19 USER Keyword in the ESD Keyword File

The USER keyword is used to identify the user of the ESP program. The user name will be written to output files. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

2.2 Environmental Concentration Data Accumulator (ECDA) Files

The purpose of the Environmental Concentration Data Accumulator (ECDA) is to provide a central storage for all environmental concentrations of analytes at the set of locations and times needed to perform impact calculations.

The file structure for the ECDA files has the following characteristics:

- Data for different analytes is stored in separate files (9 analytes would result in 9 concentration files). This design feature allows addition of an analyte to a data set without recalculation of the other analytes.
- The files have a binary, fixed record length, direct-access format.

- A mapping scheme is used to store only actual data (no placeholders with wasted storage space).

2.2.1 ECDA Data File Format

A binary ECDA file contains 12 header lines followed by data lines. The header lines contain the following information:

- Analyte ID
- Ci/m^3 or kg/m^3 (Units of concentrations in groundwater)
- Ci/m^3 or kg/m^3 (Units of concentrations in seep water
- Ci/m^3 or kg/m^3 (Units of concentrations in surface water
- Ci/m^3 or kg/m^3 (Units of concentrations in river bottom pore water)
- Ci/kg or kg/kg (Units of concentrations in river bottom sediment)
- Ci/kg or kg/kg (Units of concentrations in riparian zone soil)
- Ci/kg or kg/kg (Units of concentrations in upland soil [no irrigation])
- Ci/kg or kg/kg (Units of concentrations in upland soil [groundwater irrigation])
- Ci/kg or kg/kg (Units of concentrations in upland soil [surface water irrigation])
- Ci/m^3 or kg/m^3 (Units of concentrations in air)
- $Ci/m^2/yr$ or $kg/m^2/yr$ (Units of air deposition rate)

After the first 12 header lines, each data record in a ECDA file contains the following information: Year, Location ID, Media ID, media data (realizations 1 to the maximum). The relative order in which media data appear in the file for a given time and location is always the following:

- GWAT: concentrations in groundwater (Ci/m^3 or kg/m^3)
- SEEP: concentrations in seep water (Ci/m^3 or kg/m^3)
- SWAT: concentrations in surface water (river) (Ci/m^3 or kg/m^3)
- PWAT: concentrations in river bottom pore water (Ci/m^3 or kg/m^3)
- SEDI: concentrations in river bottom sediment ($Ci/kg_{sediment}$ or $kg_{analyte}/kg_{sediment}$)
- SORP: concentrations in riparian zone soil (land surface) (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)
- SODR: concentrations in upland soil (land surface) with no irrigation (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)
- SOGW: concentrations in upland soil (land surface) with groundwater irrigation (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)
- SOSW: concentrations in upland soil (land surface) with surface water irrigation (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)
- AIRC: concentrations in air (Ci/m^3 or kg/m^3)
- AIRD: air deposition rates (Ci/m^2 per yr or kg/m^2 per yr).

Table 2.7 provides an overview of the structure of an ECDA file in which 25 realizations were used.

Table 2.7 Structure of an ECDA File

ANALYTE ID		
11 lines, each containing the units for one medium as a character string		
Time 1	Location 1	Media L1-1, 25 realizations
		…
		Media L1-L1MAX, 25 realiz.
	Location 2	Media L2-1, 25 realizations

		…
		Media L2-L2MAX, 25 realiz.
	…	…
	Max	Media LL-1, 25 realizations
	Locations	…
		Media LL-LLMAX, 25 realiz.
Time 2	Location 1	Media L1-1, 25 realizations
		…
		Media L1-L1MAX, 25 realiz.
	Location 2	Media L2-1, 25 realizations
		…
		Media L2-L2MAX, 25 realiz.
	…	…
	Max	Media LL-1, 25 realizations
	Locations	…
		Media LL-LLMAX, 25 realiz.
…	…	…
Max Time	Location 1	Media L1-1, 25 realizations
		…
		Media L1-L1MAX, 25 realiz.
	Location 2	Media L2-1, 25 realizations
		…
		Media L2-L2MAX, 25 realiz.
	…	…
	Max	Media LL-1, 25 realizations
	Locations	…
		Media LL-LLMAX, 25 realiz.

2.2.2 ECDA Index File Format

The ECDA index file is an ASCII file that provides indexing information for the storage locations in the binary ECDA files. One index file is used for all ECDA files for a given simulation problem because the structure of the files are identical for all analytes. This file is generated by the ECDA code. The user should never modify this file.

The index file has several header lines that are followed by indexing data. All character data are enclosed in double quotation marks, and records that contain more than one value have the data separated by commas. The definition of the header lines is as follows:

- **Problem Title.** The title from the ESD keyword file.
- **Code Name.** The name of the code that generated the file.
- **Code Version.** The version number of the code that generated the file.
- **Code Date:** The modification date of the code that generated the file.
- **User Name:** The user name from the ESD keyword file.
- **Run ID.** The run ID from the code run that generated the file.
- **Block Size.** The number of records with data in a time block in the binary data file.
- **Record Length.** Record length for the binary data file.
- **Number of Realizations.** The number of realizations requested for this run.
- **Number of Times.** The number of solution times requested for this run.

- **List of Times.** A list of solution times with one time per line.
- **Number of Locations.** The number of locations requested for this run.
- **List of Locations.** A list of locations IDs, with one ID per line.

The header data are followed by record map index data. There are as many lines of index data as there are locations. The index data for locations come in the same order as the location IDs provided earlier in the file. Each line of index data contains the location ID followed by as many indices as there are media types. The indices give an offset record number. If values for a particular media are not saved at a location, then the index value is set to negative 1. Table 2.8 provides an example index file for a small data set.

Table 2.8 Example ECDA Index File

```
"Prepare Dose and Risk Factors for the ABC Study"
"ECDA"
"2.00.011"
"27 Jan 2006"
"Paul W. Eslinger"
"20060426162057"
14,"Records in a time block"
18,"Record length in the ECDA file"
1,"Number of realizations"
2,"Number of times"
2000
2050
3,"Number of locations"
"UH0001"
"RHP001"
"QHP001"
11,"Number of media"
"GWAT"
"SEEP"
"SWAT"
"PWAT"
"SEDI"
"SORP"
"SODR"
"SOGW"
"SOSW"
"AIRC"
"AIRD"
"UH0001",13,-1,-1,-1,-1,-1,14,15,16,17,18
"RHP001",19,20,-1,-1,-1,21,-1,-1,-1,22,23
"QHP001",-1,-1,24,25,26,-1,-1,-1,-1,-1,-1
```

2.2.3 ECDA Header File Format

The header file is an output file containing information used by post-processing utility codes to allow easy extraction of subsets of data stored in the ECDA files. These file is written by the ECDA code. The file contains the following sections of information:

- a header section of basic run information
- number of realizations selected

- media used
- times used
- locations used
- analytes used and analyte data file names
- record map file name.

Excerpts from a header file are given in Table 2.9. The user specifies only the name of this file; users should not modify the file after it is generated by the ECDA code. Because this file typically has at most a few thousand entries, the file size is always smaller than 200 Kb. File names for options not selected are set to the string "null".

Table 2.9 Example ECDA Header File

```
type: "ECDA"
title: "2007 Example Assessment"
user: "Eslinger-DWE-WEN"
name: "ECDA"
version: "2.00.A.4"
date: "16 Oct 2003"
id: "20040802132252"
envfile: "ESD_median.key"
realizations: 1
media: 11
"GWAT","Groundwater concentrations"
"SEEP","Seep water (riparian zone) concentrations"
"SWAT","Surface water (river) concentrations"
"PWAT","Pore water (river bottom) concentrations"
"SEDI","Sediment (river bottom) concentrations"
"SORP","Soil (riparian zone) concentrations"
"SODR","Non-irrigated upland soil concentrations"
"SOGW","Groundwater irrigated upland soil concentrations"
"SOSW","Surface water irrigated upland soil concentrations"
"AIRC","Air concentrations"
"AIRD","Air deposition rates"
times: 2
 1945
 1950
locations: 4
"UH0001","UnsuitableForAgricul"
"UH0002","UnsuitableForAgricul"
"QTV010","Transect VERNITA-1 HRM 0.3"
"QHRWI1","City of Richland Municipal Water Intake"
analytes: 3
"C14","NR","Carbon-14"
"/home/ANALYSIS4/CA1_median/ecda/C14_CA1_median.dat"
"Cs137","NR","Cesium-137"
"/home/ANALYSIS4/CA1_median/ecda/Cs137_CA1_median.dat"
"Cl36","NR","Chlorine-36"
"/home/ANALYSIS4/CA1_median/ecda/Cl36_CA1_median.dat"
recordmap: "/home/ANALYSIS4/CA1_median/ecda/ECDA_CA1_median.map"
```

2.2.4 ECDA File Size

The size of an ECDA file is limited to 2.147×10^9 bytes because the current implementation of the Fortran compilers for both the Linux and Windows operating system environments use 32 bit addressing. The ECDA file size for an analyte is a function of four quantities: the number of realizations, the number of impact solution times, the number of locations and the number of media saved at each location. The file is a binary file where the record length (in bytes) is 14 plus four times the number of realizations. The number of records is 12 (header lines) plus the product of three items: the number of impact solution times, the number of impact locations, and the number of media generated at each location. The ECDA file size can be calculated using the following equation:

$$F_s = 12 \times (4N_r + 14) + (4N_r + 14) \times N_{st} \times \left(\sum_{u=1}^{N_u} N_{um} + \sum_{r=1}^{N_r} N_{rm} + \sum_{q=1}^{N_q} N_{qm} \right)$$

Where:

F_s = The file size in bytes
N_r = The number of realizations
N_{st} = The number of impact solution times
N_u = The number of impact locations defined as upland locations
N_{um} = The number of media (maximum of 6) saved at an upland location
N_r = The number of impact locations defined as riparian locations
N_{rm} = The number of media (maximum of 5) saved at a riparian location
N_q = The number of impact locations defined as aquatic locations
N_{qm} = The number of media (maximum of 3) saved at an aquatic location

If the maximum number of media are saved at every location the file size can be calculated from the following equation:

$$F_s = 12 \times (4N_r + 14) + (4N_r + 14) \times N_{st} \times (\{6 \times N_u\} + \{5 \times N_r\} + \{3 \times N_q\})$$

2.3 Food Concentration Data Accumulator (FCDA) Files

The purpose of the Food Concentration Data Accumulator (FCDA) is to provide a central storage for all concentrations of analytes at in food products at the locations and times needed to perform human impact calculations.

The file structure for the FCDA files has the following characteristics:

- Data storage for different analytes are provided in separate files (9 analytes would result in 9 concentration files). This design feature allows addition of an analyte to a data set without recalculation of the other analytes.
- The files have a binary, fixed record length, direct-access format.
- A mapping scheme is used to store only actual data (no placeholders with wasted storage space).

2.3.1 FCDA Data File Format

A binary food concentration data file contains three header lines that are followed by concentration data. The header lines have the following definition:

- Record 1: Analyte ID – 6 Characters

- Record 2: Species ID – 6 Characters
- Record 3: Species Habitat – Up to 8 Characters (AQUATIC, RIPARIAN or UPLAND).

Each of the succeeding data records has the following information (output in the following order):

- Time: Integer (kind=4)
- Location ID: 6 Characters
- Concentration values: As many concentration values as realizations, each of type Real (kind=4).

2.3.2 FCDA Index File Format

The FCDA index file is an ASCII file that provides indexing information for the storage locations in the binary FCDA files. One index file is used for all FCDA files for a given simulation problem because the structure of the files are identical for all analytes. This file is generated by the ECEM code. The user should never modify this file.

Header type data

- Problem title: The title from the ESD keyword file.
- Code Name: The name of the code that generated the file
- Code Version: The version number of the code that generated the file
- Code Date: The modification date of the code that generated the file
- User Name: The user name from the ESD keyword file
- Run ID: The run ID from the code run that generated the file
- Block Size: The number of records with data in a time block in the binary data file for aquatic species
- Block Size: The number of records with data in a time block in the binary data file for riparian species
- Block Size: The number of records with data in a time block in the binary data file for upland species
- Record Length: Record length for the binary data file
- Number of realizations: The number of realizations requested for this run
- Number of times: From the ESD keyword file
- List of ESD times, and flag whether computed, one pair per line
- Number of locations: From the ESD keyword file
- List of ESD location ID's, flag whether computed, and location names, one triple per line
- Number of species: From the ESD keyword file
- List of ESD species ID's, flag whether computed, and species names, one triple per line

The header data are followed by record index data. The index data are split into three groups. One group is for aquatic locations, another group is for riparian locations, the other group is for upland locations. There are as many lines of index data as there are locations for the aquatic and riparian locations. There are three times as many lines of index data as for locations for the upland data. The index data for locations appear in the same order as the location IDs provided earlier in the file. Each line of index data contains the location ID followed by as many indices as there are food species types. The indices give an offset record number. If a particular medium is not saved at a location, the index value is set to negative 1. These lines contain data as follows:

- "Map: Aquatic Species"

- Map data for aquatic locations (map includes all locations). Each line has a Location ID, index for all aquatic species (-1 = not computed)
- "Map: Riparian Species"
- Map data for riparian locations (map includes all locations). Each line has a Location ID, index for all riparian species (-1 = not computed)
- "Map: Upland Species"
- Map data for upland locations (map includes 3 lines for all locations). Each line has Location ID, index for all upland species (-1 = not computed). The lines of data for all locations represent the three soil types in the following order. dry land (no irrigation), soil using groundwater for irrigation, and soil using surface water for irrigation.

An example FCDA index file is provided in Table 2.10.

Table 2.10 Example FCDA Index File

```
"ECEM Keyword File for ABC Assessment"
"ECEM"
"3.04.017"
"27 Feb 2006"
"Paul W. Eslinger"
"20060426162101"
-3,"Records in a time block - aquatic species"
-3,"Records in a time block - riparian species"
3,"Records in a time block - upland species"
14,"Record length in the FCDA file"
1,"Number of realizations"
3,"Number of header lines in binary files"
2,"Number of times"
2000,F
2050,T
3,"Number of locations"
"UH0001",T,"Representative Upland Location - Groundwater Irrigation"
"RHP001",F,"Representative Riparian Site"
"QHP001",F,"Representative Aquatic Site"
16,"Number of foods"
"UCATMT",T,"cattle (meat)"
"UCATMK",T,"cattle (milk)"
"UCHKAD",T,"chickens (adults)"
"UCHKEG",T,"chickens (eggs)"
"UEWORM",T,"earthworms"
"UARTPD",T,"terrestrial arthropods"
"UFUNGI",T,"fungi"
"UGRAIN",T,"grains"
"UGRAPE",T,"grapes"
"UGRASS",T,"grasses"
"ULFVEG",T,"leafy vegetables"
"UMLBRY",T,"mulberry"
"URTVEG",T,"root vegetables"
"UTHSLE",T,"Russian thistle"
"USHRUB",T,"shrubs"
"UTRFRT",T,"tree fruit"
```

```
"Map: Aquatic Species"
"UH0001",-1
"RHP001",-1
"QHP001",-1
"Map: Riparian Species"
"UH0001",-1
"RHP001",-1
"QHP001",-1
"Map: Upland Species"
"UH0001",4
"UH0001",5
"UH0001",6
"RHP001",-1
"RHP001",-1
"RHP001",-1
"QHP001",-1
"QHP001",-1
"QHP001",-1
```

2.3.3 FCDA Header File Format

The header file for foods is an ASCII file with the following items entered sequentially. All keywords are entered in lower case. All character strings are enclosed in double quote marks. An example file is provided in Table 2.11. The type of data for each line of the file are the following:

- **type**: "FCDA" (This line never changes.)
- **title**: The problem title from the ECEM keyword file
- **user**: The user name from the ESD keyword file
- **name**: The name of the code that generated the header file
- **version**: The version number of the code that generated the file
- **date**: The modification date of the code that generated the file
- **id**: The run ID from the code run that generated the file
- **ecemfile**: The name of the ECEM keyword file controlling the food definitions
- **realizations**: The number of realizations in the data files
- **foods**: The number of foods output from ECEM
- List of food (species) IDs, food (species) type, food (species) names, one triple per line
- **times**: The number of times output from ECEM
- List of times, one value per line
- **locations**: The number of locations output from ECEM
- List of location IDs and location names one pair per line
- **analytes**: The number of analytes processed by ECEM
- List of analyte IDs, analyte types, and analyte names, one triple per line
- Number of upland soils: From the ECDA structure
- **recordmap**: The name of the record map file for FCDA files.

Table 2.11 Example Header File for Foods

```
   type: "FCDA"
   title: "SAC Rev. 1 - Testing of the FCDA
Routines"
   user: "Paul W. Eslinger"
   name: "FCDA"
   version: "1.00.A.0"
   date: "30 Jan 2003"
   id: "20030130170205"
   ecemfile: "ECEM.key"
   realizations: 25
   foods: 12
   "AMCOOT","TA","American coot"
   "AMCOUP","TA","American coot - upland"
   "CARP  ","QA","Carp"
   "COYOTE","TA","Coyote"
   "DAPMAG","QA","Daphnia magna"
   "DENSDG","TP","Dense sedge"
   "DENSUP","TP","Dense sedge - upland"
   "FUNGI ","TP","Fungi"
   "MULBRY","TP","Mulberry"
   "MULBUP","TP","Mulberry - upland"
   "PERPHY","QP","Periphyton"
   "PHYPLK","QP","Phytoplankton"
   times: 8
   2000
   2005
   2015
   2023
   2100
   2400
   2700
   3050
   locations: 10
   "TH0001","TH0001 - Riparian - Pair with TH0002"
   "TH0002","TH0002 - River - Pair with TH0001"
   "TH0003","TH0003 - Riparian - Pair with TH0004"
   "TH0004","TH0004 - River - Pair with TH0003"
   "TH0005","TH0005 - River Only"
   "TH0006","TH0006 - River Only"
   "TH0007","TH0007 - Upland irrigated location"
   "TH0008","TH0008 - Upland irrigated location"
   "TH0009","TH0009 - Upland dry location"
   "TH0010","TH0010 - Upland dry location"
   analytes: 2
   "CrVI","NS","Hexavalent Chromium"
   "H3","NR","Tritium"
   recordmap: "ECEM_Food.Map"
```

2.3.4 FCDA File Size

The size of a FCDA file is limited to 2.147×10^9 bytes because the current implementation of the Fortran compilers for both the Linux and Windows operating system environments use 32 bit addressing. The FCDA file size for an analyte is a function of three quantities: the number of realizations, the number of

impact solution times and the number of locations. The file is a binary file where the record length (in bytes) is 10 plus four times the number of realizations. The number of records is 3 (header lines) plus the product of the number of impact solution times and the number of impact locations. The FCDA file size for aquatic species can be calculated using the following equation:

$$F_{a,s} = 3 \times (4N_r + 10) + (4N_r + 10) \times N_{st} \times N_{al}$$

Where:

F_s = The file size in bytes
N_r = The number of realizations
N_{st} = The number of impact solution times
N_{al} = The number of impact locations defined as aquatic locations

The FCDA file size for riparian species can be calculated using the following equation:

$$F_{a,s} = 3 \times (4N_r + 10) + (4N_r + 10) \times N_{st} \times N_{rl}$$

Where:

F_s = The file size in bytes
N_r = The number of realizations
N_{st} = The number of impact solution times
N_{rl} = The number of impact locations defined as aquatic locations

The FCDA file size for upland species can be calculated using the following equation:

$$F_s = 3 \times (4N_r + 10) + (4N_r + 10) \times N_{st} \times \sum_{us=1}^{N_u} N_{usm}$$

Where:

F_s = The file size in bytes
N_r = The number of realizations
N_{st} = The number of impact solution times
N_u = The number of impact locations defined as upland locations
N_{um} = The number of soil media (maximum of 3) saved at an upland location

2.4 Shared Environmental Stochastic Data

Some stochastic data are shared among several programs, including that defined by the KDSOIL (Section 5.3.8) and DILUTE (Section 5.3.3) keywords in the ESD keyword file. The following sections provide descriptions of the format of the data files containing the generated stochastic data.

2.4.1 Format of the DILUTE Library File

Entry of one or more DILUTE keywords in the ESD keyword file (see Section 5.3.3) coupled with the CREATE modifier on the FILE DILUTE keyword causes the ECDA code to generate a data file of DILUTE values for use in other codes. Table 2.12 provides an example of this file for one DILUTE keyword and two realizations. The file is a text file that starts with nine header lines. The entry on line 8 is the number of DILUTE definitions—1 in this example. The next line contains the number of realizations—3 in this example. Each succeeding line contains data for a single DILUTE definition in the form of index, identification string, data units, and generated values for each realization. Multiple data on a single line are separated by commas, and all text data are enclosed in double quotation marks.

Table 2.12 Example DILUTE File

```
"DILUTE"
"2004 Composite Analysis 1,000-year (Stochastic Inputs) Assessment"
"ECDA"
"2.00.A.4"
"16 Oct 2003"
"20040617150724"
"Eslinger-DWE-WEN"
1
3
1,"DF5m","None", 6.01588E-01, 5.10553E-01, 5.12033E-01
```

2.4.2 Format of the KDSOIL Library File

Entry of one or more KDSOIL keywords in the ESD keyword file (see Section 5.3.8) coupled with the CREATE modifier on the FILE KDSOIL keyword causes the ECDA code to generate a data file of stochastic KDSOIL values for use in other codes.

Table 2.13 provides an example of this file for 10 KDSOIL keywords and three realizations. The file is a text file that starts with 9 header lines. The entry on line 8 is the number of KDSOIL definitions—10 in this example. The next line contains the number of realizations—3 in this example. Each succeeding line contains data for a single KDSOIL definition in the form of index, identification string, data units, and generated values for each realization. Multiple data on a single line are separated by commas, and all text data are enclosed in double quotation marks.

Table 2.13 Example KDSOIL File

```
"KDSOIL"
"2004 Composite Analysis 1,000-year (Stochastic) Assessment"
"ECDA"
"2.00.A.4"
"16 Oct 2003"
"20040617150724"
"Eslinger-DWE-WEN"
10
3
1,"KDC","L/g", 8.51504E-02, 1.70702E-02, 5.09645E-02
2,"KDCl","L/g", 0.00000E+00, 0.00000E+00, 0.00000E+00
3,"KDCs","L/g", 6.42750E-01, 3.89112E+00, 2.62510E+00
4,"KDH","L/g", 0.00000E+00, 0.00000E+00, 0.00000E+00
5,"KDI","L/g", 1.37567E-05, 7.58985E-05, 6.64624E-05
6,"KDNp","L/g", 1.39180E-02, 2.26965E-02, 1.23003E-02
7,"KDSe","L/g", 5.29678E-03, 4.82762E-03, 5.18776E-03
8,"KDSr","L/g", 2.35305E-02, 2.12109E-02, 2.08005E-02
9,"KDTc","L/g", 6.34344E-06, 0.00000E+00, 2.57418E-05
10,"KDU","L/g", 8.38553E-04, 3.77616E-04, 9.35109E-04
```

2.4.3 Format of the INFILT Library File

Entry of one or more INFILTRATION keywords with the DEFINE modifier in the ESD keyword file (see Section 2.2) coupled with the CREATE modifier on the FILE INFILT keyword causes the ECDA code to generate a data file of stochastic infiltration values for use in other codes. Table 2.14 provides an

example of this file for 5 INFILTRATION keywords and three realizations. The file is a text file that starts with 9 header lines. The entry on line 8 is the number of INFILTRATION definitions—5 in this example. The next line contains the number of realizations—3 in this example. Each succeeding line contains data for a single INFILTRATION definition in the form of index, identification string, data units, and generated values for each realization. Multiple data on a single line are separated by commas, and all text data are enclosed in double quotation marks.

Table 2.14 Example INFILT File

```
"INFILT"
"Test Case Test01 for the FILLECDA Code"
"ECDA"
"4.00.001"
"31 May 2007"
"20070531112006"
"Paul W. Eslinger"
5
3
1,"ABC","mm/yr", 6.61073E-02, 1.24560E-01, 1.14312E-01
2,"Ba-dg","mm/yr", 3.94540E+01, 3.09505E+01, 3.67614E+01
3,"Ba-dn","mm/yr", 4.40370E+01, 6.03037E+01, 7.41343E+01
4,"Ba-ds","mm/yr", 8.07378E+00, 1.05555E+01, 6.72481E+00
5,"Ba-s","mm/yr", 4.75351E+00, 4.13026E+00, 2.45424E+00
```

3.0 ANIMATE – Animation of Impact Code Results

3.1 Overview

ANIMATE is a utility code that extracts data and sets up input files for the Tecplot© code for the purpose of making time-series animations from simulation outputs. Data are handled from four separate data types of the TIIA. The supported data types are shown in Table 3.1:

Table 3.1 Data Types Used in the ANIMATE Utility Code

Data Type	Description
ECDA	Media concentrations in the binary ECDA files
ECEM	Any data written to the "DETAILS" file by the ECEM code
FCDA	Food concentrations in the binary FCDA files
HUMAN	Any data written to the "DETAILS" file by the HUMAN code

3.1.1 Location in the Processing Sequence

The ANIMATE program can be used any time after one or more of the following actions have been completed:

- The ECDA program has created media concentrations in the binary ECDA files.
- The ECEM program has created and written data to the ECEM "DETAILS" file.
- The ECEM program has created food concentrations in the binary FCDA files.
- The HUMAN program has created and written data to the HUMAN "DETAILS" file.

3.1.2 How the Code Is Invoked

ANIMATE can run under either the Windows or the Linux operating system. Under the Windows operating system (Releases XP or 7), ANIMATE executes in a DOS box. A run of ANIMATE is initiated by entering the following command line:

```
ANIMATE "Keyfilename"
```

Under the Linux operating system ANIMATE is executed through any of the following Bourne Shell or C Shell commands:

```
animate-1.exe "Keyfilename"
```

For these commands, "ANIMATE.EXE" or "animate-1.exe" is the name of the executable program and "Keyfilename" is the name of a control keyword file. Both the name of the executable program and the keyword file may contain path information. If ANIMATE is invoked without entering the name of the keyword file, then the code will prompt the user for the file name. The keyword file, which should be prepared using an editor that can handle ASCII files without leaving embedded control codes, contains text control information describing the run. If ANIMATE cannot open the keyword file, then the code will terminate execution after writing an error message to the standard output device.

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3.1.3 Memory Requirements

The ANIMATE program has moderate memory requirements. The major use of memory is storing the information from all DATA keywords before any outputs are processed. If memory requirements become excessive, the problem can be subdivided into multiple runs, each using a subset of the data.

3.2 File Definitions

The ANIMATE program reads up to five input files and writes to two or more output files. These files are described in the following paragraphs.

3.2.1 Input Files

3.2.1.1 ANIMATE Keyword File

The ANIMATE keyword file contains control information. Example files are provided in each of the sections describing the keyword input for the particular data types. Detailed definitions of the keywords are provided in Sections 3.3 through 3.7.

3.2.1.2 Other Input Files

In addition to the keyword input file, the ANIMATE program also reads several additional input files. The files needed are based on the category selected for the animation. Only one category can be selected for each run of the ANIMATE code. The connectivity files for Tecplot must be prepared based on the set of locations that will be used in the contour plots. The following are the files needed to run the ANIMATE code depend on the type of animation selected:

ECDA UPLAND: Space-covering contour plots will be generated in a time sequence

- ECDA concentration file
- ECDA index file
- Connectivity file for locations
- Coordinates file, this file defines location (ID,X,Y)

HUMAN UPLAND: Space-covering contour plots will be generated in a time sequence

- HUMAN header file
- HUMAN detailed data file
- Connectivity file for locations
- Coordinates file, this file defines location (ID,X,Y)

FOOD UPLAND: Space-covering contour plots will be generated in a time sequence

- FCDA concentration file
- FCDA index file
- Connectivity file for locations
- Coordinates file, this file defines location (ID,X,Y)

ECEM UPLAND: Space-covering contour plots will be generated in a time sequence

- ECEM header file
- ECEM detailed data file
- Connectivity file for locations
- Coordinates file, this file defines location (ID,X,Y)

ECDA RIPARIAN/AQUATIC: A line plot (along the shoreline) will be generated in a time sequence

- ECDA concentration file
- ECDA index file
- Coordinates file, this file defines location (ID,X,Y)

HUMAN RIPARIAN/AQUATIC: A line plot (along the shoreline) will be generated in a time sequence

- HUMAN Header file
- HUMAN detailed data file
- Coordinates file, this file defines location (ID,X,Y)

FOOD RIPARIAN/AQUATIC: A line plot (along the shoreline) will be generated in a time sequence

- FCDA concentration file
- FCDA index file
- Coordinates file, this file defines location (ID,X,Y)

ECEM RIPARIAN/AQUATIC: A line plot (along the shoreline) will be generated in a time sequence

- ECEM Header file
- ECEM detailed data file
- Coordinates file, this file defines location (ID,X,Y)

3.2.2 Output Files

The code writes to two output files. These files are a report file and a Tecplot visualization file. The Tecplot file defines years, connectivity, and concentrations for display.

3.2.2.1 Report File

The report file contains summary information from the run of the ANIMATE code. This file contains a record of the code version, time and date of run execution, input and output file names, run information, and a summary table of results. This file also contains any error messages generated by the ANIMATE code.

3.2.2.2 Tecplot File

The Tecplot file contains the data that will be read by Tecplot to produce the animation. The file contains the coordinate information and the selected data for the animation.

3.3 Keywords for Every Run of the ANIMATE Code

In general, the keywords for ANIMATE can be entered in any order. The only restriction is that the END keyword must be the last keyword in the file.

3.3.1 CATEGORY Keyword for ANIMATE

The CATEGORY keyword (mandatory) defines the data category to be processed. The types of data that can be processed are defined in Table 3.2. The following is this keyword's syntax:

```
CATEGORY [MODIFIER]
```

Table 3.2 Modifiers Associated with the CATEGORY Keyword in ANIMATE

Modifier	Description
CULTURE	Animate a map file generated through use of the MAP keyword
ECDA	Animate environmental media concentration data (Environmental Concentration Data Accumulator – ECDA)
ECEM	Animate any of the solutions available through use of the DETAILS keyword in the ECEM code
FCDA	Animate food concentrations (Food Concentration Data Accumulator – FCDA)
HUMAN	Animate any of the solutions available through use of the DETAILS keyword in the HUMAN code

An example of this keyword that uses the environmental media concentration data:

```
CATEGORY ECDA
```

3.3.2 DEBUG Keyword for ANIMATE

The DEBUG keyword is used to activate the writing of intermediate information to the report file. The following is this keyword's syntax:

```
DEBUG [CULTURE | ECDA | ECEM | FCDA | HUMAN]
```

3.3.3 END Keyword for ANIMATE

The END keyword signifies the end of all keyword data. Nominally it will be the last keyword in the keyword file. All data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

3.3.4 LEGEND Keyword for ANIMATE

The LEGEND keyword is used to enter the names of the plot title and the header for the contour legend. The following is this keyword's syntax:

```
LEGEND [TITLE= "quote 1"] [CONTOUR="quote 2"]
```

The quote string associated with the TITLE modifier is used to enter a one-line plot title. The quote string associated with the CONTOUR modifier is used to enter a one-phrase label for the contour definitions. Some examples of the LEGEND keyword are as follows:

```
LEGEND TITLE = "Terestrial Plant" CONTOUR = "Concentration"
LEGEND TITLE = "H3 UpDrink" CONTOUR = "Dose (mrem)"
```

3.3.5 LOCATION Keyword for ANIMATE

The LOCATION keyword identifies the location type that will be used in the animation. All locations with the selected location type are used. The following is this keyword's syntax:

```
LOCATION [UPLAND | RIPARIAN | AQUATIC]
```

An example of this keyword that uses irrigated soil with groundwater:

```
LOCATION UPLAND
```

3.3.6 PICK_REL Keyword for ANIMATE

The PICK_REL keyword defines the realization to process. The following is this keyword's syntax:

```
PICK_REL value1
```

The following keyword record chooses realization number 10:

```
PICK_REL 10
```

3.3.7 REPORT Keyword for ANIMATE

The REPORT keyword is used to define the name of the output report (log) file. It must be the first keyword entered in the keyword file. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The name of the report file is entered in a quote string. File names up to 200 characters long are supported, and path names can be included. The following is an example REPORT keyword record:

```
REPORT "/SAC/SystemCodes/Cultural/Test1.rpt"
```

3.3.8 TIMES Keyword for ANIMATE

The TIMES keyword identifies the times (years) at which the calculations are to be performed for a single case. The following is this keyword's syntax:

```
TIMES [ALL | LIST [T1] {T2} … {Tn}]
```

All times in the ESD keyword file are used when the modifier ALL is present. A list of specific times can be defined by entering the modifier LIST and a set of numerical values identifying the years of interest. The specific years entered must be defined in the ESD keyword file. All times are included in the first example shown below. The second example defines a list of six years.

```
TIMES ALL
TIMES LIST 2020 2075 3014 3050 4000 12050
```

3.3.9 TITLE Keyword for ANIMATE

The TITLE keyword is used to define a single-line problem title. The problem title will be written to output files. If the title is not supplied, then the program will error terminate. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 200 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the ANIMATE code."
```

3.3.10 USER Keyword for ANIMATE

The USER keyword is used to identify the user of the program. The user name will be written to output files. If the user name is not supplied, then the program will error terminate. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

3.3.11 VERBOSE Keyword for ANIMATE

The presence of the optional VERBOSE keyword initiates additional output to the report file. The following is this keyword's syntax:

```
VERBOSE
```

3.4 Keywords Specific to ECDA Data

The keywords needed for an animation of ECDA concentration data are given in this section. These keywords are needed in addition to the keywords described in Section 3.3.

3.4.1 ANALYTE Keyword

The ANALYTE keyword is used to define the analyte for which data will be processed. The following is this keyword's syntax

```
ANALYTE ["quote"]
```

The single quote string must be a single analyte ID from the set of the analytes in the ESD keyword file. An example of this keyword is the following:

```
ANALYTE "C14"
```

3.4.2 FILE Keyword

The FILE keyword is used to enter the names of input and output files except for the report file. The following is this keyword's syntax:

```
FILE [modifier1= "quote 1"] {modifier2="quote 2"} {modifier3="quote 3"}
   {modifier4="quote 4"} {modifier5="quote 5"}
```

The file names are entered in quote strings, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. The file name associated with a modifier must be entered before the next modifier is entered.

At least one FILE keyword is required for every run of the code. At least three files must be defined for every run of the code. The modifiers associated with the FILE keyword are given in Table 3.3.

Table 3.3 Modifiers Associated with the FILE Keyword in ANIMATE for ECDA Data

Modifier	Description
CONNECT	Tecplot connectivity file (not needed with river line plot)
COORDS	Coordinate data (This defines location (ID,X,Y))
C_ECDA	ECDA concentration file
I_ECDA	ECDA map index file
RESULTS	Output file used for Tecplot visualization

3.4.3 MEDIA Keyword

The MEDIA keyword is used to define the medium for which data will be processed for a single case. The following is this keyword's syntax:

```
MEDIA ["quote 1"]
```

The single quote string is case sensitive, four characters in length. The modifiers associated with the FILE keyword are given in Table 3.4.

Table 3.4 Modifiers Associated with the MEDIA Keyword in ANIMATE for ECDA Data

Modifier	Description
GWAT	concentrations in groundwater (Ci/m^3 or kg/m^3)
SEEP	concentrations in seep water (Ci/m^3 or kg/m^3)
SWAT	concentrations in surface water (river) (Ci/m^3 or kg/m^3)
PWAT	concentrations in river bottom pore water (Ci/m^3 or kg/m^3)
SEDI	concentrations in river bottom sediment ($Ci/kg_{sediment}$ or $kg_{analyte}/kg_{sediment}$)
SORP	concentrations in riparian zone soil (land surface) (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)
SODR	concentrations in upland soil (land surface) with no irrigation (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)
SOGW	concentrations in upland soil (land surface) with groundwater irrigation (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)
SOSW	concentrations in upland soil (land surface) with surface water irrigation (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)
AIRC	concentrations in air (Ci/m^3 or kg/m^3)
AIRD	air deposition rates ($Ci/m^2/yr$ or $kg/m^2/yr$)

An example of this keyword that uses concentrations in upland soil with surface water irrigation is the following:

```
MEDIA "GWAT"
```

3.4.4 UNITS Keyword

The UNITS keyword is used to define the output units for the animation. The following is this keyword's syntax:

```
UNITS OUTPUT "quote1" FACTOR value1
```

The quote string is the desired output units, and the value is the units conversion factor to translate from the units output by the original code to the desired output units for the animation. An example of this keyword is the following:

```
UNITS OUTPUT="pCi/L" FACTOR = 1.0E9 !Convert Ci/m^3 to pCi/L
```

3.4.5 Example Keyword File for ECDA Data

An example keyword file for running an animation for ECDA concentration data is shown in Table 3.5.

Table 3.5 Example Keyword File for ANIMATE for ECDA Data

```
REPORT "Test_Animate_ECDA.rpt"
TITLE "Animation for ECDA Upland locations"
USER "Paul W. Eslinger"
VERBOSE
LOCATION UPLAND   !RIPARIAN or AQUATIC
!---------------------------------------------------------------------
CATEGORY ECDA !---> Only one category of data allowed per run of the code
FILE C_ECDA "CA_Ref_A_C14.bin"   ! Name of ECDA concentration file
FILE I_ECDA "CA_Ref_A_ECDA.idx" ! Name of ECDA map index file
DEBUG ECDA
! Files needed
FILE RESULTS "C14_Ecda_out.dat" !Output file
FILE CONNECT "All_connectivity.txt" ! TecPlot connectivity file
FILE COORDIN "All_locations.csv" ! Coordinates for the connectivity
! Pick one or more times
TIMES ALL
! Pick a single analyte
ANALYTE "C14"
! Pick a medium
MEDIA "GWAT"
! Pick a single realization animate
PICK_REL 1
! Set the output units and legend labels
UNITS OUTPUT="pCi/L" FACTOR = 1.0E9 !Convert Ci/m^3 to pCi/L
LEGEND TITLE = "Animation for ECDA Upland locations" CONTOUR =
"Concentration"
!
END
```

3.5 Keywords Specific to ECEM Data

The keywords needed for an animation of ECEM detailed data are given in this section. These keywords are needed in addition to the keywords described in Section 3.3.

3.5.1 ANALYTE Keyword

The ANALYTE keyword is used to define the analyte for which data will be processed. The following is this keyword's syntax

```
ANALYTE ["quote"]
```

The single quote string must be a single analyte ID from the set of the analytes in the ESD keyword file. An example of this keyword is the following:

```
ANALYTE "C14"
```

3.5.2 FILE Keyword

The FILE keyword is used to enter the names of input and output files except for the report file. The following is this keyword's syntax:

```
FILE [modifier1= "quote 1"] {modifier2="quote 2"} {modifier3="quote 3"}
   {modifier4="quote 4"} {modifier5="quote 5"}
```

The file names are entered in quote strings, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. The file name associated with a modifier must be entered before the next modifier is entered.

At least one FILE keyword is required for every run of the code. At least three files must be defined for every run of the code. The modifiers associated with the FILE keyword are given in Table 3.6.

Table 3.6 Modifiers Associated with the FILE Keyword in ANIMATE for ECEM Data

Modifier	Description
CONNECT	Tecplot connectivity file (not needed with river line plot)
COORDS	Coordinate data (This defines location (ID,X,Y))
HEADER	Header file
DETAIL	Detailed data
RESULTS	Output file used for Tecplot visualization

3.5.3 SOILTYPE Keyword

The SOILTYPE keyword is used to define the solution type for which data will be processed when the CATEGORY is ECEM. The following is this keyword's syntax:

```
SOILTYPE ["quote 1"]
```

The single quote string is case sensitive and six characters in length. The modifiers associated with the SOILTYPE keyword are given in Table 3.7.

Table 3.7 Modifiers Associated with the SOILTYPE Keyword in ANIMATE for ECEM Data

Modifier	Description
NONE	Applies to all aquatic locations
SORP	Riparian locations
SODR	Dry (non irrigated) upland locations

Modifier	Description
SOGW	Groundwater irrigated upland locations
SOSW	Surface water irrigated upland locations

An example of this keyword is the following:

```
SOILTYPE "SOGW"
```

3.5.4 SOLUTION Keyword

The SOLUTION is used to define the solution type for which data will be processed. The following is this keyword's syntax:

```
SOLUTION ["quote 1"]
```

The single quote string is case sensitive, six characters in length. For the CATEGORY ECEM, the modifiers associated with the SOILTYPE keyword are given in Table 3.8.

Table 3.8 Modifiers Associated with the SOLUTION Keyword in ANIMATE for ECEM Data

Modifier	Description
BURDEN	Body burdens (pCi or µg/kg wet wt)
DOSRAD	Radioactive dose (rem)
BMTISS	Ratios to tissue benchmarks (unitless)
SUMRAD	Sum of radioactive dose (rem)
CONCEN	Media concentrations (see MEDIA keyword modifiers for units)

An example of this keyword is the following:

```
SOLUTION "DOSRAD"
```

3.5.5 SPECIES Keyword

The SPECIES keyword is used to define the species for which data will be processed. The following is this keyword's syntax

```
SPECIES ["quote"]
```

The single quote string must be a single SPECIES ID from the set of the SPECIES in the ESD keyword file. Example of this keyword :

```
SPECIES "RMALRD"
```

3.5.6 UNITS Keyword

The UNITS keyword is used to define the output units for the animation. The following is this keyword's syntax:

```
UNITS OUTPUT "quote1" FACTOR value1
```

The quote string is the desired output units, and the value is the units conversion factor to translate from the units output by the original code to the desired output units for the animation. An example of this keyword is the following:

```
UNITS OUTPUT="rad/d" FACTOR = 1.0 !No conversion needed
```

3.5.7 Example Keyword File for ECEM Data

An example keyword file for running an animation for ECEM detailed data is shown in Table 3.9.

Table 3.9 Example Keyword File for ANIMATE for ECEM Data

```
REPORT "Test_Animate_ECEM.rpt"
TITLE "Animation Test for ECEM RIPARIAN locations"
USER "Paul W. Eslinger"
OS WINDOWS !UNIX ! This matches inforamtion in the header file
VERBOSE
LOCATION RIPARIAN ! UPLAND or AQUATIC
!---------------------------------------------------------------------
CATEGORY ECEM !---> Only one category of data allowed per run of the code
FILE HEADER   "Ecem_CA_Ref_A_foods.hdr"     ! Header file
FILE DETAIL   "Ecem_CA_Ref_A_det_foods.csv" ! Risk detailed data
DEBUG ECEM
! Files needed
FILE RESULTS "ECEM_RP_out.dat" !Output file
FILE CONNECT "All_connectivity.txt" ! TecPlot connectivity file
FILE COORDIN "rip_animation.csv" ! Coordinates for the connectivity
! Pick one or more times
TIMES LIST 2000 2005
! Pick a soil type
SOILTYPE "SORP"
! Pick a single analyte
ANALYTE "H3"
! Pick a species
SPECIES "RMLBRY"
! Pick a solution
SOLUTION "DOSRAD"
! Pick a single realization to animate
PICK_REL 1
! Set the output units
UNITS OUTPUT="rad/day" FACTOR = 1.0  !No units changes
LEGEND TITLE = "none" CONTOUR = "none"
!
END
```

3.6 Keywords Specific to FCDA Data

The keywords needed for an animation of FCDA food concentration data are given in this section. These keywords are needed in addition to the keyword described in Section 3.3.

3.6.1 ANALYTE Keyword

The ANALYTE keyword is used to define the analyte for which data will be processed. The following is this keyword's syntax

```
ANALYTE ["quote"]
```

The single quote string must either be a single analyte ID from the set of the analytes in the ESD keyword file, or the string "-Rads-" if the combined dose over multiple radioactive analytes is desired. Two examples of this keyword are the following:

```
ANALYTE "C14"
ANALYTE "-Rads-"
```

3.6.2 FILE Keyword

The FILE keyword is used to enter the names of input and output files except for the report file. The following is this keyword's syntax:

```
FILE [modifier1= "quote 1"] {modifier2="quote 2"} {modifier3="quote 3"}
   {modifier4="quote 4"} {modifier5="quote 5"}
```

The file names are entered in quote strings, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. The file name associated with a modifier must be entered before the next modifier is entered.

At least one FILE keyword is required for every run of the code. At least three files must be defined for every run of the code. The modifiers associated with the FILE keyword are given in Table 3.10.

Table 3.10 Modifiers Associated with the FILE Keyword in ANIMATE for FCDA Data

Modifier	Description
CONNECT	Tecplot connectivity file (not needed with river line plot)
COORDS	Coordinate data (This defines location (ID,X,Y))
C_FCDA	FCDA concentration file
I_FCDA	FCDA map index file
RESULTS	Output file used for Tecplot visualization

3.6.3 SOIL Keyword

The SOIL keyword is used to the solution type for which data will be processed when the CATEGORY is FCDA. The following is this keyword's syntax:

```
SOIL ["quote 1"]
```

The single quote string is case sensitive and is six characters in length. The modifiers associated with the SOIL keyword are given in Table 3.11.

Table 3.11 Modifiers Associated with the SOIL Keyword in ANIMATE for ECEM Data

Modifier	Description
SODR	Dry (non irrigated) upland locations
SOGW	Groundwater irrigated upland locations
SOSW	Surface water irrigated upland locations

An example of this keyword is the following:

```
SOIL "SOGW"
```

3.6.4 SPECIES Keyword

The SPECIES keyword is used to define the species for which data will be processed. The following is this keyword's syntax:

```
SPECIES ["quote"]
```

The single quote string must be a single SPECIES ID from the set of the SPECIES in the ESD keyword file. An example of this keyword is the following:

```
SPECIES "RMALRD"
```

3.6.5 UNITS Keyword

The UNITS keyword is used to define the output units for the animation. The following is this keyword's syntax:

```
UNITS OUTPUT "quote1" FACTOR value1
```

The quote string is the desired output units, and the value is the units conversion factor to translate from the units output by the original code to the desired output units for the animation. An example of this keyword is the following:

```
UNITS OUTPUT="pCi/kg" FACTOR = 1.0 !No conversion needed
```

3.6.6 Example Keyword File for FCDA Data

An example keyword file for running an animation for FCDA food concentration data is shown in Table 3.12.

Table 3.12 Example Keyword File for ANIMATE for FCDA Data

```
REPORT "Test_Animate_FCDA.rpt"
TITLE "Animation Test for FCDA Upland locations"
USER "Paul W. Eslinger"
OS WINDOWS !UNIX ! This matches information in the header file
VERBOSE
LOCATION UPLAND  !RIPARIAN or AQUATIC
!---------------------------------------------------------------------
CATEGORY FCDA !---> Only one category of data allowed per run of the code
FILE C_FCDA "Food_H3_ULFVEG.fod" ! Name of FCDA concentration file
FILE I_FCDA "Ecem_CA_Ref_A_map_foods.dat" ! Name of FCDA map index file
DEBUG FCDA
! Files needed
FILE RESULTS "H3_ULFVEG_out.dat" !Output file
FILE CONNECT "All_connectivity.txt" ! TecPlot connectivity file
FILE COORDIN "All_locations.csv" ! Coordinates for the connectivity
! Pick one or more times
TIMES LIST 1945 1990 1995
! Pick a single analyte
ANALYTE "H3"
! Pick a soil type
SOIL "SOGW" !"SODR" SOSW"
! Pick a species
SPECIES "ULFVEG"
! Pick a single realization to animate
```

```
PICK_REL 1
! Set the output units
UNITS OUTPUT="pCi/kg" FACTOR = 1.0 !No conversion needed
LEGEND TITLE = "Terestrial Plant" CONTOUR = "Concentration"
!
END
```

3.7 Keywords Specific to HUMAN Data

The keywords needed for an animation of HUMAN detailed data are given in this section. These keywords are needed in addition to the keywords described in Section 3.3.

3.7.1 ANALTYPE Keyword

The ANALTYPE keyword is used to define the analyte type for which data will be processed. The following is this keyword's syntax

```
ANALTYPE ["quote"]
```

The single quote string is case sensitive. The modifiers associated with the ANALTYPE keyword are given in Table 3.13.

Table 3.13 Modifiers Associated with the ANALTYPE Keyword in ANIMATE for HUMAN Data

Modifier	Description
ALL	The analyte field is used for a quantity that is a sum over analytes
CAR	The analyte is a carcinogenic chemical
CONMEDIA	The analyte field is used to select an environmental medium
CONFOODS	The analyte field is used to select a food species
HAZ	The analyte is a hazardous chemical
RAD	The analyte is a radionuclide

An example of this keyword is the following:

```
ANALTYPE "Rad"
```

3.7.2 ANALYTE Keyword

The ANALYTE keyword is used to define the analyte for which data will be processed. The following is this keyword's syntax

```
ANALYTE ["quote"]
```

The single quote string must either be a single analyte ID from the set of the analytes in the ESD keyword file, or the string "-Rads-" if the combined dose over multiple radioactive analytes is desired. Two examples of this keyword are the following:

```
ANALYTE "C14"
ANALYTE "-Rads-"
```

3.7.3 FILE Keyword

The FILE keyword is used to enter the names of input and output files except for the report file. The following is this keyword's syntax:

```
FILE [modifier1= "quote 1"] {modifier2="quote 2"} {modifier3="quote 3"}
   {modifier4="quote 4"} {modifier5="quote 5"}
```

The file names are entered in quote strings, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. The file name associated with a modifier must be entered before the next modifier is entered.

At least one FILE keyword is required for every run of the code. At least three files must be defined for every run of the code. The modifiers associated with the FILE keyword are given in Table 3.14.

Table 3.14 Modifiers Associated with the FILE Keyword in ANIMATE for HUMAN Data

Modifier	Description
CONNECT	Tecplot connectivity file (not needed with river line plot)
COORDS	Coordinate data (This defines location (ID,X,Y))
HEADER	Header file created by the HUMAN code
DETAIL	Detailed data
RESULTS	Output file used for Tecplot visualization

3.7.4 SOLUTION Keyword

The SOLUTION is used to define the solution type for which data will be processed. The following is this keyword's syntax:

```
SOLUTION ["quote 1"]
```

The single quote string is case sensitive. The modifiers associated with the SOLUTION keyword are given in Table 3.15.

Table 3.15 Modifiers Associated with the SOLUTION Keyword in ANIMATE for HUMAN Data

Modifier	Description
ANADOSE	Analyte dose
ANARISK	Analyte risk
ANAHQ	Analyte hazard quotient
DOSEING	Ingestion dose
DOSEINH	Inhalation dose
DOSEEXT	External dose
DOSEDER	Dermal dose
HQING	Ingestion hazard quotient
HQINH	Inhalation hazard quotient
HQDER	Dermal hazard quotient
POPDOSE	Population dose (radioactive)

Modifier	Description
POPRISK	Population risk (radioactive)
RISKING	Ingestion risk
RISKINH	Inhalation risk
RISKEXT	External risk
RISKDER	Dermal risk
SUMDOSE	Dose summed over analyes
SUMRISK	Risk summed over analyes
SUMHQ	Hazard quotient summed over analyes

An example of this keyword is the following:

```
SOLUTION "ANARISK"
```

3.7.5 UNITS Keyword

The UNITS keyword is used to define the output units for the animation. The following is this keyword's syntax:

```
UNITS OUTPUT "quote1" FACTOR value1
```

The quote string is the desired output units, and the value is the units conversion factor to translate from the units output by the original code to the desired output units for the animation. An example of this keyword is the following:

```
UNITS OUTPUT="pCi/L" FACTOR = 1.0E9 !Convert Ci/m^3 to pCi/L
```

3.7.6 Example Keyword File for HUMAN Data

An example keyword file for running an animation for HUMAN detailed data is shown in Table 3.16.

Table 3.16 Example Keyword File for ANIMATE for HUMAN Data

```
REPORT "Test_Animate_HUMAN_UPLAND.rpt"
TITLE "Animation Test for HUMAN UPLAND locations"
USER "Paul W. Eslinger"
OS WINDOWS !UNIX ! This matches inforamtion in the header file
VERBOSE
LOCATION UPLAND ! RIPARIAN or AQUATIC
!-------------------------------------------------------------------------
CATEGORY HUMAN  !---> Only one category of data allowed per run of the code
FILE HEADER   "Human_CA_Ref_A_UpDrink_SACVIEW.Hdr"     ! Header file
FILE DETAIL   "Human_CA_Ref_A_UpDrink_Dtl.csv"         ! Risk detailed data
! Files needed
FILE RESULTS "H3_UpDrink_out.dat" !Output file use for tecplot visualization
FILE CONNECT "All_connectivity.txt" ! TecPlot connectivity file
FILE COORDIN "All_locations.csv" ! Coordinates for the connectivity (This
defines location (ID,X,Y))
! Pick one or more times
TIMES ALL
! Pick a single analyte
```

```
ANALYTE "H3"
! Pick an analyte type
ANALTYPE "CONMEDIA"
! Pick a solution
SOLUTION "GWAT"
! Pick a single realization to animate
PICK_REL 1
! Set the output units
UNITS OUTPUT="pCi/L" FACTOR = 1.0E9 !Convert Ci/m^3 to pCi/L
LEGEND TITLE = "H3 UpDrink" CONTOUR = "Concentration"
!
END
```

4.0 CONSUME – Ecological Species Consumption Data

4.1 Overview

The CONSUME program reads a text file containing ecological species information, including a full predation matrix, and reformats the data into CONSUME keyword records for use in ECEM. The predation matrix (the fraction of the intake for an ecological specie that comes from consuming other species) is also checked for errors during this process. Typically, the underlying data for ECEM are maintained in a spreadsheet. This program converts data from the spreadsheet into a format that can be inserted into an ECEM keyword file.

4.1.1 Location in the Processing Sequence

The CONSUME program is a preprocessor to the ECEM code.

4.1.2 Memory Requirements

The CONSUME code uses dynamic memory allocation. It is expected that most, if not all, of the runs of the CONSUME code will require less than 2 MB of memory.

4.2 File Definitions

The CONSUME code reads one file and writes one file.

4.2.1 Input File

The CONSUME code reads a text data file containing ecological species information in a comma-separated format. An example input data file for 12 ecological species is provided in Table 4.1. The first line in the file is a user name of up to 16 characters. Enclose the name in double quotes to preserve embedded spaces. The second line contains an integer (N_S) giving the number of species to process. This input is followed by a definition line for each of the N_S species. Each line contains the following:

- The user name (up to 16 characters)
- The species ID (up to 6 characters)
- The type of the species; valid entries for this string are
  - TA – if the species is a terrestrial animal
  - TP – if the species is a terrestrial plant
  - QA – if the species is an aquatic animal
  - QP – if the species is an aquatic plant.
- The species location; valid entries for this string are
  - RIPARIAN – riparian zone (river shore)
  - UPLAND – upland
  - AQUATIC – river.
- The species long name (up to 72 characters).

The definition lines are followed by consumption lines for each of the N_S species. The order of the consumption lines must match with the order in which the species are defined in the file. Each line contains N_S+2entries. The first N_S entries give the fraction of the intake for the species that comes from each of the other species. Valid entries are in the range 0 to 1. Plants always have all zeros, and animal species typically have entries that sum to 1. An exception to this rule is the adult salmon that moves up the river without consuming any food. The entry in the N_S+1 position is the amount of sediment consumed by the species, expressed as a fraction of intake. This value should be zero for all species that are not aquatic animals. Valid values are in the range 0 to 1. The entry in the N_S+2 position is the amount of soil consumed by the species, expressed as a fraction of intake. This value should be zero for all species that are not terrestrial animals. Valid values are in the range 0 to 1.

Table 4.1 Example Input File for CONSUME

```
“John Doe”
12
"RCTWOD","TP","RIPARIAN","black cottonwood"
"RCRESS","TP","RIPARIAN","Columbia yellowcress"
"RSEDGE","TP","RIPARIAN","dense sedge"
"RFERN ","TP","RIPARIAN","fern"
"RFUNGI","TP","RIPARIAN","fungi"
"HRVMSE","TA","RIPARIAN","Harvest mouse"
"RMLBRY","TP","RIPARIAN","mulberry"
"RREEDC","TP","RIPARIAN","reed canarygrass"
"RRUSHS","TP","RIPARIAN","rushes"
"RSWCLV","TP","RIPARIAN","Sweet Clover (Melalotus alba)"
"RARTPD","TA","RIPARIAN","terrestrial arthropods"
"RRTULE","TP","RIPARIAN","tule"
0,0,0,0,0,0,0,0,0,0,0,0,0,0
0,0,0,0,0,0,0,0,0,0,0,0,0,0
0,0,0,0,0,0,0,0,0,0,0,0,0,0
0,0,0,0,0,0,0,0,0,0,0,0,0,0
0,0,0,0,0,0,0,0,0,0,0,0,0,0
0,0,0.3,0,0,0,0,0.3,0,0.1,0.3,0,0,0.02
0,0,0,0,0,0,0,0,0,0,0,0,0,0
0,0,0,0,0,0,0,0,0,0,0,0,0,0
0,0,0,0,0,0,0,0,0,0,0,0,0,0
0,0,0,0,0,0,0,0,0,0,0,0,0,0
0.1,0.1,0.1,0.1,0.1,0,0.2,0.1,0.1,0,0,0.1,0,0.5
0,0,0,0,0,0,0,0,0,0,0,0,0,0
```

4.2.2 Output File

The CONSUME code writes one data file. This file is a text file that is always named “consume.rpt” and contains the reformatted consumption data, an echo of the predation matrix, and any error messages. Excerpts from a report file are provided in Table 4.2. The typical mode of operation is to extract the CONSUME keyword records from this file and paste them into an input file for the ECEM code.

Table 4.2 Excerpts from a CONSUME Report File

```
! Consumption formatted as CONSUME keywords for ECEM
!   Program: Consume
!   Version: 4.0.001
!   Revised: 9 Jul 2012
!   User:    Paul W. Eslinger
!   Date:    07-19-2012
!   Time:    14:20:41
!   File:    Test_Consume.kwd
!
CONSUME ID="PERCH" PREY
  "DETFAC"  0.02400
  "ANCHOV"  0.15000
  "LZFISH"  0.10500
  "STRDRM"  0.10000
  "EPIFAN"  0.16000
  "SEARBN"  0.19000
  "THRDFN"  0.15900
  "SARDNS"  0.11200
  SEDING    0.10000
!
CONSUME ID="ANCHOV" PREY
  "FITPLC"  1.00000
  SEDING    0.00000
```

4.3 Code Execution

CONSUME can run under either the Windows or Linux operating system. Under the Windows operating system (Releases XP or 7), CONSUME executes in a DOS box. A run of CONSUME is initiated by entering the following command line:

```
CONSUME "Data File"
```

Under the Linux operating system CONSUME is executed through the following Bourne Shell or C Shell commands:

```
consume-1.exe "Data File"
```

For these commands, “CONSUME.EXE” or “consume-1.exe” is the name of the executable program. One argument (file name) must be provided on the command line. The argument is the name of the data file to be processed.

5.0 ECDA – Environmental Concentration Data Accumulator Setup

5.1 Overview

The ECDA code creates the binary environmental concentration data accumulator (ECDA) files and initializes the contents for each environmental medium. In addition, the ECDA code optionally creates the stochastic data libraries of soil distribution coefficients (K_d), shoreline seep water dilution factors and surface soil net water infiltration rates.

5.1.1 Location in the Processing Sequence

The ECDA code typically is run before any other code in an assessment. It must be run before any of the following codes can execute: SOIL, RIPSAC, or any of the impacts codes.

5.1.2 How the Code Is Invoked

ECDA can run under either the Windows or the Linux operating system. Under the Windows operating system (Releases 2000 or XP), ECDA executes in a DOS box. A run of ECDA is initiated by entering the following command line:

```
ECDA "Keyfilename"
```

Under the Linux operating system, ECDA is executed through any of the following Bourne Shell or C Shell commands:

```
ecda-1.exe "Keyfilename"
```

For these commands, “ECDA.EXE” or “ecda-1.exe” is the name of the executable program, and “Keyfilename” is the name of a control keyword file. Both the name of the executable program and keyword file may contain path information. If ECDA is invoked without entering the name of the keyword file, then the code will prompt the user for the file name. The keyword file, which should be prepared using an editor that can handle ASCII files without leaving embedded control codes, contains text control information describing the run. If ECDA cannot open the keyword file, then the code will terminate execution after writing an error message to the standard output device.

5.1.3 Memory Requirements

The ECDA program has minimal memory requirements. A run of the code to create files using 1000 locations, 100 realizations, and 15 analytes required less than 4 MB of memory.

5.2 File Definitions

The ECDA program reads one input file and writes multiple output files. These files are described in the following sections.

5.2.1 Input Files for ECDA

The ECDA program reads the ESD keyword file that contains the basic control information for the entire assessment. An example file is provided in Table 5.1.

Table 5.1 Example Keyword File for ECDA

```
TITLE  "Test Case Test01 for the FILLECDA Code"
USER   "Paul W. Eslinger"
REALIZAT 5 ! Number of realizations
!
PERIOD START=2000 STOP=2050 CLOSURE=2050
!
ANALYTE ID="CCl4"  NAME="Carbon Tetrachloride" TYPE="OS" COMPUTE
  MOLWGT=1.538230E+02  HALFLIFE=0.000000E+00  HENRY=3.080280E+03
  MOLDIFF=8.800000E-06 HENRY=1.0
ANALYTE ID="Tc99"  NAME="Technetium-99"  TYPE="NR" COMPUTE
  HALFLIFE=2.130000E+05  DFIMM=3.663852E-04 DFSED=6.700000E-22
  GAMMA=0.0 MOLDIFF=1.05E-05  HENRY=0.0
!
TIMES 2000 2010 2015 2020 2030 2050
!
FILE KDSOIL NAME="KdSoil_Test01.dat" SEED=232323.0 CREATE
ECHO KDSOIL
KDSOIL ID="Dist01-01" 2 1.0E-10 1.0E-09
  "Distribution type 1 - Constant" UNITS="L/g"
KDSOIL ID="Dist01-02" 2 0.0002  0.00024
  "Soil-water Kd for iodine" UNITS="L/g"
!
FILE DILUTE NAME="Dilute_Test01.dat" SEED=123445.0 CREATE
ECHO DILUTE
DILUTE ID="DF_01" 2 1.47 2.42
  "Dilution factor number 01" UNITS="None"
DILUTE ID="DF_02" 2 2.47 3.42
  "Dilution factor number 02" UNITS="None"
!
FILE INFILT NAME="infilt_Test01.dat" SEED=1275.0 CREATE
ECHO INFILT
INFILTRATION DEFINE UNIT="mm/yr" CLASS="ABC" 6 0.05 0.1 0.2
  "Soil Surface covered by Asphalt, Building, or Concrete"
INFILTRATION DEFINE UNIT="mm/yr" CLASS="Ba-dg" 6 13 26 52
  "Burbank loamy sand (Ba), disturbed - with cheatgrass"
!
! Initialize the ECDA files
FILLECDA GWAT FIXED =  0.0
FILLECDA PWAT FIXED =  0.0
FILLECDA SWAT FIXED =  0.0
FILLECDA SEEP FIXED =  0.0
FILLECDA SEDI FIXED =  0.0
FILLECDA SORP FIXED =  0.0
FILLECDA SODR FIXED =  0.0
FILLECDA SOGW FIXED =  0.0
FILLECDA SOSW FIXED =  0.0
FILLECDA AIRC FIXED =  0.0
FILLECDA AIRD FIXED =  0.0
!
```

```
FILE HEADER NAME="ECDA_Test01.hdr" CREATE
FILE I_ECDA NAME="ECDA_Test01.idx" CREATE
FILE C_ECDA ANALYTE="CCl4" NAME="CCl4_Test01.bin" CREATE
FILE C_ECDA ANALYTE="Tc99" NAME="Tc99_Test01.bin" CREATE
!
IRRIGATE SPRING=121 FALL=256 RATE=76.0 NET=0.20 START=2000
  THETAIRG=0.5 THETADRY=0.2
!
LOCATION ID="UH0002" EASTING=575272.00  NORTHING=153617.00  MILE=-1
  NAME="UnsuitableForAgricul" GWAT SODR SOGW SOSW AIRC AIRD
  TYPE="UPLAND"  AREA=1436021.9 IRG_SWAT="QHP001"
  APSD    = 0.040  POROSITY = 0.350  FOC = 1.000  VEGCOV = 0.500
  MSWIND = 3.440   NECF    = 1.000  RHOS     = 1.500  SRH = 0.018
  TEMP   = 012.0  MZWIND = 3.440 TEMP = 12.0
!
LOCATION ID="RHP001" EASTING=557280.81  NORTHING=144134.20  MILE=389.05
  NAME="Riparian Benton Upriver Vernita Bridge"
  GWAT SEEP SORP AIRC AIRD TYPE="RIPARIAN" AREA=9360
  APSD    = 0.040  POROSITY = 0.350  FOC = 1.000  VEGCOV = 0.500
  MSWIND = 3.440   NECF    = 1.000  RHOS     = 1.500  SRH = 0.018
  TEMP   = 012.0  MZWIND = 3.440  TEMP = 12.0
!
LOCATION ID="QHP001" EASTING=557374.25 NORTHING=144903.27 MILE=389.05
  NAME="AquaticBentonUpriverVernitaBridge"
  SWAT PWAT SEDI TYPE="AQUATIC" AREA=2500 COXYGEN=0.011
!
END
```

5.2.2 Output Files for ECDA

The ECDA code writes a number of output files. A report file is always written. The number of other files written depend on the input options. The following list summarizes the output files:

- **Report file**: A report file, named "ecda.rpt" is written for every run of the code. This file is a text file containing information about the run progress. Error messages are written to this file as well.
- **ECDA Data files**: A separate ECDA file is written for every analyte if the CREATE and C_ECDA modifiers are present on the FILE keyword. The file format is described by Eslinger et al. (2006a, Section 2.2.1). These binary files contain the media concentrations calculated by the transport codes that are saved for use in the impacts codes.
- **ECDA Index file**: This file is written if a file name is entered in the keyword file (FILE keyword, I_ECDA modifier). The file format is described in Section 2.2.2. This file contains indexing information to quickly locate data for specific times and locations in the binary ECDA files.
- **ECDA Header file**: This file is written if a file name is entered in the keyword file (FILE keyword, I_ECDA modifier). The file format is described in Section 2.2.3. This file is used to facilitate retrieving and displaying data.
- **Dilution Library File**: This file is written if the CREATE modifier is present in the keyword file (FILE keyword, DILUTE modifier). The file format is described in Section 2.4.1. This file contains a library of generated dilution factors that describe the mixing of groundwater and river water in the riparian zone modeling that are used in the RIPSAC code.

- **Infiltration Library File**: This file is written if the CREATE modifier is present in the keyword file (FILE keyword, INFILT modifier). The file format is described in Section 2.4.3 This file contains a library of generated infiltration values that describe the net infiltration of water through the upper soil layer.
- **Kdsoil Library File**: This file is written if the CREATE modifier is present in the keyword file (FILE keyword, KDSOIL modifier). The file format is described in Section 2.4.2. This file contains a library of generated solid-aqueous partition coefficients (K_d values) that are used in a number of other TIAA programs.

5.3 Keyword Definitions for the ECDA Code

The ECDA code gets all of its control information from keywords in the ESD keyword file. In general, keywords for the ECDA code can be entered in any order. The only restriction is that the END keyword must be the last keyword in the file. The following keyword descriptions have been modified from those described in Section 2.1 to restrict the definition to information used by the ECDA code.

5.3.1 ANALYTE Keyword for ECDA

The ANALYTE keyword is used to define the analytes to be used in the simulation. The following is this keyword's syntax:

```
ANALYTE [ID="quote 1"] [TYPE="quote 2"] [NAME="quote 3"]
```

A separate ANALYTE keyword must be entered for every analyte to be included in the simulation. Table 5.2 provides the modifiers associated with the ANALYTE keyword.

Table 5.2 Modifiers Associated with the ANALYTE Keyword for ECDA

Modifier	Description
ID	The quote string associated with the ID modifier is an analyte identification string up to six characters in length. The analyte identification string is case sensitive, and spaces or hyphens change the definition. All data in the analyte identification strings must satisfy the following conventions: • Only the first entry in the analyte identification string is capitalized. • No embedded spaces or hyphens are used, even for radionuclides. • Individual elements are defined using the standard element abbreviation.
TYPE	The quote string associated with the TYPE modifier string is a two-character analyte type indicator. The following are the valid entries for this string: • NR – if the analyte is a radioactive element or an inorganic compound containing a radionuclide • NS – if the analyte is a stable (nonradioactive) element or inorganic compound • OR – if the analyte is an organic compound containing a radionuclide • OS – if the analyte is an organic compound, containing a stable (nonradioactive) elemental analyte or compound
NAME	The quote string associated with the NAME modifier is an analyte name or description up to 72 characters in length.

The following ANALYTE keywords select the analytes tritium, uranium-235, and chemical uranium for analysis:

```
ANALYTE ID="H3"  NAME="Tritium"  TYPE= "NR"
ANALYTE ID="U235"  NAME="Uranium-235"  TYPE="NR"
ANALYTE ID="U"  NAME="Uranium"  TYPE="NS"
```

5.3.2 DEBUG Keyword for ECDA

The DEBUG keyword initiates output of detailed information on the processing by the code. The following is this keyword's syntax:

```
DEBUG {ECDA}
```

This keyword has no effect if the modifier ECDA is not present. The following keyword will initiate debug outputs:

```
DEBUG ECDA
```

5.3.3 DILUTE Keyword for ECDA

The DILUTE keyword is used to enter the definition of a statistical distribution for stochastic water dilution variables used in the riparian zone water mixing model. The following is this keyword's syntax:

```
DILUTE [ID="quote1"] [Dist_Index Parameters] {TRUNCATE U1 U2}
   {LABEL="quote2"}  [UNITS="quote3"]
```

The quote string associated with the ID modifier is a unique character string of up to 20 characters that will be used to identify this stochastic variable for subsequent uses. It is case sensitive, and embedded spaces are significant. The quote string associated with the optional modifier LABEL contains a description for the stochastic variable that can be up to 64 characters long. An entry for quote2 is not required, although it is used for labeling purposes if present. However, if the modifier LABEL is present, the associated quote string must be entered as well. The quote string associated with the UNITS modifier contains a units descriptor for the data. The strings "none" or "unitless" should be used if the variable is unitless. Section 19.0 contains further information about generating stochastic values.

A dilution factor that is triangular on the triple (0.2, 0.5, 0.99) could use the following keyword entry:

```
DILUTE ID="ID#1" 6 0.2 0.5 0.99 LABEL="Example dilution factor"
   UNITS="none"
```

The stochastic values generated from information on the DILUTE keyword are used only in the RIPSAC code.

5.3.4 ECHO Keyword for ECDA

The ECHO keyword is used to initiate output of summary information code when processing the statistical distributions defined by KDSOIL, DILUTE and INFILTRATION keywords. The following is this keyword's syntax:

```
ECHO {KDSOIL} {DILUTE} {INFILT}
```

If the KDSOIL modifier is present then variable definitions and summary statistics on generated values will be written to the report file for every distribution specified on a KDSOIL keyword. If the DILUTE modifier is present, then variable definitions and summary statistics on generated values will be written to the report file for every distribution specified on a DILUTE keyword. If the INFILT modifier is present, then variable definitions and summary statistics on generated values will be written to the report file for every distribution specified on an INFILTRATION (DEFINE) keyword. Example uses of this keyword are the following:

```
ECHO KDSOIL
ECHO DILUTE
ECHO DILUTE KDSOIL INFILT
```

5.3.5 END Keyword for ECDA

The END keyword signifies the end of all keyword data. It should be the last keyword in the keyword file. Any data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

There are no modifiers or quote strings associated with the END keyword.

5.3.6 FILE Keyword for ECDA

The FILE keyword is used to enter the names of many of the files used in a simulation run. The following is this keyword's syntax:

```
FILE [NAME="quote 1"] {ANALYTE="quote 2"}
   [ HEADER | KDSOIL | DILUTE | C_ECDA | I_ECDA ] {CREATE}
```

The file names must be entered with the complete path. One FILE keyword is required for every analyte for which concentrations are to be generated. Every file definition requires the entry of a separate FILE keyword. Table 5.3 provides the file type modifiers associated with the FILE keyword.

Table 5.3 Modifiers Associated with the FILE Keyword for ECDA

Modifier	Description
NAME	The quote string associated with the NAME modifier is a file name (including path) up to 200 characters in length.
ANALYTE	If the file name is associated with the C_ECDA modifier, the ANALYTE modifier must also be entered to indicate which analyte is to be associated with the ECDA concentration data file.
HEADER	This modifier indicates that the FILE keyword is defining a header file that facilitates extraction of human-readable concentration data by post-processor programs.
KDSOIL	This modifier indicates that the FILE keyword is defining a file to contain stochastic realizations of all of the random variables defined using the KDSOIL keyword.
INFILT	This modifier indicates that the FILE keyword is defining a file to contain stochastic realizations of all of the random variables defined using the INFILTRATION (DEFINE) keyword.

Modifier	Description
DILUTE	This modifier indicates that the FILE keyword is defining a file to contain stochastic realizations of all of the random variables defined using the DILUTE keyword.
C_ECDA	This modifier indicates that the FILE keyword is defining an ECDA concentration data file. Concentrations for each analyte are contained in separate files. The ANALYTE modifier is used to associate an analyte with this file.
I_ECDA	This modifier indicates that the FILE keyword is defining a record index file for mapping into all ECDA concentration files.
CREATE	When this modifier is present, the file will be created. If the CREATE modifier is not present, no actions occur for that file.

The following example entries define the concentration files for a suite of analytes:

```
FILE C_ECDA ANALYTE="H3" NAME="/test/ecda/H3_median.dat"  CREATE
FILE C_ECDA ANALYTE="C14" NAME="/test/ecda/C14_median.dat"  CREATE
FILE C_ECDA ANALYTE="I129" NAME="/test/ecda/I129_median.dat" CREATE
FILE C_ECDA ANALYTE="Tc99" NAME="/test/ecda/Tc99_median.dat" CREATE
```

If present, the CREATE flag causes the following actions:

- Deletion of any existing file by that name and creation of a new file.
- If the file is associated with the HEADER, DILUTE, KDSOIL, INFILT, or I_ECDA modifiers, new data are written to the file.
- If the file is associated with the C_ECDA modifier, the concentration data are initialized to the values identified by the FILLECDA keyword.

The following example entries define the files for soil-water K_d values and the water dilution factors for the river-shore module:

```
FILE KDSOIL NAME="KDSOIL.CSV" SEED=23232.0 CREATE
FILE DILUTE NAME="DILUTE.CSV" SEED=12345.0 CREATE
```

The following example entries define the Header file and ECDA record number index files:

```
FILE HEADER NAME="/test/ecda/Sacview_median.hdr" CREATE
FILE I_ECDA  NAME="/test/ecda/ECDA_median.map"  CREATE
```

5.3.7 FILLECDA Keyword for ECDA

The FILLECDA keyword controls filling ECDA files with fixed or random values as they are initialized. The following is this keyword's syntax:

```
FILLECDA [GWAT|SWAT|AIRC|AIRD|PWAT|SEDI|SORP|SEEP|SODR|SOGW|SOSW]
   [FIXED=N1 | RANDOM=N2]
```

Concentrations can be set to zero, an invalid value (negative number), or other specified values. Other codes that read concentrations check for negative values and error terminate if negative values are encountered. Initializing these files to negative concentrations can be a usedful check that later actions enter all valid concentration data that are needed. A separate FILLECDA keyword must be entered for each media. Table 5.4 describes the modifiers associated with the FILLECDA keyword. These keywords provide global initialization of the ECDA files. The separate FILLECDA code can be used to enter user-defined values in support of a specific analysis.

Table 5.4 Modifiers Associated with the FILLECDA Keyword in the ESD File

Modifier	Description
GWAT	Presence of this optional modifier indicates that groundwater concentrations will be initialized with the specified value.
SWAT	Presence of this optional modifier indicates that surface water concentrations will be initialized with the specified value.
AIRC	Presence of this optional modifier indicates that atmospheric concentrations will be initialized with the specified value.
AIRD	Presence of this optional modifier indicates that atmospheric deposition rates will be initialized with the specified value.
PWAT	Presence of this optional modifier indicates that river bottom pore water concentrations will be initialized with the specified value.
SEDI	Presence of this optional modifier indicates that sediment concentrations (on the river bottom) will be initialized with the specified value.
SORP	Presence of this optional modifier indicates that riparian zone soil concentrations (on the land surface) will be initialized with the specified value.
SEEP	Presence of this optional modifier indicates that seep water concentrations (on the land surface) will be initialized with the specified value.
SODR	Presence of this optional modifier indicates that upland soil concentrations from non-irrigated soils will be initialized with the specified value.
SOGW	Presence of this optional modifier indicates that upland soil concentrations using groundwater for irrigation will be initialized with the specified value.
SOSW	Presence of this optional modifier indicates that upland soil concentrations using surface water for irrigation will be initialized with the specified value.
RANDOM	This modifier initializes the values of the media using random numbers on the interval (0,1). The numerical value N_2 is used to initialize the random number generator and must be a whole number in the range 1 to 9999999. This option is usually restricted to code testing where a unique concentration value is desired for every entry for the media.
FIXED	The numerical value, N_1, associated with this modifier is used to initialize all entries for the selected media. The units associated with each media are defined in Section 2.2.1. If a fixed entry is used, the same value is used for the media for every time, location and realization. The most typical values used are 0 (no concentration) or -1 (invalid concentration).

The following example entries assign values to use in initialization of the ECDA files:

```
FILLECDA GWAT FIXED =  0.0
FILLECDA PWAT FIXED =  0.0
FILLECDA SWAT FIXED =  0.0
FILLECDA SEEP FIXED = -1.0
FILLECDA SEDI FIXED =  0.0
FILLECDA SORP FIXED = -1.0
FILLECDA SODR FIXED = -1.0
FILLECDA SOGW FIXED = -1.0
FILLECDA SOSW FIXED = -1.0
FILLECDA AIRC FIXED =  0.0
```

```
FILLECDA AIRD FIXED =  0.0
```

5.3.8 INFILTRATION Keyword in ECDA

The INFILTRATION keyword defines the stochastic distribution for net natural infiltration rates through surface soil. The infiltration rates are tagged with an ID (called a CLASS) and they are assumed to be constant with time. If irrigation is used at one or more locations, then an infiltration rate must be specified for each location. Multiple locations can use one infiltration rate by assigning that specific ID. Definitions of infiltration rates use the following syntax:

```
INFILTRATION DEFINE [CLASS="quote 1"]  [UNIT="quote 2"]
   [Dist_Index Parameters]  {TRUNCATE U1 U2}  {"quote 3"}
```

The quote string associated with the CLASS modifier contains a user-specified ID for the infiltration class. The data for this class will be referenced by the ID. The quote string associated with the UNIT modifier must contain the data units. Units of mm/yr should be used. The quote string identified as quote3 contains a descriptive label for this infiltration class and must be the third quote string in the keyword entry.

The remaining entries for this syntax are used to define a statistical distribution for the infiltration rate. Additional information about these entries is provided in Section 19.1. Some example uses of this syntax are the following:

```
INFILTRATION DEFINE UNIT="mm/yr" CLASS="Hanford" 1 0.1 "Hanford Barrier"
INFILTRATION DEFINE UNIT="mm/yr" CLASS="Hs-dn" 1 55
   "Hanford Sand (Hs), disturbed with no vegation"
```

5.3.9 KDSOIL Keyword in ECDA

The KDSOIL keyword is used to enter the definition of a statistical distribution for the solid-aqueous distribution coefficient (K_d) to be used for calculating soil concentrations from groundwater concentrations. The following is this keyword's syntax:

```
KDSOIL [ID="quote1"] [Dist_Index Parameters] {TRUNCATE U1 U2}
   {LABEL="quote2"}  [UNITS="quote3"]
```

The quote string associated with the ID modifier is a unique character string of up to 20 characters that will be used to identify this stochastic variable for subsequent uses. It is case sensitive, and embedded spaces are significant. The quote string associated with the optional modifier LABEL contains a description for the stochastic variable that can be up to 64 characters long. An entry for quote2 is not required, although it is used for labeling purposes if present. However, if the modifier LABEL is present, the associated quote string must be entered as well. The quote string associated with the UNITS modifier contains a units descriptor for the data. The strings "none" or "unitless" should be used if the variable is unitless. Section 1.0 contains further information about generating stochastic values.

A K_d that is triangular on the triple (0.2, 0.5, 0.99) could use the following keyword entry:

```
KDSOIL ID="ID#1" 6 0.2 0.5 0.99 LABEL="Example Kd" UNITS= "L/g"
```

The data entered by this keyword are used in the river model MASS2 and in the riparian zone model RIPSAC.

5.3.10 LOCATION Keyword for ECDA

The LOCATION keyword identifies the locations where concentrations will be generated for use in the impacts modules. The following is this keyword's syntax:

```
LOCATION [ID="quote1"] [EASTING=N1] [NORTHING=N2] {GWAT} {SWAT}
   {AIRC} {AIRD} {PWAT} {SEDI} {SORP} {SEEP} {SODR} {SOGW} {SOSW}
   [NAME="quote2"]
```

Table 5.5 provides the modifiers and associated data for the LOCATION keyword.

Table 5.5 Modifiers Associated with the LOCATION Keyword in the ESD File

Modifier	Description
ID	The location identification string is entered using the ID modifier. This string is limited to 6 characters and must be unique. It is used to associate other data with a specific location.
EASTING	This entry is associated with the easting coordinate for the location. These coordinates are expressed in terms of the Lambert projection of the Washington State Plane North American Datum of 1983, expressed in meters.
NORTHING	This entry is associated with the northing coordinate for the location. These coordinates are expressed in terms of the Lambert projection of the Washington State Plane North American Datum of 1983, expressed in meters.
NAME	The quote string associated with the NAME modifier contains a descriptive name of up to 64 characters in length that is used for labeling purposes.
GWAT	Presence of this optional modifier indicates that groundwater concentrations will be computed at this location.
SWAT	Presence of this optional modifier indicates that surface water concentrations will be computed at this location.
AIRC	Presence of this optional modifier indicates that atmospheric concentrations will be computed at this location.
AIRD	Presence of this optional modifier indicates that atmospheric deposition rates will be computed at this location.
PWAT	Presence of this optional modifier indicates that river bottom pore water concentrations will be computed at this location.
SEEP	Presence of this optional modifier indicates that seep water concentrations (on the land surface) will be computed at this location.
SODR	Presence of this optional modifier indicates that upland soil concentrations from non-irrigated soils will be initialized with the specified value.
SORP	Presence of this optional modifier indicates that riparian zone soil concentrations (on the land surface) will be computed at this location.
SEDI	Presence of this optional modifier indicates that sediment concentrations (on the river bottom) will be computed at this location.
SOGW	Presence of this optional modifier indicates that soil concentrations using groundwater for irrigation will be computed at this location.

Modifier	Description
SOSW	Presence of this optional modifier indicates that soil concentrations using surface water for irrigation will be computed at this location. Refer to the IRG_SWAT modifier to specify the surface water location.

The following example keywords define three impact locations:

```
LOCATION ID="HL0151" NAME="Upland location"
   EASTING=594737.5  NORTHING=127827.4  GWAT
LOCATION ID="HL0417" NAME="Riparian zone location"
   EASTING=557375.3  NORTHING=144885.2  GWAT SORP SEEP
LOCATION ID="HL0413" NAME="Richland municipal water intake"
   EASTING=595445.1  NORTHING=109753.5  SWAT PWAT SEDI
```

5.3.11 PERIOD Keyword for ECDA

The PERIOD keyword identifies the start and stop times for the entire simulation. The following is this keyword's syntax:

```
PERIOD [START=year1]  [STOP=year2]  [CLOSURE=year3]
```

The modifier START and the associated value $year_1$ identify the start year for the simulation. The start of the simulation period must be 1944 or later, or the inventory code will error terminate. The modifier STOP and the associated value $year_2$ identify the end year for the simulation. Start and stop years should be entered as whole numbers with the stop year no smaller than the start year. The modifier CLOSURE and the associated value $year_3$ identify the year that site closure occurs. The year of site closure cannot be smaller than the start year. The following example PERIOD keyword simulates from 1944 through 3050 with site closure occurring at 2050:

```
PERIOD START=1944 STOP=3050 CLOSURE 2050
```

5.3.12 REALIZAT Keyword for ECDA

The REALIZAT (or REALIZATION) keyword identifies the number of realizations to be simulated. The following is this keyword's syntax:

```
REALIZAT N1
```

The number of realizations is given by the single numerical entry N1. The valid number of realizations is 1 to 9999. Run times and disk storage requirements are directly proportional to the number of realizations. The following is an example REALIZAT keyword requesting 25 realizations:

```
REALIZAT 25
```

5.3.13 TITLE Keyword for ECDA

The TITLE keyword is used to define a single-line problem title. The problem title will be written to output files. If the title is not supplied, then the program will error terminate. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 200 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the ECDA code."
```

5.3.14 USER Keyword for ECDA

The USER keyword is used to identify the user of the program. The user name will be written to output files. If the user name is not supplied, then the program will terminate with an error. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

6.0 ECDA_ASCII – Environmental Concentration Data Accumulator File Conversions

6.1 Overview

The ECDA_ASCII program converts binary environmental concentration files into text format. The sole purpose of the conversion is to create a file that is human readable in a text editor.

6.1.1 Location in the Processing Sequence

The ECDA_ASCII program can be executed any time after the ECDA files have been created. However, other programs such as RIPSAC, SOIL and FILLECDA write concentration data to these files. Thus, ECDA_ASCII is usually run after all of the other codes have been executed.

6.1.2 How the Code Is Invoked

ECDA_ASCII can run under either the Windows or the Linux operating system. Under the Windows operating system (Releases XP or 7), ECDA_ASCII executes in a DOS box. A run of ECDA_ASCII is initiated by entering the following command line:

```
ECDA_ASCII
```

Under the Linux operating system ECDA_ASCII is executed through any of the following Bourne Shell or C Shell commands:

```
ecda_ascii.exe
```

For these commands, “ECDA_ASCII .EXE” or “ecda_ascii.exe” is the name of the executable program.

6.1.3 Memory Requirements

The ECDA_ASCII code uses dynamic memory allocation. However, only one line of the input file is in memory at any given time, so the memory requirements are minimal. It is expected that most, if not all, of the runs of the ECDA_ASCII code will require less than 2 MB of memory.

6.2 File Definitions

The ECDA_ASCII code reads one file and writes one file.

6.2.1 Input Files

The ECDA_ASCII code reads an environmental concentration data accumulator (ECDA) file. This file is in binary format and is created by the ECDA program. Other programs such as FILLECDA, RIPSAC and SOIL write concentration data to these ECDA files.

6.2.2 Output Files

The ECDA_ASCII code writes one data file. This file is a text translation of the binary ECDA file. An example of the first 20 lines of the output text file when only the groundwater media is selected is provided in Table 6.1. The numbers in the left column are record numbers that are not in the original data set. The file starts with an analyte identifier followed by the units of the 11 possible media. The data for multiple realizations are written on each line. This file only contained one realization of data.

Table 6.1 Excerpts from an ECDA_ASCII Output File

```
File: N:\CA1_median\ecda\Eu152_CA1_median.dat
       1 Eu152
       2 Ci/m^3
       3 Ci/m^3
       4 Ci/m^3
       5 Ci/m^3
       6 Ci/kg
       7 Ci/kg
       8 Ci/kg
       9 Ci/kg
      10 Ci/kg
      11 Ci/m^3
      12 Ci/m^2/yr
      13    1945 UH0001 GWAT  0.00000E+00
      19    1945 UH0002 GWAT  0.00000E+00
      25    1945 UH0003 GWAT  0.00000E+00
      31    1945 UH0004 GWAT  0.00000E+00
      37    1945 UH0005 GWAT  0.00000E+00
      43    1945 UH0006 GWAT  0.00000E+00
      49    1945 UH0007 GWAT  0.00000E+00
```

6.3 Code Execution

The ECDA_ASCII program runs in an interactive mode. A screen image from a run of the code on a Windows machine is provided in Figure 6.1. The user must provide answers to five prompts:

1. The name of the binary ECDA file must be provided. A full pathname is required unless the ECDA file is in the same directory where the ECDA_ASCII code was invoked.
2. The name of the output ASCII file must be provided. The user can select any name. An extension of ".txt" is recommended.
3. The number of realizations for the simulation must be provided. An entry of 0 will terminate program execution.
4. The media for which data are to be translated must be provided (either ALL or one of the 4-character abbreviations provided below). The entry ALL will translate data for all media. The individual media options are as follows (also see Section 2.2.1):
   - GWAT – concentrations in groundwater
   - SEEP – concentrations in seep water
   - SWAT – concentrations in surface water
   - PWAT – concentrations in river bottom pore water
   - SEDI – concentrations in river bottom sediment
   - SORP – concentrations in riparian zone soil (land surface)

- SODR – concentrations in upland soil (land surface) with no irrigation
- SOGW – concentrations in upland soil (land surface) with groundwater irrigation
- SOSW – concentrations in upland soil (land surface) with surface water irrigation
- AIRC – concentrations in air
- AIRD – air deposition rates

5. The locations for which media to translate must be provided (either ALL or one of the 6-character location ID's defined in the ESD keyword file). The entry ALL will translate data for all locations.
6. The number of data records to be translated must be provided. Care must be taken when translating a large ECDA file such that the output ASCII file does not exceed 2.1 gigabytes in size. If the output file exceeds that size, the program will error terminate.

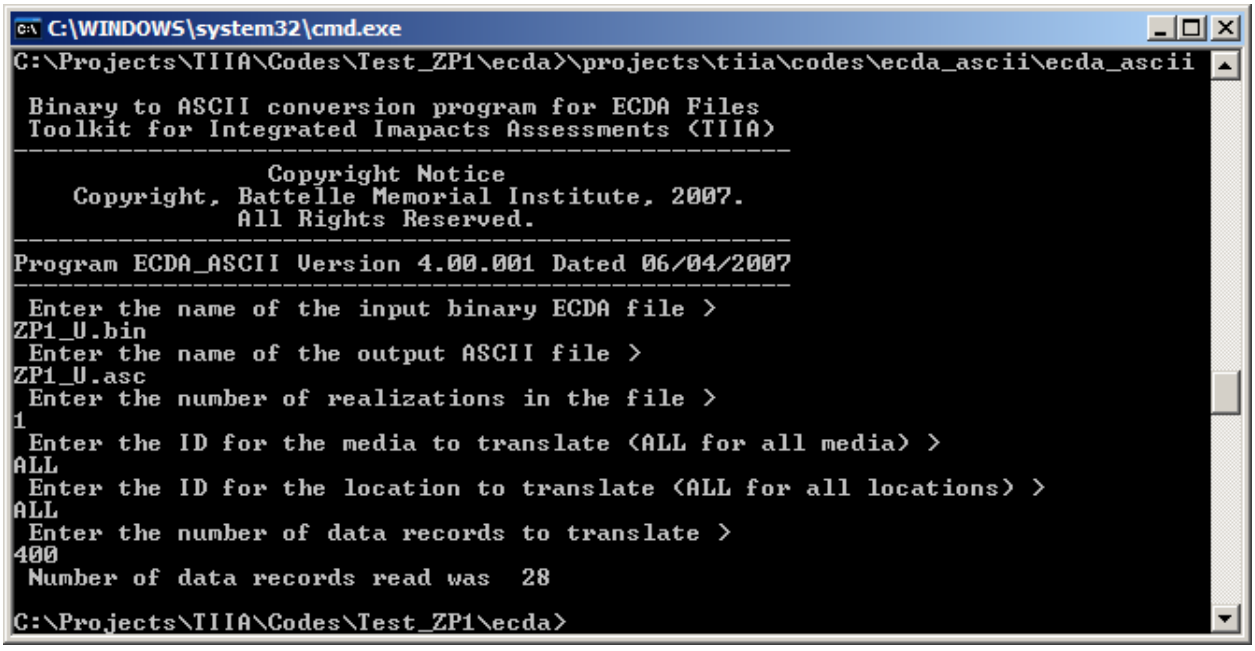

Figure 6.1 Screen Image of an ECDA_ASCII Run

7.0 ECEM – Ecological Impact Model

The ecological risk model is a detailed, food-web based chronic exposure model. It is intended for use in situations where the environmental contamination conditions are static or only slowly varying. The models are not appropriate for estimating risks from short-term accidental releases.

The ECEM code addresses pathways related to long-term contamination from sources in air, surface water, and groundwater, with the associated contaminated media of seeps, springs, soils, and sediments. With these as starting points, the code calculates contaminant concentrations in aquatic foods, terrestrial crops, and animal products. Exposure pathways explicitly modeled include external irradiation, dermal contact, inhalation, and ingestion via a food web. Organisms include plants, herbivores, and carnivores or omnivores (consumers of both flesh and plant material) in upland, terrestrial, and aquatic environments. An organism's exposure to contaminated food, sediment, surface water, or pore water is a function of its life style. The model assumes equilibrium conditions, meaning that exposures are estimated based on the assumption that the organism spends enough time in a given location that the concentration of contaminants in its tissue is in equilibrium with the environment (i.e., no net gain or loss of contaminant from the organism).

The ECEM code provides results for radioactive contaminants; non-radioactive but carcinogenic contaminants; and non-radioactive, non-carcinogenic, but still hazardous contaminants. Radiation impact to an individual organism is calculated as radiation dose; carcinogenic chemical impact is calculated as body burden or dose; risks from hazardous chemicals are provided as body burden, dose, or Environmental Hazard Quotient—the dimensionless ratio of the estimated intake to a standard Reference Dose.

The ECEM code is designed to accept multiple realizations of concentration of contaminants in the environment. It allows the definition of stochastic exposure parameters, which combine with the uncertainty in the input media concentrations to provide a full range of uncertainty on the final dose or risk to the hypothetical exposed individual organism.

7.1 Mathematical Formulation for the Ecological Impact Model

The following sections give the intake and exposure equations for the ecological impact model. The equations are given for both terrestrial and aquatic species. The concentration equations given in this section are based on equilibrium concepts rather than dynamic formulations.

7.1.1 Terrestrial Species

Terrestrial species are subdivided into plant and animal species. The exposure equations for terrestrial species are given in this section.

7.1.1.1 Terrestrial Plants

The analyte concentrations in terrestrial plants can come from rain splash, root uptake or foliar absorption from vapor, soil contact, air deposition onto the plant surface, and irrigation water deposition onto the plant surface. The concentrations also depend on whether the analyte is organic or inorganic.

7.1.1.1.1 Contaminant Deposition Caused by Rain Splash

The equilibrium concentration of contaminant c in above-ground parts of plant species i from rain splash is calculated using the following equation:

$$C_{par}(i,c) = EC_{soil}(c) \times K_{ps1}(i) \tag{7.1}$$

where

$C_{par}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from rain splash (µg/kg or pCi/kg plant wet)
$EC_{soil}(c)$ = concentration of contaminant c in surface soil (top ~1 cm) (µg/kg or pCi/kg dry)
$K_{ps1}(i)$ = plant-soil partition coefficient for rain splash on fresh-weight basis for plant species i (kg soil/kg plant wet)

If the plant is an emergent plant (rooted in soil but grows in water), then $C_{par}(i,c)$ is set to zero.

7.1.1.1.2 Root Uptake to Above-Ground Plant Tissue

The equilibrium concentration in above-ground plant parts from root uptake is calculated using the following equations. For organic contaminants, the equation is:

$$C_{pau}(i,c) = EC_{soil}(c) \times K_{ps2}(c) \tag{7.2}$$

For inorganic contaminants except tritium, the equation is:

$$C_{pau}(i,c) = EC_{soil}(c) \times B_v(i,c) \times \left(1 - f_w(i)\right) \tag{7.3}$$

where

$C_{pau}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from root uptake (µg/kg or pCi/kg plant wet)
$EC_{soil}(c)$ = concentration of contaminant c in surface soil (top ~1 cm) (µg/kg or pCi/kg dry)
$K_{ps2}(c)$ = plant-soil partition coefficient for root-zone soil to above-ground plant parts for organic contaminant c - fresh weight basis (kg soil/kg plant wet)
$B_v(i,c)$ = bioconcentration factor for vegetative parts of plant species i for inorganic contaminant c – dry weight basis (kg-soil/kg plant dry)
$f_w(i)$ = weight fraction of plant species i that is water (wet to dry conversion)

For the inorganic contaminant tritium, the equation is:

$$C_{pau}(i,c) = EC_{water}(c) \times f_w(i) \times 1 \tag{7.4}$$

where

$C_{pau}(i,c)$ = equilibrium tritium concentration in above-ground plant parts from root uptake (pCi/kg wet)
$EC_{water}(c)$ = tritium concentration in the water source (pCi/L)
$f_w(i)$ = weight fraction of plant species i that is water (wet to dry conversion)
1 = density of water (L/kg)

If the plant is an emergent plant (rooted in soil but grows in water), then the concentration of the analyte in sediment, $EC_{sed}(c)$, is used in the equation for $C_{pau}(i,c)$ rather than $EC_{soil}(c)$.

The plant-soil partition coefficient for root-zone soil to above-ground plant parts for organic contaminants (fresh weight basis) is calculated using the following regression model (McKone 1993):

$$K_{ps2}(c) = 7.7 \times \left(10^{K_{ow}(c)}\right)^{-0.58} \quad (7.5)$$

where $K_{ow}(c)$ = log base 10 of the octanol-water partition coefficient for contaminant c (unitless)

7.1.1.1.3 Foliar Uptake from Soil by Vapor

The equilibrium concentration in above-ground plant parts from vapor uptake is calculated using the following equation (Hope 1995):

$$C_{pav}(i,c) = (EC_{vap}(i,c) + EC_{airc}(c)) \times K_{pa1}(i,c) \quad (7.6)$$

where:

$C_{pav}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from vapor uptake (µg/kg or pCi/kg plant wet)
$EC_{vap}(i,c)$ = concentration of contaminant c in the gas phase for exposure to species i (µg/m^3 or pCi/m^3)
$EC_{airc}(c)$ = concentration of contaminant c in air (µg/m^3 or pCi/m^3)
$K_{pa1}(i,c)$ = plant-air partition coefficient to above-ground parts of plant species i for organic contaminant c (m^3/kg wet weight)

The plant-air partition coefficient for transfer of analytes in the air to above-ground plant parts for organic contaminants is calculated using the following equation (Bacci et al. 1990 and Riederer 1990):

$$K_{pa1}(i,c) = \left[f_{pa}(i) + \left(f_{pw}(i) + \left[f_{pl}(i) \times 10^{K_{ow}(c)}\right]\right) \times \left[\frac{R \times (T + 273.15)}{H(c)}\right]\right] \Big/ \rho_p(i) \quad (7.7)$$

where

$K_{pa1}(i,c)$ = plant-air partition coefficient to above-ground parts of plant species i for organic contaminant c (m^3/kg wet weight)
$f_{pa}(i)$ = volume fraction of plant species i tissue is air (unitless)
$f_{pw}(i)$ = volume fraction of plant species i tissue that is water (unitless)
$f_{pl}(i)$ = volume fraction of plant species i tissue that is lipid (unitless)
$K_{ow}(c)$ = log base 10 of the octanol-water partition coefficient for contaminant c (unitless)

R = universal gas constant (Pa-m^3/mol-K)
T = temperature (K)
H(c) = Henry's law constant for contaminant c (Pa-m^3/mol)
$\rho_p(i)$ = plant species i tissue density (kg/m^3)

The concentration of gas-phase contaminant is calculated using the following equation (EPA 1991):

$$EC_{vap}(i,c) = \frac{EC_{soil}(c) \times 10^4}{\left(\frac{LS \times V \times D_h(i)}{A}\right) \times \left(\frac{[\pi \times \varsigma(c) \times I]^{0.5}}{2 \times D_{ei}(c) \times E \times K_{as}(c) \times 10^{-3}}\right)} \quad (7.8)$$

where
$EC_{vap}(i,c)$ = concentration of contaminant c in the gas phase for exposure to species i (µg/m^3 or pCi/m^3)
$EC_{soil}(c)$ = concentration of contaminant c in surface soil (top 15 cm) (µg/kg or pCi/kg dry)
LS = length of side of contaminated area (m)
V = wind speed in mixing zone (m/s)
$D_h(i)$ = diffusion height for species i (m)
A = area of contamination (m^2)
$\zeta(c)$ = effective diffusion rate for contaminant c (cm^2/s)
I = exposure interval (s)
$D_{ei}(c)$ = effective diffusivity for contaminant c (cm^2/s)
E = soil porosity (unitless)
$K_{as}(c)$ = soil/air partition coefficient for contaminant c (g soil/cm^3 air)
10^4 = unit conversion factor (cm^2/ m^2)
10^{-3} = unit conversion factor (kg/g)

The effective diffusion rate is calculated from the expression:

$$\varsigma(c) = \frac{D_{ei}(c) \times E}{E + \left(\rho_s \times \left[\frac{1 - E}{K_{as}(c)}\right]\right)} \quad (7.9)$$

where
$\zeta(c)$ = effective diffusion rate for contaminant c (cm^2/s)
$D_{ei}(c)$ = effective diffusivity for contaminant c (cm^2/s)
E = soil porosity (unitless)
ρ_s = denotes the soil density (g/cm^3)
$K_{as}(c)$ = soil/air partition coefficient for contaminant c (g soil/cm^3 air)

The soil/air partition coefficient is calculated (EPA 1991) from the expression:

$$K_{as}(c) = \frac{41 \times H(c)}{101{,}325 \times K_d(c)} \quad (7.10)$$

where

$K_{as}(c)$ = soil/air partition coefficient for contaminant c (g soil/cm^3 air)
$H(c)$ = Henry's law constant for contaminant c (Pa-m^3/mol)
$K_d(c)$ = soil-water partition coefficient for contaminant c (cm^3/g)
41 = unit conversion factor (mol/m^3-atm)
101,325 = unit conversion factor (Pa/atm)

Furthermore, K_d for organic contaminants is calculated (regression model in Baker et al. 1997) using the expression:

$$K_d(c) = s_{oc} \times 10^{0.094} \times \left(10^{K_{ow}(c)}\right)^{0.903} \quad (7.11)$$

where
$K_d(c)$ = soil-water partition coefficient for organic contaminant c (cm^3/g)
$K_{ow}(c)$ = log base 10 of the octanol-water partition coefficient for organic contaminant c (unitless)
s_{oc} = soil organic carbon content (unitless)

The effective diffusivity is calculated from the expression:

$$D_{ei}(c) = D_i(c) \times E^{0.33} \quad (7.12)$$

where:
$D_{ei}(c)$ = effective diffusivity for contaminant c (cm^2/s)
$D_i(c)$ = molecular diffusivity for contaminant c (cm^2/s)
E = soil porosity (unitless)

7.1.1.1.4 Foliar Adsorption of Particulates from Soil

The equilibrium concentration in above-ground plant parts from foliar adsorption of particulates from soil is calculated from the expression:

$$C_{pap}(i,c) = EC_{par}(i,c) \times K_{pa2}(i) \quad (7.13)$$

where
$C_{pap}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from foliar adsorption (µg/kg or pCi/kg plant wet)
$EC_{par}(i,c)$ = concentration of particulate-bound contaminant c in air for exposure to species i (µg/m^3 or pCi/m^3)
$K_{pa2}(i)$ = plant-air partition coefficient for above-ground parts of plant species i for particulate-bound contaminants (m^3/kg plant wet)

The air concentration of particulate-bound contaminant is calculated (EPA 1991) as:

$$EC_{par}(i,c) = \frac{EC_{soil}(c)}{PEF(i)} \quad (7.14)$$

where

$EC_{par}(i,c)$ = concentration of particulate-bound contaminant c in air for exposure to species i ($\mu g/m^3$ or pCi/m^3)

$EC_{soil}(c)$ = concentration of contaminant c in surface soil (top ~1 cm) ($\mu g/kg$ or pCi/kg dry)

PEF(i) = the particulate emission factor for species i (m^3/kg)

Furthermore, PEF is calculated from the following expression (EPA 1991):

$$PEF(i) = \frac{LS \times V \times D_h(i) \times 3600}{A} \times 1000 \Bigg/ \left[Rf \times (1 - Cf) \times \left(\frac{U_m}{U_t} \right)^3 \times F(x) \right] \qquad (7.15)$$

where

PEF(i) = the particulate emission factor for species i (m^3/kg)
LS = length of side of contaminated area (m)
V = wind speed in mixing zone (m/s)
$D_h(i)$ = diffusion height for species i (m)
A = contaminated area (m^2)
Rf = respirable fraction (g/m^2-hr)
Cf = fraction of vegetative cover (unitless)
U_m = mean annual wind speed (m/s)
U_t = erosion threshold wind speed at 10 m (m/s)
F(x) = Cowherd function (Cowherd et al. 1985) (unitless)
3600 = unit conversion factor (s/hr)
1000 = unit conversion factor (g/kg)

The erosion threshold wind speed is calculated (Cowherd et al. 1985) from:

$$U_t = 2.5 \times TFV \times \ln\left(\frac{10}{SRH} \right) \qquad (7.16)$$

where

U_t = erosion threshold wind speed at 10 m (m/s)
TFV = the threshold friction velocity (m/s)
SRH = surface roughness height (m)
10 is a modeling factor with units of meters.

Furthermore, TFV is calculated from a regression model (Cowherd et al. 1985) using the following equation:

$$TFV = NECF \times \left(\frac{64 + 0.0055 \times APSD \times 1000}{100} \right) \qquad (7.17)$$

where

TFV = the threshold friction velocity (m/s)
NECF = nonerodible elements correction factor (unitless)
APSD = the aggregate particle size distribution (mm)
1000 = conversion factor (mm/m)

7.1.1.1.5 Foliar Adsorption of Particulates from Air Deposition

The equilibrium concentration of contaminant c in above-ground parts of plant species i from foliar adsorption of particulates from air deposition is calculated from the expression:

$$C_{pad}(i,c) = \frac{EC_{aird}(c) \times F_{dint}(i,c)}{BM(i) \times \lambda_{wd}(i,c)} \quad (7.18)$$

where:

$C_{pad}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from air deposition (µg/kg or pCi/kg plant wet)
$EC_{aird}(c)$ = air deposition rate of contaminant c (µg/m^2/yr or pCi/m^2/yr)
$F_{dint}(i,c)$ = foliar dry interception of contaminant c for plant species i (unitless)
BM(i) = standing biomass of plant species i (kg/m^2)
$\lambda_{wd}(i,c)$ = weathering constant for dry deposition of contaminant for plant species i (yr^{-1})

7.1.1.1.6 Foliar Adsorption of Particulates from Water Deposition

The equilibrium concentration in above-ground plant parts from foliar adsorption of particulates from water deposition (upland irrigation) is calculated from the expression:

$$C_{paw}(i,c) = \frac{EC_{water}(c) \times (IRR/GS) \times F_{wint}(i,c) \times 10}{BM(i) \times \lambda_{ww}(i,c)} \quad (7.19)$$

where:

$C_{paw}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from irrigation water deposition (µg/kg or pCi/kg plant wet)
$EC_{water}(c)$ = concentration of contaminant c in irrigation water (µg/L or pCi/L)
IRR = amount of irrigation water applied in a year (cm)
GS = length of the growing season (yr)
$F_{wint}(i,c)$ = foliar wet interception of contaminant c for plant species i (unitless)
BM(i) = standing biomass of plant species i (kg/m^2)
$\lambda_{ww}(i,c)$ = weathering constant for wet deposition of contaminant c for plant species i (yr^{-1})
10 = unit conversion factor (L/m^3 x m/cm)

7.1.1.1.7 Total Plant Burden

The total plant burden can be expressed either as an internal burden or the burden as eaten by herbivores. The internal burden of contaminant c in plant species i is calculated from the following expression:

$$C_{pai}(i,c) = C_{pav}(i,c) + C_{pau}(i,c) + \left(C_{par}(i,c) + C_{pap}(i,c) + C_{pad}(i,c)\right) \times KLI_d(i,c) + C_{paw}(i,c) \times KLI_w(i,c) \quad (7.20)$$

where

$C_{pai}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i (µg/kg or pCi/kg tissue)

$C_{pav}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from vapor uptake (µg/kg or pCi/kg plant wet)

$C_{pau}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from root uptake (µg/kg or pCi/kg plant wet)

$C_{par}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from rain splash (µg/kg or pCi/kg plant wet)

$C_{pap}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from foliar adsorption (µg/kg or pCi/kg plant wet)

$C_{pad}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from air deposition (µg/kg or pCi/kg plant wet)

$KLI_d(i,c)$ = leaf to internal plant transfer factor for dry deposition of contaminant c for plant species i (unitless)

$C_{paw}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from irrigation water deposition (µg/kg or pCi/kg plant wet)

$KLI_w(i,c)$ = leaf to internal plant transfer factor for wet deposition of contaminant c for plant species i (unitless)

The total burden of contaminant c in plant species i as eaten by herbivores is calculated from the following expression:

$$C_{pat}(i,c) = C_{pav}(i,c) + C_{pau}(i,c) + C_{par}(i,c) + C_{pap}(i,c) + C_{pad}(i,c) + C_{paw}(i,c) \qquad (7.21)$$

where

$C_{pat}(i,c)$ = equilibrium concentration of contaminant c in and on plant tissue for plant species i (µg/kg or pCi/kg tissue)

$C_{pav}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from vapor uptake (µg/kg or pCi/kg plant wet)

$C_{pau}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from root uptake (µg/kg or pCi/kg plant wet)

$C_{par}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from rain splash (µg/kg or pCi/kg plant wet)

$C_{pap}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from foliar adsorption (µg/kg or pCi/kg plant wet)

$C_{pad}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from air deposition (µg/kg or pCi/kg plant wet)

$C_{paw}(i,c)$ = equilibrium concentration of contaminant c in above-ground parts of plant species i from irrigation water deposition (µg/kg or pCi/kg plant wet)

7.1.1.2 Terrestrial Animals

The body burden for terrestrial animals can come from any combination of dermal contact, ingestion, and inhalation. The equations for these exposure routes are provided in this section.

7.1.1.2.1 Dermal Contact with Soil

The equilibrium body burden in a terrestrial animal species i from dermal contact with contaminant c in soil is calculated from the following equation (modified from Hope [1995]):

$$C_{ders}(i,c) = D_{ders}(i,c) / K_e(i,c) \quad (7.22)$$

where

$C_{ders}(i,c)$ = equilibrium body burden in species i from dermal contact with contaminant c in soil (µg/kg or pCi/kg body weight)

$D_{ders}(i,c)$ = absorbed daily dose for species i from dermal contact with contaminant c in soil (µg/kg/d or pCi/kg/d)

$K_e(i,c)$ = depuration rate of contaminant c for species i (d^{-1})

The annual-average absorbed daily dose for species i from dermal contact with contaminant c in soil is calculated using the following equation (modified from EPA [1991]):

$$D_{ders}(i,c) = EC_{soil}(c) \times SA(i) \times P_{cs}(i) \times S_a(i) \times CF \times \alpha_{dc}(i,c) \times \theta(i) \times \psi(i) / W(i) \quad (7.23)$$

where

$D_{ders}(i,c)$= absorbed daily dose for species i from dermal contact with contaminant c in soil (µg/kg/d or pCi/kg/d)

$EC_{soil}(c)$= concentration of contaminant c in surface soil (top ~1 cm) (µg/kg or pCi/kg dry)

$SA(i)$ = surface area of species i (cm^2)

$P_{cs}(i)$ = fraction of species i's surface area in contact with soil per day (d^{-1})

$S_a(i)$ = skin adherence factor for species i (mg/cm^2)

CF = unit conversion factor (10^{-6} kg/mg)

$\alpha_{dc}(i,c)$ = dermal absorption factor for contaminant c and species i (unitless)

$\theta(i)$ = area use factor for species i (ratio of contaminant area to home range - unitless)

$\psi(i)$ = seasonality factor for species i (fraction of year spent at the contaminated site – unitless)

$W(i)$ = body weight of species i (kg wet weight)

7.1.1.2.2 Dermal Contact with Water

The equilibrium body burden in species i from dermal contact with contaminant c in water is calculated from the following equation (Hope 1995):

$$C_{derw}(i,c) = D_{derw}(i,c) / K_e(i,c) \quad (7.24)$$

where

$C_{derw}(i,c)$ = equilibrium body burden in species i from dermal contact with contaminant c in water (µg/kg or pCi/kg body weight)

$D_{derw}(i,c)$ = absorbed daily dose for species i from dermal contact with contaminant c in water (µg/kg/d or pCi/kg/d)

$K_e(i,c)$ = depuration rate of contaminant c for species i (d^{-1})

Furthermore, the value for $D_{derw}(i,c)$ is calculated from the following equation (modified from EPA [1991c] to include use and seasonality factors):

$$D_{derw}(i,c) = EC_{water}(c) \times SA(i) \times P_{cw}(i) \times ET_w(i) \times CF \times \alpha_{dw}(i,c) \times \theta(i) \times \psi(i) / W(i) \quad (7.25)$$

where

$D_{derw}(i,c)$ = absorbed daily dose for species i from dermal contact with contaminant c in water (µg/kg/d or pCi/kg/d)
$EC_{water}(c)$ = concentration of contaminant c in water (µg/L or pCi/L)
$SA(i)$ = surface area of species i (cm^2)
$P_{cw}(i)$ = fraction of surface area of species i available for contact with water (unitless)
$ET_w(i)$ = average exposure time to water per day for species i (hr/d)
CF = volumetric conversion factor for water (1 L/1,000 cm^3)
$\alpha_{dw}(i,c)$ = dermal absorption factor of contaminant c in water for species i (cm/hr)
$\theta(i)$ = area use factor for species i (ratio of contaminant area to home range – unitless)
$\psi(i)$ = seasonality factor for species i (fraction of year spent at the contaminated site – unitless)
$W(i)$ = body weight of species i (kg wet weight)

7.1.1.2.3 Total Dermal Dose

The equilibrium body burden in species i from dermal exposure to contaminant c is calculated from the equation:

$$C_{der}(i,c) = C_{ders}(i,c) + C_{derw}(i,c) \quad (7.26)$$

where

$C_{der}(i,c)$ = equilibrium body burden in species i from dermal exposure to contaminant c (µg/kg or pCi/kg body weight)
$C_{ders}(i,c)$ = equilibrium body burden in species i from dermal contact with contaminant c in soil (µg/kg or pCi/kg body weight)
$C_{derw}(i,c)$ = equilibrium body burden in species i from dermal contact with contaminant c in water (µg/kg or pCi/kg body weight)

The total daily dose for species i from dermal absorption of contaminant c is calculated from the equation:

$$D_{der}(i,c) = D_{ders}(i,c) + D_{derw}(i,c) \quad (7.27)$$

where

$D_{der}(i,c)$ = total daily dose for species i of dermally-absorbed contaminant c (µg/kg/d or pCi/kg body weight/d)
$D_{ders}(i,c)$ = absorbed daily dose for species i s from dermal contact with contaminant c in soil (µg/kg/d or pCi/kg/d)
$D_{derw}(i,c)$ = absorbed daily dose for species i from dermal contact with contaminant c in water (µg/kg/d or pCi/kg/d)

7.1.1.2.4 Inhalation of Air and Vapor

The equilibrium body burden for species i from inhalation of contaminant c in air and vapor is calculated from the following equation (Hope 1995):

$$C_{iv}(i,c) = D_{iv}(i,c) \times \left(\frac{\alpha_{vap}(i,c)}{K_e(i,c)} \right) \quad (7.28)$$

where

$C_{iv}(i,c)$ = equilibrium body burden for species i from vapor inhalation of contaminant c (µg/kg or pCi/kg)
$D_{iv}(i,c)$ = applied daily dose to species i from vapor inhalation of contaminant c (µg/kg/d or pCi/kg/d)
$\alpha_{vap}(i,c)$ = inhalation absorption factor of contaminant c for species i (unitless)
$K_e(i,c)$ = depuration rate of contaminant c for species i (d^{-1})

The applied daily dose to species i from vapor inhalation of contaminant c is calculated from the following equation (modified from Hope [1995]):

$$D_{iv}(i,c) = \left[\frac{\left((EC_{vap}(i,c) + EC_{airc}(c)) \times IR(i) \right)}{W(i)} \right] \times \theta(i) \times \psi(i) \quad (7.29)$$

where

$D_{iv}(i,c)$ = applied daily dose to species i from vapor inhalation of contaminant c (µg/kg/d or pCi/kg/d)
$EC_{vap}(i,c)$ = concentration of contaminant c in the gas phase (µg/m^3 or pCi/m^3)
$EC_{airc}(c)$ = concentration of contaminant c in air (µg/m^3 or pCi/m^3)
$IR(i)$ = resting inhalation rate for species i (m^3/d)
$W(i)$ = body weight of species i (kg wet weight)
$\theta(i)$ = area use factor for species i (ratio of contaminant area to home range – unitless)
$\psi(i)$ = seasonality factor for species i (fraction of year spent at the contaminated site – unitless)

7.1.1.2.5 Inhalation of Particulates

The equilibrium contaminant body burden for species i from inhalation of particulates is calculated from the following equation (Hope 1995):

$$C_{ip}(i,c) = D_{ip}(i,c) \times \left(\frac{\alpha_{par}(i,c)}{K_e(i,c)} \right) \quad (7.30)$$

where

$C_{ip}(i,c)$ = equilibrium body burden for species i from particulate inhalation of contaminant c (µg/kg or pCi/kg)
$D_{ip}(i,c)$ = applied daily dose to species i from particulate inhalation of contaminant c (µg/kg/d or pCi/kg/d)
$\alpha_{par}(i,c)$ = inhalation particulate absorption factor of contaminant c in species i (unitless)
$K_e(i,c)$ = depuration rate of contaminant c for species i (d^{-1})

The applied daily dose to species i from particulate inhalation of contaminant c is calculated as (modified from Hope [1995]):

$$D_{ip}(i,c) = \left[\frac{\left(EC_{par}(i,c) \times IR(i)\right)}{W(i)} \right] \times \theta(i) \times \psi(i) \quad (7.31)$$

where

$D_{ip}(i,c)$ = applied daily dose to species i from particulate inhalation of contaminant c (µg/kg/d or pCi/kg/d)

$EC_{par}(i,c)$= air concentration of particulate-bound contaminant c for exposure to species i (µg/m^3 or pCi/m^3)

$IR(i)$ = resting inhalation rate of species i (m^3/d)

$W(i)$ = body weight of species i (kg wet weight)

$\theta(i)$ = area use factor for species i (ratio of contaminant area to home range – unitless)

$\psi(i)$ = seasonality factor for species i (fraction of year spent at the contaminated site – unitless)

7.1.1.2.6 Total Inhalation Dose

The total equilibrium burden for species i from inhalation of contaminant c is calculated as:

$$C_{inh}(i,c) = C_{iv}(i,c) + C_{ip}(i,c) \quad (7.32)$$

where

$C_{inh}(i,c)$ = equilibrium body burden for species i from inhalation of contaminant c (µg/kg or pCi/kg body weight)

$C_{iv}(i,c)$ = equilibrium body burden for species i from vapor inhalation of contaminant c (µg/kg or pCi/kg)

$C_{ip}(i,c)$ = equilibrium body burden for species i from particulate inhalation of contaminant c (µg/kg or pCi/kg)

The total inhalation applied dose to species i from inhalation of contaminant c is calculated as:

$$D_{inh}(i,c) = D_{iv}(i,c) + D_{ip}(i,c) \quad (7.33)$$

where

$D_{inh}(i,c)$ = total applied dose to species i from inhalation of contaminant c (µg/kg or pCi/kg body weight/d)

$D_{iv}(i,c)$ = applied daily dose to the species from vapor inhalation of contaminant c (µg/kg/d or pCi/kg/d)

$D_{ip}(i,c)$ = applied daily dose to species i from particulate inhalation of contaminant c (µg/kg/d or pCi/kg/d)

7.1.1.2.7 Ingestion of Water

The equilibrium contaminant body burden for species i from ingestion of contaminant c in water is calculated from the following expression:

$$C_{ingw}(i,c) = D_{ingw}(i,c) \times \left(\frac{\alpha_{ing}(i,c)}{K_e(i,c)} \right) \quad (7.34)$$

where

$C_{ingw}(i,c)$ = equilibrium body burden for species i from ingestion of contaminant c in water (µg/kg or pCi/kg)

$D_{ingw}(i,c)$ = applied daily dose to species i from ingestion of contaminant c in water (µg/kg/d or pCi/kg/d)

$\alpha_{ing}(i,c)$ = ingestion absorption factor of contaminant c for species i (unitless)

$K_e(i,c)$ = depuration rate of contaminant c for species i (d^{-1})

The applied daily dose to species i from ingestion of contaminant c in water is calculated from the equation (modified from EPA [1993a] to incorporate site use fractions):

$$D_{ingw}(i,c) = \left[\frac{\left(EC_{water}(c) \times WI(i)\right)}{W(i)}\right] \times \theta(i) \times \psi(i) \tag{7.35}$$

where

$D_{ingw}(i,c)$ = applied daily dose to species i from ingestion of contaminant c in water (µg/kg/d or pCi/kg/d)

$EC_{water}(c)$ = concentration of contaminant c in water (µg/L or pCi/L)

$WI(i)$ = water ingestion rate of species i (L/d)

$W(i)$ = body weight of species i (kg wet weight)

$\theta(i)$ = area use factor for species i (ratio of contaminant area to home range – unitless)

$\psi(i)$ = seasonality factor for species i (fraction of year spent at the contaminated site – unitless)

7.1.1.2.8 Ingestion of Soil

The contaminant body burden of species i from ingestion of contaminant c in soil is calculated from the equation (modified from Hope [1995]):

$$C_{ings}(i,c) = D_{ings}(i,c) \times \left(\frac{\alpha_{ing}(i,c)}{K_e(i,c)}\right) \tag{7.36}$$

where

$C_{ings}(i,c)$ = equilibrium body burden of species i from ingestion of contaminant c in soil (µg/kg or pCi/kg body weight)

$D_{ings}(i,c)$ = applied daily dose to species i from ingestion of contaminant c in soil (µg/kg/d or pCi/kg/d)

$\alpha_{ing}(i,c)$ = ingestion absorption factor for contaminant c and species i (unitless)

$K_e(i,c)$ = depuration rate of contaminant c for species i (d^{-1})

The applied daily dose to species i from ingestion of contaminant c in soil is calculated from the equation (modified from EPA [1993a] to incorporate site use fractions):

$$D_{ings}(i,c) = EC_{soil}(c) \times SI(i) \times NIR_{total}(i) \times F_{dw}(i) \times \theta(i) \times \psi(i) \tag{7.37}$$

where

$D_{ings}(i,c)$ = applied daily dose to species i from ingestion of contaminant c in soil (µg/kg/d or pCi/kg/d)
$EC_{soil}(c)$ = concentration of contaminant c in soil (µg/kg or pCi/kg)
$SI(i)$ = soil ingestion rate for species i (kg soil ingested/kg dry diet)
$NIR_{total}(i)$ = total normalized ingestion rate for species i (kg prey wet weight/kg predator body weight/d)
$F_{dw}(i)$ = conversion factor, dry diet to wet diet for species i (kg dry/kg wet)
$\theta(i)$ = area use factor for species i (ratio of contaminant area to home range – unitless)
$\psi(i)$ = seasonality factor for species i (fraction of year spent at the contaminated site – unitless)

The total normalized ingestion rate for species i is calculated from the equation (EPA 1993):

$$NIR_{total}(i) = \frac{FMR(i)}{W(i) \times \sum_{j \neq i} \left(P(i,j) \times ME(j)\right)} \quad (7.38)$$

where

$NIR_{total}(i)$= total normalized ingestion rate for species i (kg prey wet weight/kg predator body weight/d)
$FMR(i)$ = free-living metabolic rate of predator species i (kcal/d)
$W(i)$ = body weight of species i (kg wet weight)
$P(i,j)$ = wet weight or volume fraction of i's diet consisting of prey j (unitless)
$ME(j)$ = metabolizable energy from prey j (kcal/kg prey wet wt)

The metabolizable energy from prey j is calculated from (EPA 1993):

$$ME(j) = GE(j) \times AE(j) \quad (7.39)$$

where

$ME(j)$ = metabolizable energy from prey j (kcal/kg prey wet wt)
$GE(j)$ = gross energy from prey j (kcal/kg wet weight)
$AE(j)$ = assimilation efficiency of prey j (unitless)

7.1.1.2.9 Ingestion of Food

The equilibrium body burden for species i from ingestion of contaminant c in food is calculated (from Hope [1995]) as:

$$C_{ingf}(i,c) = D_{ingf}(i,c) \times \left(\frac{\alpha_{ing}(i,c)}{K_e(i,c)}\right) \quad (7.40)$$

where

$C_{ingf}(i,c)$ = equilibrium body burden for species i from ingestion of contaminant c in food (µg/kg or pCi/kg body wet weight)

$D_{ingf}(i,c)$ = applied daily dose to species i from ingestion of contaminant c in food (µg/kg/d or pCi/kg/d)
$\alpha_{ing}(i,c)$ = ingestion absorption factor for species i and contaminant c (unitless)
$K_e(i,c)$ = contaminant-specific depuration rate of contaminant c for species i (d^{-1})

The applied daily dose to species i from ingestion of contaminant c in food is calculated from the equation (modified from Hope [1995] using EPA [1993a]):

$$D_{ingf}(i,c) = \theta(i) \times \psi(i) \times \sum_{j} \left(C(j,c) \times NIR(i,j) \right) \tag{7.41}$$

where
$D_{ingf}(i,c)$ = applied daily dose to species i from ingestion of contaminant c in food (µg/kg/d or pCi/kg/d)
$\theta(i)$ = area use factor for species i (ratio of contaminant area to home range – unitless)
$\psi(i)$ = seasonality factor for species i (fraction of year spent at the contaminated site – unitless)
$C(j,c)$ = average concentration of contaminant c in jth food item (µg/kg or pCi/kg wet weight)
$NIR(i,j)$ = normalized ingestion rate of jth food type on a wet-weight basis (kg prey/kg body weight predator/d)

The normalized ingestion rate of jth food type on a wet-weight basis is calculated from (EPA 1993) as:

$$NIR(i,j) = P(i,j) \times NIR_{total}(i) \tag{7.42}$$

where
$NIR(i,j)$ = normalized ingestion rate of jth food type on a wet-weight basis (kg prey/kg body weight predator/d)
$P(i,j)$ = wet weight or volume fraction of i's diet consisting of prey j (unitless)
$NIR_{total}(i)$= total normalized ingestion rate for species i (kg prey wet weight/kg predator body weight/d)

7.1.1.2.10 Total Ingestion Dose

The applied daily dose for species i from ingestion of contaminant c is calculated from the equation:

$$D_{ing}(i,c) = D_{ingf}(i,c) + D_{ings}(i,c) + D_{ingw}(i,c) \tag{7.43}$$

where
$D_{ing}(i,c)$ = applied daily dose for species i from ingestion of contaminant c (µg/kg/d or pCi/kg/d)
$D_{ingf}(i,c)$ = applied daily dose to species i from ingestion of contaminant c in food (µg/kg/d or pCi/kg/d)
$D_{ings}(i,c)$ = applied daily dose to species i from ingestion of contaminant c in soil (µg/kg/d or pCi/kg/d)
$D_{ingw}(i,c)$ = applied daily dose to species i from ingestion of contaminant c in water (µg/kg/d or pCi/kg/d)

7.1.1.2.11 Total Terrestrial Animal Dose

The total applied daily dose for species i and contaminant c is calculated from the equation:

$$D(i,c) = D_{der}(i,c) + D_{inh}(i,c) + D_{ing}(i,c) \quad (7.44)$$

where

$D(i,c)$ = total applied daily dose for species i and contaminant c (µg/kg/d or pCi/kg/d)
$D_{der}(i,c)$ = total daily dose for species i of dermally-absorbed contaminant c (µg/kg/d or pCi/kg body weight/d)
$D_{inh}(i,c)$ = total applied daily dose to species i from inhalation of contaminant c (µg/kg/d or pCi/kg/d)
$D_{ing}(i,c)$ = total applied daily dose to species i from ingestion of contaminant c (µg/kg/d or pCi/kg/d)

7.1.1.2.12 Total Terrestrial Animal Burden

The equilibrium body burden of contaminant c for terrestrial animal species i is calculated from the equation:

$$C(i,c) = C_{ingf}(i,c) + C_{ings}(i,c) + C_{ingw}(i,c) + C_{inh}(i,c) + C_{der}(i,c) \quad (7.45)$$

where

$C(i,c)$ = equilibrium body burden for species i from ingestion of contaminant c (µg/kg wet wt or pCi/kg wet wt)
$C_{ingf}(i,c)$ = equilibrium body burden for species i from ingestion of contaminant c in food (µg/kg or pCi/kg body weight)
$C_{ings}(i,c)$ = equilibrium body burden to species i from ingestion of contaminant c in soil (µg/kg or pCi/kg body weight)
$C_{ingw}(i,c)$ = equilibrium body burden for species i from ingestion of contaminant c in water (µg/kg or pCi/kg)
$C_{inh}(i,c)$ = equilibrium body burden for species i from inhalation of contaminant c (µg/kg or pCi/kg body weight)
$C_{der}(i,c)$ = equilibrium body burden for species i from dermal exposure to contaminant c (µg/kg or pCi/kg body weight)

There are a few animal products that are modeled using a secondary calculation. The secondary animal product is calculated as a transfer factor times the primary species body burden. For example, to estimate a milk concentration, the body burden for a cow is multiplied by a transfer factor combining feed to meat and meat to milk transfer. The total concentration in the animal product is:

$$C_s(i,c) = C(i,c) \times T(i,c) \quad (7.46)$$

where

$C_s(i,c)$ = total equilibrium body burden of contaminant c for secondary species to species i (µg/kg wet wt or pCi/kg wet wt)
$C(i,c)$ = total equilibrium body burden of contaminant c in the primary species i (µg/kg or pCi/kg)

T(i,c) = secondary transfer factor for contaminant c and species i (µg or pCi/kg secondary /µg or pCi/kg primary)

The total animal body burden or concentration in the animal product is the concentration written to the food files for human consumption of terrestrial animals.

7.1.2 Water-Respiring/Transpiring Species

The basic models used in the risk assessment model to estimate exposures of aquatic organisms to metal or organic contaminants in sediments, pore water, surface water, and the subsequent transfer through the food chain consist of mass-balance equilibrium models originally derived by Thomann (1989) and Thomann et al. (1992, 1995). The basic equilibrium models presented in those papers were further modified by the authors to provide a system of equations generally applicable when only sediment data are available. The essential assumption used in that modification is that the aquatic system is not depurating contaminants, such that the three abiotic compartments (sediment, pore water, and surface water) are in static equilibrium (Thomann et al. 1992). This assumption may only be valid for large lacustrine systems; clearly, it is invalid for streams. However, the basic models may be used directly with only minor modification to address these more dynamic systems.

7.1.2.1 Body Burden for Aquatic Animals

The body burden of contaminant c in a predator species i, V(i,c), is calculated from direct exposure to contaminated water, ingestion of contaminated prey, and ingestion of contaminated sediment, using the following equation:

$$V(i,c) = \left[BCF(i,c) \times (b_{pore}(i) \times EC_{pore}(c) + [1 - b_{pore}(i)] \times EC_{surf}(c))\right] + \left[\frac{\sum_{j \neq i} \left(P(i,j) \times \alpha(i,c) \times I(i,j) \times V(j,c)\right)}{K(i,c) + G(i)}\right] + \left[EC_{sed}(c) \times SD(i) \times \alpha(i,c) \times \left(\frac{\sum_{j \neq i} \left(P(i,j) \times I(i,j)\right)}{K(i,c) + G(i)}\right)\right] \quad (7.47)$$

where

V(i,c) = body burden of contaminant c in predator species i (metals: µg/kg or pCi/kg dry weight [Thomann et al. 1995]; organics: µg/g lipid [Thomann et al. 1992])

BCF(i,c)= bioconcentration factor for species i and contaminant c (inorganics: L/kg dry weight; organics: L/g lipid)

$b_{pore}(i)$ = relative exposure of species i to pore water (unitless)

$EC_{pore}(c)$= concentration of contaminant c in pore water (µg/L or pCi/L)

$EC_{surf}(c)$= concentration of contaminant c in surface water (µg/L or pCi/L)

P(i,j) = wet weight or volume fraction of i's diet consisting of prey j (unitless)

α(i,c) = chemical assimilation efficiency for contaminant c consumed along with prey by species i (g contaminant assimilated/g contaminant ingested)

I(i,j) = feeding rate of species i on prey item j (organic model: g prey lipid/g predator lipid/d, metal model: g prey dry weight/g predator dry weight/d)

V(j,c) = body burden of contaminant c in prey species j (metals: µg/kg or pCi/kg dry weight [Thomann et al. 1995]; organics: µg/g lipid [Thomann et al. 1992]) or in sediment

(metals: µg/kg dry sediment [Thomann et al. 1995]; organics: µg/g organic carbon [Thomann et al. 1992])

$EC_{sed}(c)$= concentration of contaminant c in sediment (µg/kg or pCi/kg)

SD(i) = feeding rate of species i on sediment as a fraction of total diet intake (kg sediment dry weight/kg prey dry weight/d)

K(i,c) = species i loss rate of contaminant c, including depuration and metabolism (d^{-1})

G(i) = growth rate of species i (d^{-1})

The species i loss rate of organic contaminant c, including depuration and metabolism, is calculated from the equation (Thomann 1989):

$$K(i,c) = \left[k_u(i,c) \Big/ \left(\frac{10^{K_{ow}(c)}}{1000} \right) \right] + K_m(i,c) \tag{7.48}$$

where

K(i,c) = species i loss rate of contaminant c, including depuration and metabolism (d^{-1})

$k_u(i,c)$ = uptake from dissolved sources of contaminant c for species i (metals: L/g dry weight/d [Thomann et al. 1995]; organics: L/g lipid/d [Thomann et al. 1992])

$K_{ow}(c)$ = log base 10 of the octanol-water partition coefficient for contaminant c (unitless)

$K_m(i,c)$ = chemical loss rate in species i due to metabolism and fecal loss (d^{-1})

1000 = Unit conversion factor (g/L)

The contaminant uptake from dissolved sources for species i for organic contaminants is calculated from the equation (Thomann 1989):

$$k_u(i,c) = \frac{2.67 \times f_{oc}(i) \times \rho(i) \times E(i,c)}{awd(i) \times C_0 \times f_L(i)} \tag{7.49}$$

where

$k_u(i,c)$ = uptake of dissolved sources of contaminant c for species i (L/g lipid/d)

$f_{oc}(i)$ = fraction organic carbon in species i (g organic carbon/g dry weight)

$\rho(i)$ = oxygen respiration rate for species i (g O_2/g lipid/d)

E(i,c) = chemical transfer efficiency for contaminant c in species i (g/g per g O_2/g lipid)

awd(i) = wet-to-dry weight ratio for species i (g wet/g dry)

C_0 = oxygen concentration in the river (g O_2/L)

$f_L(i)$ = fraction lipid in species i (g lipid/g wet)

2.67 = grams of oxygen per gram of carbon (g O_2/g organic carbon)

The chemical transfer efficiency E(i,c) is calculated from $K_{ow}(c)$ log base 10 of the octanol-water partition coefficient for contaminant c (unitless) using linear interpolation from a lookup table obtained from (Thomann 1989). This lookup table is provided in Table 7.1. Values of $K_{ow}(c)$ outside the range defined in the table are mapped to the closest table value.

Table 7.1 Relationship between the chemical transfer efficiency and the octanol-water partition coefficient.

$Log_{10}\ K_{ow}(c)$	E(i,c)
2.0	0.025119
2.5	0.044668
3.0	0.079433
3.5	0.141254
4.0	0.251189
4.5	0.8
5.0	0.8
5.5	0.8
6.0	0.8
6.5	0.8
7.0	0.6
7.5	0.4
8.0	0.4
8.5	0.05
9.0	0.01

This equation (Equation 7.49) is not used in the model for metal uptake; instead, the BCF relationship is used and BCFs are obtained from the literature.

The growth rate of species i is given by the regression equation (Thomann 1989):

$$G(i) = \delta \times wm(i)^{-\beta} \tag{7.50}$$

where δ and β are regression parameters and wm(i) is the wet body mass of species i (g wet weight).

The feeding rate of species i on biotic prey item j for organic contaminants is calculated from the following equation (Thomann et al. 1992):

$$I(i,j) = \left(\frac{G(i)+\rho(i)}{a(i)}\right) \times \left(\frac{awd(j)}{awd(i)}\right) \times \left(\frac{f_L(j)}{f_L(i)}\right) \times \left(\frac{f_{oc}(i)}{f_{oc}(j)}\right) \tag{7.51}$$

where

- I(i,j) = feeding rate of species i on prey item j (organic model: g prey lipid/g predator lipid/d)
- G(i) = growth rate of species i (d^{-1})
- $\rho(i)$ = oxygen respiration rate for species i (d^{-1})
- a(i) = organic carbon assimilation rate for species i (g organic carbon assimilated/g organic carbon ingested)
- awd(j)= wet-to-dry weight ratio for prey species j (g wet/g dry)
- awd(i)= wet-to-dry weight ratio for predator species i (g wet/g dry)
- $f_L(j)$ = fraction lipid in prey species j (g lipid/g wet)
- $f_L(i)$ = fraction lipid in predator species i (g lipid/g wet)
- $f_{oc}(j)$ = fraction organic carbon in prey species j (g organic carbon/g dry weight)

$f_{oc}(i)$ = fraction organic carbon in predator species i (g organic carbon/g dry weight)

The oxygen respiration rate for species i is calculated from the equation:

$$\rho(i) = \phi \times wm(i)^{-\gamma} \tag{7.52}$$

where ϕ and γ are regression parameters (Thomann 1989) and wm(i) is the wet body mass of species i (g wet weight).

The bioconcentration factor for species i and organic contaminant c is calculated from the equation:

$$BCF(i,c) = \frac{k_u(i,c)}{K(i,c) + G(i)} \tag{7.53}$$

where

BCF(i,c) = bioconcentration factor for species i and organic contaminant c (L/g lipid)
$k_u(i,c)$ = uptake of dissolved sources of contaminant c for species i (L/g lipid/d)
K(i) = loss rate of contaminant for species i, including depuration and metabolism (d^{-1})
G(i) = growth rate of species i (d^{-1})

The equation for I(i,j) for organic contaminants returns values with units of (g prey lipid/g predator lipid/d). The equivalent units for the metal uptake model of Thomann et al. (1995) are (g prey dry weight/ g predator dry weight/d). For the purposes of evaluating metal uptake in aquatic systems, the following conversion was applied to produce consumption rates in the correct units for the feeding rate of species i on biotic prey item j for metallic contaminants:

$$I_{metal}(i,j) = I(i,j) \times \left(\frac{awd(i)}{awd(j)}\right) \times \left(\frac{f_L(i)}{f_L(j)}\right) = \left(\frac{G(i) + \rho(i)}{a(i)}\right) \times \left(\frac{f_{oc}(i)}{f_{oc}(j)}\right) \tag{7.54}$$

where

$I_{metal}(i,j)$ = feeding rate of species i on prey item j (inorganics model: g prey dry weight/ g predator dry weight/d)
I(i,j) = feeding rate of species i on prey item j (organic model: g prey lipid/g predator lipid/d)
awd(i) = wet-to-dry weight ratio for predator species i (g wet/g dry)
awd(j) = wet-to-dry weight ratio for prey species j (g wet/g dry)
$f_L(i)$ = fraction lipid in predator species i (g lipid/g wet)
$f_L(j)$ = fraction lipid in prey species j (g lipid/g wet)
G(i) = growth rate of species i (d^{-1})
$\rho(i)$ = oxygen respiration rate for species i (d^{-1})
a(i) = organic carbon assimilation rate for species i (g organic carbon assimilated/g organic carbon ingested)
$f_{oc}(i)$ = fraction organic carbon in predator species i (g organic carbon/g dry weight)
$f_{oc}(j)$ = fraction organic carbon in prey species j (g organic carbon/g dry weight)

7.1.2.2 Body Burden for Aquatic Plants

The body burden for aquatic plant species i, V(i,c), is calculated from the following equation for all analytes except tritium:

$$V(i,c) = BCF(i,c) \times (b_{pore}(i) \times EC_{pore}(c) + [1 - b_{pore}(i)] \times EC_{surface}(c)) \quad (7.55)$$

where

- V(i,c) = body burden in aquatic plant species i of contaminant c (inorganics: µg/kg or pCi/kg dry weight [Thomann et al. 1995]; organics: µg/g lipid [Thomann et al. 1992])
- BCF(i,c) = bioconcentration factor for species i and contaminant c (inorganics: L/kg dry weight; organics: L/g lipid)
- $b_{pore(}(i)$ = relative exposure of species i to pore water (unitless)
- $EC_{pore}(c)$ = concentration of contaminant c in pore water (µg/L or pCi/L)
- $EC_{surface}(c)$ = concentration of contaminant c in surface water (µg/L or pCi/L)

The body burden for aquatic plant species i, V(i,c), for tritium is calculated from the following equation:

$$V(i,c) = (1 - 1/awd(i)) \times (b_{pore}(i) \times EC_{pore}(c) + [1 - b_{pore}(i)] \times EC_{surface}(c)) \quad (7.56)$$

where

- V(i,c) = body burden in aquatic plant species i of contaminant c (inorganics: µg/kg or pCi/kg dry weight [Thomann et al. 1995]; organics: µg/g lipid [Thomann et al. 1992])
- awd(i) = wet-to-dry weight ratio for species i (g wet/g dry)
- $b_{pore(}(i)$ = relative exposure of species i to pore water (unitless)
- $EC_{pore}(c)$ = concentration of contaminant c in pore water (µg/L or pCi/L)
- $EC_{surface}(c)$ = concentration of contaminant c in surface water (µg/L or pCi/L)

7.1.2.3 Body Burden as Consumed

The equilibrium body burden is calculated for all aquatic species for consumption by terrestrial species and by humans. These concentrations are written to the FOOD files for input into the HUMAN code.

The equilibrium body burden for species i from ingestion of inorganics is calculated from the equation:

$$C(i,c) = V(i,c)/awd(i) \quad (7.57)$$

where

- C(i,c) = body burden for species i from ingestion of contaminant c (µg/kg or pCi/kg wet)
- V(i,c) = body burden in predator species i of contaminant c (µg/kg or pCi/kg dry weight)
- awd(i) = wet-to-dry weight ratio for species i (g wet/g dry)

For the inorganic contaminant tritium in aquatic plants, the equation is:

$$C(i,c) = V(i,c) \times (1.0 - 1.0/awd(i)) \quad (7.58)$$

The equilibrium body burden for species i from ingestion of organics is calculated from the equation:

$$C(i,c) = V(i,c) \times 1000 \times f_L(i) \quad (7.59)$$

where

C(i,c) = equilibrium body burden for species i from ingestion of contaminant c (µg/kg or pCi/kg wet)
V(i,c) = body burden of contaminant c in species i (µg/g lipid)
$f_L(i)$ = fraction lipid in species i (g lipid/g wet)
1000 = unit conversion factor (g wet/kg wet)

7.1.2.4 Ecological Hazard Quotient

The ecological hazard quotient calculation allows comparison of a body burden to a benchmark body burden threshold. This value is calculated differently for organic and inorganic nonradioactive analytes

The ratio of tissue value to benchmark value for both plant and animal aquatic species for organic, nonradioactive, contaminants is calculated from the following equation:

$$EHQ(i,c) = V(i,c) \times 1000 \times f_L(i) / BB(i,c) \quad (7.60)$$

where

EHQ(i,c) = ratio of body burden to benchmark value for species i and contaminant c (no units)
V(i,c) = the body burden of contaminant c in species i (µg/g lipid)
$f_L(i)$ = the fraction lipid in species i (g lipid/g wet)
BB(i,c) = the benchmark body burden value for species i and contaminant c (µg/kg lipid)
1000 = unit conversion factor (g/kg)

The tissue benchmark value for both plant and animal aquatic species for inorganic, nonradioactive, contaminants is calculated from the following equation:

$$EHQ(i,c) = \frac{V(i,c)}{BB(i,c) \times awd(i)} \quad (7.61)$$

where

EHQ(i,c) = the ratio of body burden value to benchmark value for species i and contaminant c (unitless)
V(i,c) = total body burden of contaminant c (in species i µg/kg wet or pCi/kg wet)
BB(i,c) = benchmark body burden value for species i and contaminant c (µg/kg dry)
awd(i) = wet-to-dry weight ratio for species i (g wet/g dry)

7.1.3 Radiological Dose Estimation

The exposure equations return estimates of ingestion exposure to radiological contaminants in units of pCi/kg body mass/day (i.e., in units of radioactive decay rate density). However, radiological effects result from radioactive energy density absorbed by a body in a unit of time, which is usually expressed in units of rad/day. Consequently, decay rates must be converted to energy equivalents. Similarly, an organism can receive external energy from radioactive decay occurring in the abiotic media (air, water, or soil).

7.1.3.1 Internal Dose

The internal total-body dose rate to an organism is the sum of the individual dose rates from each radionuclide in the body. The equation is written as follows:

$$R_{int}(i) = \sum_{c} \left(C(i,c) \times E(i,c) \right) \tag{7.62}$$

where

$R_{int}(i)$ = radiological dose to species i from internal radioactive decay (rad/d)
$C(i,c)$ = body burden of radionuclide c in species i (pCi/kg)
$E(i,c)$ = effective absorbed energy rate for radionuclide c per unit activity in species i (kg-rad/ pCi/d)

Doses are summed across all radionuclides. As shown in Baker and Soldat (1992), the effective absorbed energy rate for nuclide c per unit activity in organism i can be calculated from the following equation:

$$E(i,c) = 1\ Ci/10^{12}\ pCi \times 3.7\times10^{10}\ disintegrations/s/Ci \times 86{,}400\ s/d \times 1.602\times10^{-11}\ kg\text{-}rad/MeV \times \varepsilon_{i,c}$$

$$E(i,c) = 5.12\times10^{-8} \times \varepsilon(i,c) \tag{7.63}$$

where

$E(i,c)$ = effective absorbed energy rate for radionuclide c per unit activity in species i (kg-rad/pCi/d)
$\varepsilon(i,c)$ = is the effective absorbed energy (MeV/disintegration)

7.1.3.2 External Dose

7.1.3.3 External Dose from Water Immersion for Aquatic Organisms

The external radiological dose to aquatic species i from exposure to radioactive decay in water is calculated using the equation:

$$R_{imm}(i) = \sum_{c} \left[\left(b_{pore}(i) \times EC_{pore}(c) + (1 - b_{pore}(i)) \times EC_{surface}(c) \right) \times DF_{imm}(c) \times CF_{imm} \right] \tag{7.64}$$

where the sum extends over all radiological contaminants (with index c):

$R_{imm}(i)$ = external radiological dose to species i from exposure to radioactive decay in water (rad/d)
$b_{pore}(i)$ = relative exposure to pore water for species i (unitless)
$EC_{pore}(c)$ = concentration of radionuclide c in pore water (pCi/L)
$EC_{surface}(c)$ = concentration of radionuclide c in surface water (pCi/L)
$DF_{imm}(c)$ = water immersion dose factor for radionuclide c (mrad/yr per pCi/m^3)
CF_{imm} = 2.737851×10^{-9} (conversion factor: from (mrad-m^3)/(L-yr) to rad/d)

7.1.3.4 External Dose from Water Immersion for Terrestrial Organisms

The external radiological dose to terrestrial organism i from exposure to radioactive decay in water is calculated using the equation:

$$R_{imm}(i) = F_{water}(i) \times ET_{water}(i) \times CF_{imm} \times \sum_{c} \left[EC_{water}(c) \times DF_{imm}(c) \right] \quad (7.65)$$

where the sum extends over all radiological contaminants (with index c):

$R_{imm}(i)$ = external radiological dose to species i from exposure to radioactive decay in water (rad/d)
$EC_{water}(c)$= concentration of radionuclide c in water (pCi/L)
$DF_{imm}(c)$ = water immersion dose factor for radionuclide c (mrad/yr per µCi/m^3)
$F_{water}(i)$ = fraction of species i exposed to water (unitless)
$ET_{water}(i)$ = average exposure time to water per day for species i (hr/d)
CF_{imm} = unit conversion factor: 1.140771×10^{-10} = (0.001 rad/mrad x 10^{-6} µCi/pCi x 1000 L/m^3) / (24 hr/d x 365.25 d/yr)

7.1.3.5 External Dose from Contact with Sediment for Aquatic Organisms

External dose received from contact with sediment is calculated for aquatic species as the combination of external dose received above the sediment and below the sediment. The equations (EPA 1993) are:

$$RAbove_{sed}(i) = F_{above}(i) \times CF_{sedelev}(i) \times DSF \times SWD \times CF_{above} \times \sum_{c} \left[EC_{sed}(c) \times DF_{sed}(c) \right]$$

$$RBelow_{sed}(i) = (1 - F_{above}(i)) \times MCF \times CF_{below} \times \sum_{c} \left[EC_{sed}(c) \times \gamma(c) \right] \quad (7.66)$$

$$R_{sed}(i) = RAbove_{sed}(i) + RBelow_{sed}(i)$$

where the sum extends over all radiological contaminants (with index c):

$RAbove_{sed}(i)$ = external radiological dose to species i from exposure above the sediment (rad/d)
$RBelow_{sed}(i)$ = external radiological dose to species i from exposure below the sediment (rad/d)
$R_{sed}(i)$ = external radiological dose to species i from exposure to radioactive decay in sediment (rad/d)
$F_{above}(i)$ = fractional time for exposure of species i above the sediment (unitless)
$CF_{sedelev}(i)$ = $0.8 \times b_{pore}(i) + 0.2$, where $b_{pore}(i)$ is the relative exposure to pore water (unitless)
DSF = directional source factor for 1-sided exposure (0.5)
SWD = sediment conversion factor for wet weight to dry weight (0.75)
CF_{above} = unit conversion factor applicable above the sediment: 5.12×10^{8} (1.6×10^{3} kg/m3 x 86,400 s/d x 3.7×10^{-2} Bq/pCi x 100 rem/Sv x 1 rad/rem)
$EC_{sed}(c)$ = concentration of radionuclide c in sediment (pCi/kg)
$DF_{sed}(c)$ = sediment dose factor for 15 cm depth for radionuclide c (Sv/s per Bq/m^3)
MCF = medium correction factor for sediment exposure (1.05)
CF_{below} = unit conversion factor applicable below the sediment: 5.12×10^{-8} (1×10^{-12} Ci/pCi x 3.7×10^{10} disintegration/s/Ci x 86,400 s/d x 1.602×10^{-11} kg-rad/MeV)
$\gamma(c)$ = gamma energy for radionuclide c (MeV/disintegration)

7.1.3.6 External Dose from Contact with Soil for Terrestrial Organisms

The external dose received from contact with sediment is calculated for terrestrial species as the combination of external dose received above the sediment and below the sediment. The equations (EPA 1993) are:

$$\begin{aligned} \mathrm{RAbove}_{soil}(i) = {} & F_{above}(i) \times CF_{soilelev}(i) \times DRF_{rough} \times CF_{above} \times \sum_{c} \left[EC_{soil}(c) \times DF_{sed}(c) \right] \\ \mathrm{RBelow}_{soil}(i) = {} & (1 - F_{above}(i)) \times MCF \times CF_{below} \times \sum_{c} \left[EC_{soil}(c) \times \gamma(c) \right] \\ R_{soil}(i) = {} & \mathrm{RAbove}_{soil}(i) + \mathrm{RBelow}_{soil}(i) \end{aligned} \quad (7.67)$$

where the sum extends over all radiological contaminants (with index c):

$\mathrm{RAbove}_{soil}(i)$ = external radiological dose to species i from exposure above the soil (rad/d)
$\mathrm{RBelow}_{soil}(i)$ = external radiological dose to species i from exposure to below the soil (rad/d)
$R_{soil}(i)$ = external radiological dose to species i from exposure to radioactive decay in soil (rad/d)
$F_{above}(i)$ = fractional time for exposure of species i above the sediment (unitless)
$CF_{soilelev}(i)$= 2 if $Diffht_i < 1$ or 1 if $Diffht_i >= 1$
DRF_{rough} = dose rate reduction fraction accounting for ground roughness (0.7)
CF_{above} = unit conversion factor applicable above the sediment: 5.12×10^{8} (1.6×10^{3} kg/m3 x 86,400 s/d x 3.7×10^{-2} Bq/pCi x 100 rem/Sv x 1 rad/rem)
$EC_{soil}(c)$ = concentration of radionuclide c in soil (pCi/kg)
$DF_{sed}(c)$ = sediment dose factor for 15 cm depth for nuclide c (Sv/s per Bq/m^3)
MCF = medium correction factor for sediment exposure (1.05)
CF_{below} = unit conversion factor applicable below the sediment: 5.12×10^{-8} (1×10^{-12} Ci/pCi x 3.7×10^{10} disintegration/s/Ci x 86,400 s/d x 1.602×10^{-11} kg-rad/MeV)
$\gamma(c)$ = gamma energy for nuclide c (MeV/disintegration)

7.1.3.7 Total Radiological Dose

Finally, total radiological dose is obtained by summing the above quantities:

$$R_{total}(i) = R_{imm}(i) + \mathrm{Rext}_{ext}(i) + R_{int}(i) \quad (7.68)$$

where:

$R_{imm}(i)$ = external radiological dose to species i from exposure to radioactive decay in water (rad/d)
$R_{sed}(i)$ = external radiological dose to species i from exposure to radioactive decay in sediment (rad/d)
$R_{int}(i)$ = radiological dose to species i from internal radioactive decay (rad/d)

7.2 Code Execution Environment

7.2.1 Location in the Processing Sequence

The Ecological Contaminant Exposure Model (ECEM) code requires access to a number of data files developed by other codes. In particular, the ECDA files shown on Figure 1.1 must have been created

under the control of the same ESD keyword file that the ECEM code reads to determine processing options.

7.2.2 How the Code Is Invoked

ECEM can run under either the Windows or the Linux operating system. Under the Windows operating system (Releases XP or 7), ECEM executes in a DOS box. A run of ECEM is initiated by entering the following command line:

```
ECEM "Keyfilename"
```

Under the Linux operating system, ECEM is executed through any of the following Bourne Shell or C Shell commands:

```
ecem-1.exe "Keyfilename"
```

For these commands, ECEM or "ecem.exe" is the name of the executable program, and "Keyfilename" is the name of an ecological scenario keyword file. Both the name of the executable program and the keyword file may contain path information. If ECEM is invoked without entering the name of the keyword file, the code will prompt the user for the file name. The keyword file, which should be prepared using an editor that can handle ASCII files without leaving embedded control codes, contains text control information describing the run. If ECEM cannot open the keyword file, then the code will terminate execution after writing an error message to the standard output device.

If the string "-help" is entered instead of the keyword file name a few help lines are written to the standard output. The help lines identify the correct command line options for the code. Code execution terminates after the help message has been displayed when the "-help" option is used.

7.2.3 Memory Requirements

The ECEM code uses dynamic memory allocation, so the memory requirements depend on the problem being analyzed. A reasonably large example run where the ECEM code required 2.54 MB of memory (on a Windows 2000 machine) used 10 analytes, 60 time steps, 11 realizations, and 168 locations. It is expected that most, if not all, of the runs of the ECEM code will require less than 4 MB of memory. This run took about 10 minutes to execute on a 933-megahertz system.

7.3 Data Files

The ECEM code reads four or more input files and writes up to five output files. The number of input files depends on the number of contaminants being analyzed. The number of output files depends on the options selected in the ECEM code. These files are described in the following sections.

7.3.1 Input Files

The input files for the ECEM code are keyword files and a suite of concentration data related files. One keyword file controls the case the ECEM code will execute, and it points to the ESD keyword file. The suite of concentration data files are all identified in the ESD keyword file – the user of the ECEM only needs to identify the ESD keyword file. The following are the input files:

- **ESD Keyword File**: The ESD keyword file contains the control information that the inventory and environmental transport codes use to generate concentration data files. Examples of keywords in the ESD file that control the impact codes, including the ECEM code, are provided in Section 2.1.
- **ECDA Concentration Files**: The ECDA files contain all the concentration data available for the impact codes. The concentrations for all analytes are based on the same time and location data. There is a "index" file for the ECEM code containing indexing information for each of the concentration data files. The format of this file is described in Section 2.2.2. In addition, there is a separate concentration data file for every analyte used in the impacts scenario. For example, when running a scenario with seven analytes, there will be one map file and seven concentration data files. The format of an ECDA data file is described in Section 2.2.1.
- **ECEM Keyword File**: The ECEM Keyword file controls the scenario to be analyzed by the ECEM code. The options and data available are constrained by the case defined in the ESD Keyword file. Section 7.3.1.3 describes the contents of the ECEM keyword file.

7.3.1.1 ESD Keyword File

The ECEM code reads keywords from the environmental settings file. These keywords are read from a different file and can have a different definition from a keyword defined for internal use in the ECEM code. The environmental settings keywords are defined in Section 2.1. The following keywords are required:

- ANALYTE – definition of analytes in the environmental simulations
- END – end of the environmental settings keywords
- FILE – file names for the concentration file for each analyte
- IRRIGATE – definition of the first and last days of the growing season and the year irrigation starts
- LOCATION – locations at which concentrations were generated for the ecological impacts
- PERIOD – Time definitions for the entire simulation case
- RADIUS – effective energy by organism radius
- REALIZAT – number of realizations for which concentration data were generated for ecological impact calculations
- SPECIES – definition of species for the ecological impacts calculations
- TIMES – times at which concentrations were generated for the ecological impacts
- TITLE – environmental simulation title

7.3.1.2 ECDA Concentration Files

The ECDA provides a central storage location for concentration data for all analytes at the environmental locations and times needed to perform social-cultural analyses. The ECDA files are described in Section 2.2.

7.3.1.3 ECEM Keyword File

The ECEM keyword definition file contains control information for the desired impact simulation. Individual keywords are defined in Section 7.4. Table 7.2 contains excerpted keywords for a run of ECEM using 7 realizations, 15 locations, 10 analytes and 57 ecological species. The complete file is 4400 lines long.

Table 7.2 Excerpted Records from an ECEM Keyword File

```
REPORT "/home/ANALYSIS5/CA_Ref_A/foods/Ecem_CA_Ref_A_foods.rpt"
TITLE  "Reference Case A - Hanford plus Background Food Run"
USER   "Paul W. Eslinger"
EXECUTE
! Random Seed for Stochastics
SEED 4453190
! Number of Realizations
REALIZATION 1
!  File Definitions (use full path in name)
FILE HEADER     "/home/ANALYSIS5/CA_Ref_A/foods/Ecem_CA_Ref_A_foods.hdr"
FILE VALUES     "/home/ANALYSIS5/CA_Ref_A/foods/Ecem_CA_Ref_A_val_foods.csv"
FILE DETAILS    "/home/ANALYSIS5/CA_Ref_A/foods/Ecem_CA_Ref_A_det_foods.csv"
! Environmental Settings Definition keyword file
FILE ESD "/home/ANALYSIS5/CA_Ref_A/ESD_CA_Ref_A.key"
FOODS MAP= "Ecem_CA_Ref_A_map_foods.dat"
      PATH="/home/ANALYSIS5/CA_Ref_A/foods/"
      HEADER="Ecem_CA_Ref_A_FCDA_foods.hdr"
TIMES
  1945  1950  1955  1960  1965  1970  1975  1980  1985  1990
!  Analyte Definitions
ANALYTE ID="H3" ELEMENT="H" PARTICLE= 0 OUTPUT
ANALYTE ID="C14" ELEMENT="C" PARTICLE= 0 OUTPUT
ANALYTE ID="Sr90" ELEMENT="Sr" PARTICLE= 0 OUTPUT
ANALYTE ID="U233" ELEMENT="U" PARTICLE= 0 OUTPUT
ANALYTE ID="U235" ELEMENT="U" PARTICLE= 0 OUTPUT
GROWTH DELTA 0.002 ! Reference = Thomann et al. 1992
GROWTH BETA 0.25   ! Reference = Thomann et al. 1992
RESPIRE PHI 0.032  ! Reference = Thomann 1989
RESPIRE GAMMA 0.2  ! Reference = Thomann 1989
!  Other varialbes for terrestrial plants
VARIABLE COWHDFX 0.0497 ! Units="unitless"  Default value (EPA,1991) RAGS,
Part B.
VARIABLE LENGTH  45     ! Units="m"  Default value (EPA,1991) RAGS, Part B.
! Upland Locations
LOCATION PRIMARY="UH0002" OUTPUT
! Riparian (Hanford) and Aquatic (Hanford) Locations
LOCATION PRIMARY="RHP001" SECOND="QHP001" OUTPUT
!-------------------------| Species Definitions |-------------------------!
SPECIES ID="QCARPS" OUTPUT ! carp
SPECIES ID="UMDLRK" !OUTPUT ! Western meadowlark
!-----------------------------------------------------------------------!
!  Consume Keywords
CONSUME ID="QCARPS" PREY
  "QCPBSN"  0.15000
  "QMAYFL"  0.25000
  "QPERIP"  0.50000
  "QMLFOL"  0.10000
```

```
  SEDING    0.16000
CONSUME ID="UHVMSE" PREY
  "UEWORM"  0.05000
  "UFUNGI"  0.02500
  "UGRAIN"  0.20000
  "UGRASS"  0.22500
  "ULFVEG"  0.02500
  "UMLBRY"  0.05000
  "URTVEG"  0.02500
  "UTHSLE"  0.02500
  "USHRUB"  0.20000
  "UARTPD"  0.15000
  "UTRFRT"  0.02500
  SOILING   0.02000
!   Values used for KOW
STOCHASTIC "C     KOW" 1 0
!   Values  used for Aquatic Animal ALPHAIJ
STOCHASTIC "Sr90  QCARPSALPHAIJ" 1 0.25
!   Values used for Aquatic Animal BCF
STOCHASTIC "Se79  QMAYFLBCF" 1 114
!   VAlues used for Aquatic Animal Bpore
STOCHASTIC "QCARPSBPORE" 1 0.05
STOCHASTIC "QCATFSBPORE" 1 0.1
!   Values used for Aquatic Animal Fabove
STOCHASTIC "QCARPSFABOVE" 1 1
STOCHASTIC "QCATFSFABOVE" 1 1
STOCHASTIC "QCLAMSFABOVE" 1 0.5
STOCHASTIC "QCPBSNFABOVE" 1 0.7
STOCHASTIC "QCRYFSFABOVE" 1 0.7
STOCHASTIC "QDPMAGFABOVE" 1 1
STOCHASTIC "QHYALEFABOVE" 1 0.5
STOCHASTIC "QLMSUCFABOVE" 1 1
STOCHASTIC "QMAYFLFABOVE" 1 0.5
STOCHASTIC "QMWTFSFABOVE" 1 1
STOCHASTIC "QMUSELFABOVE" 1 0.5
STOCHASTIC "QLMPJVFABOVE" 1 0.1
STOCHASTIC "QRBTADFABOVE" 1 1
STOCHASTIC "QRBTEGFABOVE" 1 0
STOCHASTIC "QRBTJVFABOVE" 1 1
STOCHASTIC "QSAMADFABOVE" 1 1
STOCHASTIC "QSAMEGFABOVE" 1 0
STOCHASTIC "QSAMJVFABOVE" 1 1
STOCHASTIC "QSBASSFABOVE" 1 1
STOCHASTIC "QWTDTPFABOVE" 1 0.7
STOCHASTIC "QSTURGFABOVE" 1 0.9

!   Values used for Aquatic Animal Deprate
STOCHASTIC "H3    QLMPJVDEPRATE" 1 0.15
!   Values used for Aquatic Plant Bpore
STOCHASTIC "QPERIPBPORE" 1 1
STOCHASTIC "QPHYPKBPORE" 1 0
STOCHASTIC "QMLFOLBPORE" 1 0.5
!   Values used for Aquatic Plant Fabove
STOCHASTIC "Cl36  QMLFOLBCF" 1 300
!   Values used for Terrestrial Animal Alphads
STOCHASTIC "Se79  UCHKADALPHADS" 1 0
!   Values used for Terrestrial Animal Alphadw
```

```
STOCHASTIC "U233  RWTDADALPHADW" 1 0
!   Values used for Terrestrial Animal Alphaing
STOCHASTIC "Pa231 RROBINALPHAING" 1 5.000000E-02
!   Values used for Terrestrial Animal Alphapar
STOCHASTIC "Np237 RKSTRLALPHAPAR" 1 0.00048
!   Values used for Terrestrial Animal Alphavap
STOCHASTIC "Np237 UMDLRKALPHAVAP" 1 0.00048
!   Values used for Terrestrial Animal Deprate
STOCHASTIC "Cs137 RACOOTDEPRATE" 1 0.04
!   Values used for Terrestrial Animal Fabove
STOCHASTIC "RVOLESFABOVE" 1 0.8
!   Values used for Terrestrial Animal Transfer
STOCHASTIC "H     UCHKEGTRANSFER" 1 1.071
!   Values used for Terrestrial Plant Bcfveg
STOCHASTIC "Cs    RLFVEGBCFVEG" 1 4.100000E-02
!   Values used for Terrestrial Plant Biomass
STOCHASTIC "UFUNGIBIOMASS" 1 0.1697 ! Data from NUREG/CR-5512 (Table 6.54,
rye)
!   Values used for Terrestrial Plant Leaf Interception - Dry
STOCHASTIC "Cl36  RRUSHSIFRACDRY" 1 8.477322E-02
!   Values used for Terrestrial Plant Leaf Interception - Wet
STOCHASTIC "Ra226 RWILOWIFRACWET" 1 0.35
!   Values used for Terrestrial Plant Leaf Transfer - Dry
STOCHASTIC "Ra226 UMLBRYKLIDRY" 1 0.1
!   Values used for Terrestrial Plant Leaf Transfer - Wet
STOCHASTIC "C14   URTVEGKLIWET" 1 0.1
!   Values used for Terrestrial Plant Parms
STOCHASTIC "RRTULEKPA2" 1 0.0034
!   Values used for Terrestrial Plant Leaf Weathering - Dry
STOCHASTIC "Tc99  URTVEGLWEATHDRY" 1 18.000000
!   Values used for Terrestrial Plant Leaf Weathering - WetSTOCHASTIC "C14
RCRESSLWEATHWET" 1 18.000000
STOCHASTIC "Ra226 RGRASSLWEATHWET" 1 18.000000
! End of Inputs
END
```

7.3.2 Output Files

Up to five output files can be written by the ECEM code. The number of files depends on the options selected in the scenario being analyzed. The following are the output files:

- **Report File**: This required file contains a summary of the scenario being analyzed and contains any error messages. An example report file for the ECEM code is provided in Table 7.3.
- **Stochastic Values File**: This optional file contains the values for every stochastic variable generated in the ECEM code. The description of the VALUES modifier on the FILE keyword (see Section 7.4.7) explains how to activate writing this file. A subset of the data written to this file for a run using five realizations is provided in Table 7.4.
- **Header File**: This required file contains information used by post-processor programs to allow easy extraction of subsets of the results computed by the ECEM code. An example of this file is given in Table 7.5.
- **Detailed Data**: This optional file contains the detailed values for the dose and risk values generated in the ECEM code. The description of the DETAILS modifier on the FILE keyword

(see Section 7.4.7) explains how to activate writing this file. A subset of the data written to this file for a run using five realizations is provided in Table 7.6.

- **Summary Statistics Data**: This optional file contains the summary statistics for the dose and risk values generated in the ECEM code. The description of the STATISTI modifier on the FILE keyword (see Section 7.4.7) explains how to activate writing this file. A subset of the data written to this file for a run using five realizations is provided in Table 7.7.
- **FCDA Data Files**: The FCDA files contain all the food concentration data created by the ECEM code. The concentrations for all food species are based on the same analyte, time, and location data. There is a separate food concentration data file for every species requested in the ecological impacts keyword file. The file format for these file is provided in Section 2.3.1.
- **FCDA Index File**: This optional file provides an index map into the FCDA binary data files. This file is required if FCDA files are created by ECEM. The file format for this file is provided in Section 2.3.2.
- **FCDA Header File**: This required file contains information used by post-processor programs to allow easy extraction of the food concentrations computed by the ECEM code. The file format for this file is provided in Section 2.3.3.

7.3.2.1 ECEM Report File

Excerpted records for an example report file for the ECEM code are provided in Table 7.3. This file contains information for a run of the ECEM code using 12 analytes, 1 realization, 3555 locations, and 1 solution times. The size of this file is about 298 KB in size. The size of this file grows rapidly when debug options are selected. A run using all debug options having a large number of locations, analytes, solution times, and realizations could easily generate a report file larger than the 2.1-GB file size limit under the Windows operating system.

Table 7.3 Excerpted Records from an ECEM Report File

```
      EEEEEEE   CCCCC   EEEEEEE  MM   MM
      E        C     C  E        M M M M
      E        C        E        M  M  M
      EEEEE    C        EEEEE    M  M  M
      E        C        E        M     M
      E        C     C  E        M     M
      EEEEEEE   CCCCC   EEEEEEE  M     M

          ECEM       Version 3.04.017
         Last Modified on 27 Feb 2006
-----------------------------------------------
    Ecological Contaminant Exposure Model
 Stochastic Ecological Pathways Risk Analysis
-----------------------------------------------
   Developed By Battelle Memorial Institute
    Pacific Northwest National Laboratories
             Richland, Washington
-----------------------------------------------
              Copyright Notice
Copyright c Battelle Memorial Institute, 2000.
           All Rights Reserved.
-----------------------------------------------
```

```
        Current Run ID = 20060425144621   User Name = Paul W. Eslinger
               System Date = 04/25/2006   System Time = 14:46:21

           The software used to generate this output is experimental
              and has not been formally tested or peer reviewed.

                              Review Signatures

Input Prepared By: _____________________________       Date: _________________

Input Reviewed By: _____________________________       Date: _________________

======================== Echo of the Problem Definition ========================
Title: Reference Case A - Hanford plus Background Food Run
User:  Paul W. Eslinger
1 Realizations requested

File Name for Input Keyword Data
File: Ecem_CA_Ref_A_foods.key

File Name for the Report File
File: /home/ANALYSIS5/CA_Ref_A/foods/Ecem_CA_Ref_A_foods.rpt

File Name for Media Concentrations for analyte with ID="File Name for Generated
Stochastic Values"
File: /home/ANALYSIS5/CA_Ref_A/foods/Ecem_CA_Ref_A_val_foods.csv

File Name for Media Concentrations for analyte with ID="H3"
File: /home/ANALYSIS5/CA_Ref_A/ecda/CA_Ref_A_H3.bin

File Name for Media Concentrations for analyte with ID="C14"
File: /home/ANALYSIS5/CA_Ref_A/ecda/CA_Ref_A_C14.bin

File Name for Media Concentrations for analyte with ID="Cl36"
File: /home/ANALYSIS5/CA_Ref_A/ecda/CA_Ref_A_Cl36.bin

...
Debug Flag Information
   No  : Concentration Data
   No  : Stochastic Calculations
   No  : Air Concentration Calculations
...
   No  : Equations in subroutine NS_TP
   No  : Equations in subroutine NS_QA
   No  : Equations in subroutine NS_TA

Summary Statistics Output Flag Information
   No  : BURDEN : Body burden
   No  : BMTISS : Aquatic species tissue benchmark
...
   No  : DOSING : Ingestion dose by analyte
   No  : DOSINH : Inhalation dose by nuclide

Detailed Data Output Flag Information
   No  : BURDEN : Body burden
   No  : BMTISS : Aquatic species tissue benchmark
...
   No  : DOSING : Ingestion dose by analyte
   No  : DOSINH : Inhalation dose by nuclide

Growing season information for food calulations
       121 : Day of year (Julian calendar) the growing season starts
```

```
       256 : Day of year (Julian calendar) the growing season ends
    0.3726 : Fraction of year assigned to the growing season
   76.0000 : Amount of irrigation water applied in a year (cm)

Starting Problem Execution

    Date: 04/25/2006
    Time: 14:47:02.093

Time Slices Requested: (Index, Calendar Year)
      1 : 1945
      2 : 1950
      3 : 1955
 ...
    306 : 11950
    307 : 12000
    308 : 12050
A total of 308 times have been requested.

Locations Requested: (Index, ID, Type, Name)
      1 : UH0002 : UPLAND   : "UnsuitableForAgricul"
      2 : UH0003 : UPLAND   : "UnsuitableForAgricul"
      3 : UH0004 : UPLAND   : "AgExclusionBuffer"
 ...
   4314 : QTV009 : AQUATIC  : "Transect VERNITA-1 HRM 0.3"
   4315 : QTV010 : AQUATIC  : "Transect VERNITA-1 HRM 0.3"
   4316 : QHRWI1 : AQUATIC  : "City of Richland Municipal Water Intake - River"
A total of 4273 locations have been requested.

Analytes Requested:
Index   ID   Element Type Description
----- ------ ------- ---- ------------------------------------------------
    1 H3      H       NR  Tritium
    2 C14     C       NR  Carbon-14
    3 Cl36    Cl      NR  Chlorine-36
    4 Se79    Se      NR  Selenium-79
    5 Sr90    Sr      NR  Strontium-90
    6 Tc99    Tc      NR  Technetium-99
    7 I129    I       NR  Iodine-129
    8 Cs137   Cs      NR  Cesium-137
   10 Ra226   Ra      NR  Radium-226
   11 Pa231   Pa      NR  Protactinium-231
   12 U233    U       NR  Uranium-233
   13 U235    U       NR  Uranium-235
   14 U238    U       NR  Uranium-238
   15 Np237   Np      NR  Neptunium-237
A total of 14 analytes have been requested.

Species information listed in order of computation
Order Out Type Habitat     ID    Long Name
----- --- ---- --------  ------  ------------------------------------------------
    1 No   QP  AQUATIC  "QPERIP" periphyton
    2 No   QP  AQUATIC  "QPHYPK" phytoplankton
...
   78 No   TA  UPLAND   "UCYOTE" coyote
   66 No   TA  UPLAND   "UBDGER" American badger
A total of 135 species have been requested.

No Thresholds Requested that Match with Requested Species and Analytes

Concentration data units conversion factors
```

```
    1 : H3     : NR : Ground water  :  1.00000E+09 : From Ci/m^3       to pCi/L
    1 : H3     : NR : Surface water :  1.00000E+09 : From Ci/m^3       to pCi/L
    1 : H3     : NR : Seep water    :  1.00000E+09 : From Ci/m^3       to pCi/L
    1 : H3     : NR : Sediment      :  1.00000E+12 : From Ci/kg        to pCi/kg
    1 : H3     : NR : Pore water    :  1.00000E+09 : From Ci/m^3       to pCi/L
    1 : H3     : NR : Soil-Riparian :  1.00000E+12 : From Ci/kg        to pCi/kg
    1 : H3     : NR : Soil-Dry Land :  1.00000E+12 : From Ci/kg        to pCi/kg
    1 : H3     : NR : Soil-GW Irrig :  1.00000E+12 : From Ci/kg        to pCi/kg
    1 : H3     : NR : Soil-SW Irrig :  1.00000E+12 : From Ci/kg        to pCi/kg
    1 : H3     : NR : Air Concen.   :  1.00000E+12 : From Ci/m^3       to pCi/m^3
    1 : H3     : NR : Air Deposit.  :  1.00000E+12 : From Ci/m^2/yr    to pCi/m^2/yr

Header information from the map file
   FCDA_PTITLE   = "Reference Case A - Hanford plus Background Food Run"
   FCDA_PRGNAM   = "ECEM"
   FCDA_PRGVER   = "3.04.017"
   FCDA_PRGDAT   = "27 Feb 2006"
   FCDA_USRNAM   = "Paul W. Eslinger"
   FCDA_CRUNID   = "20060425144621"
   FCDA_BLOCK_AQ = 753
   FCDA_BLOCK_RP = 692
   FCDA_BLOCK_UP = 8484
   FCDA_NHEAD    = 3
   FCDA_RECLEN   = 14
   FCDA_NREAL    = 1

Creating food files

  Unit:  23  Analyte: "H3    "  Species: "QCARPS"  File:
"/home/ANALYSIS5/CA_Ref_A/foods/Food_H3_QCARPS.fod"
  Unit:  24  Analyte: "H3    "  Species: "QCATFS"  File:
"/home/ANALYSIS5/CA_Ref_A/foods/Food_H3_QCATFS.fod"
  Unit:  25  Analyte: "H3    "  Species: "QLMSUC"  File:
"/home/ANALYSIS5/CA_Ref_A/foods/Food_H3_QLMSUC.fod"
...
  Unit: 622  Analyte: "Np237 "  Species: "UMLBRY"  File:
"/home/ANALYSIS5/CA_Ref_A/foods/Food_Np237_UMLBRY.fod"
  Unit: 623  Analyte: "Np237 "  Species: "URTVEG"  File:
"/home/ANALYSIS5/CA_Ref_A/foods/Food_Np237_URTVEG.fod"
  Unit: 624  Analyte: "Np237 "  Species: "UTRFRT"  File:
"/home/ANALYSIS5/CA_Ref_A/foods/Food_Np237_UTRFRT.fod"

Ending Problem Execution

    Date: 04/25/2006
    Time: 21:08:05.697

Message originating in routine ECEM
Message: Normal Termination
```

7.3.2.2 ECEM Stochastic Values File

The stochastic values file is an optional output file that contains the values for every stochastic variable generated in the ECEM code. The description of the VALUES modifier on the FILE keyword (see Section 7.4.7) explains how to activate writing this file. The values are written as text in comma-separated format so they can be imported easily into a spreadsheet or other software. Each line of the file consists of the ID of the stochastic variable followed by a value for every generated realization. Table 7.4 provides a subset of the data written to this file for a run using four realizations. Because this file has at

most a few thousand entries, the file size is always smaller than 1 MB. For this example case, there were 57 species and 10 analytes. The resulting output file contained 2195 stochastic variables.

Table 7.4 Excerpted Records from the ECEM Stochastic Values File

```
"H3    KOW", 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00
"H3    BCFVEG", 4.76008E+00, 5.14824E+00, 4.68511E+00, 4.90057E+00
"H3    AMCOOTALPHAING", 2.99159E-01, 3.20625E-01, 3.12601E-01, 3.32825E-01
"H3    AMCOOTALPHAPAR", 2.95370E-01, 3.02699E-01, 3.07821E-01, 3.18973E-01
"H3    AMCOOTALPHAVAP", 3.03127E-01, 2.97189E-01, 3.12049E-01, 3.33042E-01
"H3    AMCOOTALPHADW", 1.42924E-03, 1.53292E-03, 1.56314E-03, 1.49832E-03
"H3    AMCOOTALPHADS", 7.90622E-04, 8.16154E-04, 7.95349E-04, 7.57446E-04
"H3    AMCOOTDEPRATE", 1.37955E-01, 1.47876E-01, 1.49062E-01, 1.52669E-01
"H3    CARP  BCF", 9.91170E-01, 9.75634E-01, 1.03975E+00, 9.55665E-01
"AMCOOTFABOVE", 1.00000E+00, 1.00000E+00, 1.00000E+00, 1.00000E+00
"AMKSTLFABOVE", 1.00000E+00, 1.00000E+00, 1.00000E+00, 1.00000E+00
"AMWPELFABOVE", 1.00000E+00, 1.00000E+00, 1.00000E+00, 1.00000E+00
"BEAVERFABOVE", 5.00000E-01, 5.00000E-01, 5.00000E-01, 5.00000E-01
"BLCTWDKPS1", 3.28382E-03, 3.15453E-03, 3.69783E-03, 3.46070E-03
"BLCTWDKPA2", 3.30129E+03, 3.26486E+03, 3.53984E+03, 3.13465E+03
"TARTPDFABOVE", 5.00000E-01, 5.00000E-01, 5.00000E-01, 5.00000E-01
"TULE  KPS1", 3.35116E-03, 3.41507E-03, 3.26583E-03, 3.50039E-03
"TULE  KPA2", 3.45243E+03, 3.23831E+03, 3.13824E+03, 3.35585E+03
"TULE  FABOVE", 1.00000E+00, 1.00000E+00, 1.00000E+00, 1.00000E+00
"WEASELFABOVE", 1.00000E+00, 1.00000E+00, 1.00000E+00, 1.00000E+00
"WMLFOLBPORE", 4.92350E-01, 4.97657E-01, 5.28679E-01, 5.16139E-01
"WOTDADFABOVE", 1.00000E+00, 1.00000E+00, 1.00000E+00, 1.00000E+00
"WOTDTPBPORE", 4.93585E-01, 5.35813E-01, 4.94853E-01, 4.74527E-01
"WAQGS FABOVE", 8.00000E-01, 8.00000E-01, 8.00000E-01, 8.00000E-01
"WSTRGNBPORE", 9.33988E-02, 9.83106E-02, 1.03638E-01, 1.07242E-01
```

7.3.2.3 ECEM Header File

The ECEM header file is an output file containing information used by post-processor programs to allow easy extraction of subsets of the results computed by the ECEM code. This file is required for every run of the ECEM code. An example of this file is given in Table 7.5. The file contains the following sections of information:

- A header section of basic run information
- Number of realizations
- Solution times selected
- Locations used
- Analytes processed
- Species with output selected
- Solutions selected
- Output file names.

The user only specifies the name of this file; users should not modify the file after it is generated by the ECEM code. Because this file has at most a few hundred entries, the file size is always much smaller than 1 MB. File names for options not selected are set to null.

Table 7.5 Example Header File from ECEM

```
type: "Ecological"
title: "ECEM keyword file - History2 Assessments"
```

```
user: "Paul W. Eslinger"
name: "ECEM"
version: "3.04.018"
date: "18 Jul 2006"
id: "20060718094745"
envfile: "/home/ANALYSIS6/History2_Best/ESD_History2_Best.key"
realizations:    1
times:   40
 1945
 1950
...
 2018
 2019
 2020
locations:    5
"UH0138","AgExclusionBuffer"
"RHP026","Riparian Benton Downriver 100BC"
"QHP025","AquaticBenton100BC"
"QHP026","AquaticBentonDownriver100BC"
"QHP215","AquaticBenton300Area"
analytes:    5
"H3    ","NR","Tritium"
"Tc99  ","NR","Technetium-99"
"I129  ","NR","Iodine-129"
"U     ","NS","Uranium"
"-Rads-","XX","Sum of radionuclides"
species:    1
"UCHKEG","TA","chickens (eggs)"
media:   11
"AIRC","Air concentration"
"AIRD","Air deposition"
"GWAT","Groundwater concentration"
"PWAT","Pore water concentration"
"SEDI","Sediment concentration"
"SEEP","Seep (spring) water concentration"
"SORP","Riparian soil concentration"
"SODR","Dry (nonirrigated) soil concentration"
"SOGW","Goundwater irrigated soil concentration"
"SOSW","Surface water irrigated soil concentration"
"SWAT","Surface water concentration"
solutions:    3
"DOSRAD","Radioactive dose"
"CONCEN","Media concentration"
"SUMRAD","Sum of radioactive dose"
summary: "NULL"
detail: "/home/ANALYSIS6/History2_Best/ecem/Ecem_History2_Best_det.csv"
```

7.3.2.4 ECEM Detailed Data

The detailed data file is an optional output file that contains the detailed values for body burdens and dose generated in the ECEM code. The description of the DETAILS modifier on the FILE keyword (see Section 7.4.7) explains how to activate writing this file. The solution types that can be written to the file are described in Section 7.4.4. The values are written as text in comma-separated format so they can be imported easily into a spreadsheet or other software. Each line of the file consists of six identifiers followed by a value for every generated realization. A subset of the data written to this file for a run

using two realizations is provided in Table 7.6. The header line occupies one line in the file even though it occupies two lines in the table. The following are the six identifiers on each line:

- Time: Year for which the data are valid
- Location ID: The location identifier where the data are valid
- Analyte ID: The identification of the analyte for which the data were computed
- Species ID: The identification for the species for which data were computed
- Solution type: A flag for solution type
- Units: The units associated with the computed data.

Table 7.6 Excerpted Records from an ECEM Detailed Data File

```
"Time","Location ID","Soil Type","Analyte ID","Specie","Solution Type","Units","Values
by realization"
1990,"UH0138","NONE","H3","AIRD","CONCEN","pCi/m^2/yr", 0.00000E+00
1990,"UH0138","NONE","H3","GWAT","CONCEN","pCi/L", 8.53571E+04
1990,"UH0138","SODR","H3","SODR","CONCEN","pCi/kg", 0.00000E+00
1990,"UH0138","SOGW","H3","SOGW","CONCEN","pCi/kg", 0.00000E+00
1990,"UH0138","SOSW","H3","SOSW","CONCEN","pCi/kg", 0.00000E+00
2020,"UH0138","NONE","Tc99","AIRC","CONCEN","pCi/m^3", 0.00000E+00
2020,"UH0138","NONE","Tc99","AIRD","CONCEN","pCi/m^2/yr", 0.00000E+00
2020,"UH0138","NONE","Tc99","GWAT","CONCEN","pCi/L", 7.86180E+01
2020,"UH0138","SODR","Tc99","SODR","CONCEN","pCi/kg", 0.00000E+00
2020,"UH0138","SOGW","Tc99","SOGW","CONCEN","pCi/kg", 1.30067E+02
2020,"UH0138","SOSW","Tc99","SOSW","CONCEN","pCi/kg", 9.43818E-02
2020,"UH0138","SODR","Tc99","UCHKEG","BURDEN","pCi/kg", 0.00000E+00
2020,"UH0138","SODR","Tc99","UCHKEG","DOSRAD","rad/day", 0.00000E+00
2020,"UH0138","SOGW","Tc99","UCHKEG","BURDEN","pCi/kg", 1.39743E+04
2020,"UH0138","SOGW","Tc99","UCHKEG","DOSRAD","rad/day", 6.01008E-05
2020,"UH0138","SOSW","Tc99","UCHKEG","BURDEN","pCi/kg", 1.13824E+00
2020,"UH0138","SOSW","Tc99","UCHKEG","DOSRAD","rad/day", 4.89538E-09
```

This file can have several rows of information for every combination of time, location, species, and analyte. Therefore, this file can become very large. As an example, a 2,800 KB file was generated for a case involving 14 locations, 10 analytes, 7 realizations, 12 times, and 4 output species. The file size directly scales with the number of analytes, locations, species, and times. The file size grows more slowly than a direct scaling by the number of realizations. The file size can be reduced by selecting fewer times, locations, output species, or solution types.

7.3.2.5 ECEM Summary Statistics

This optional file contains summary statistics for dose generated in the ECEM code. The description of the STATISTI modifier on the FILE keyword (see Section 7.4.7) explains how to activate writing this file. The solution types that can be written to the file are described in Section 7.4.17. The values are written as text in comma-separated format so they can be imported easily into a spreadsheet or other software. Each line of the file consists of six identifiers followed by summary statistics (nine percentiles, mean value, and standard deviation). A subset of the data written to this file for a run using five realizations is provided in Table 7.7. The following are the six identifiers on each line:

- Time: Year for which the data are valid
- Location ID: The location identifier where the data are valid
- Analyte ID: The identification of the analyte for which the data were computed
- Species ID: The identification for the species for which data were computed

- Solution type: A flag for solution type
- Units: The units associated with the computed data.

The data for each record in this file are too long to present without line-wrapping in this document. Each record in the file occupies two lines in Table 7.7.

Table 7.7 Excerpted Records from the ECEM Summary Statistics File

"Time","Location ID","Specie ID","Analyte ID","Result Type","Units","Minimum","5th Percentile","10th Percentile",
"25th Percentile","Median","75th Percentile","90th Percentile","95th Percentile","Maximum","Mean","Standard Deviation"
1990,"RH0050","RCANGS","H3 ","BURDEN","pCi/kg", 2.54241E+01, 2.54241E+01, 2.54241E+01, 2.54241E+01,
2.73537E+04, 3.38985E+04, 4.51161E+04, 4.51161E+04, 8.01585E+04, 3.32611E+04, 2.48229E+04
1990,"RH0050","RCANGS","H3 ","DOSRAD","rad/day", 7.54994E-09, 7.54994E-09, 7.54994E-09, 7.54994E-09,
8.12296E-06, 1.00665E-05, 1.33977E-05, 1.33977E-05, 2.38039E-05, 9.87721E-06, 7.37140E-06
1990,"RH0050","MAYFLY","H3 ","BURDEN","pCi/kg", 1.22778E+01, 1.22778E+01, 1.22778E+01, 1.22778E+01,
6.70630E+03, 8.25514E+03, 1.05390E+04, 1.05390E+04, 1.76211E+04, 7.74609E+03, 5.44027E+03
1990,"RH0050","MAYFLY","H3 ","BMTISS","unitless", 1.23215E+01, 1.23215E+01, 1.23215E+01, 1.23215E+01,
6.88845E+03, 8.12850E+03, 1.02607E+04, 1.02607E+04, 1.80153E+04, 7.76516E+03, 5.52208E+03
1990,"RH0050","MAYFLY","H3 ","DOSRAD","rad/day", 3.64601E-09, 3.64601E-09, 3.64601E-09, 3.64601E-09,
1.99150E-06, 2.45145E-06, 3.12967E-06, 3.12967E-06, 5.23275E-06, 2.30028E-06, 1.61554E-06
1990,"RH0050","SALMJV","H3 ","BURDEN","pCi/kg", 6.28882E+00, 6.28882E+00, 6.28882E+00, 6.28882E+00,
1.38113E+03, 1.89246E+03, 2.46386E+03, 2.46386E+03, 4.66751E+03, 1.82576E+03, 1.46418E+03
1990,"RH0050","SALMJV","H3 "," BMTISS ","unitless", 6.32028E+00, 6.32028E+00, 6.32028E+00, 6.32028E+00,
1.48005E+03, 1.87565E+03, 2.34242E+03, 2.34242E+03, 4.54303E+03, 1.81281E+03, 1.40662E+03
1990,"RH0050","SALMJV","H3 ","DOSRAD","rad/day", 1.86753E-09, 1.86753E-09, 1.86753E-09, 1.86753E-09,
4.10141E-07, 5.61986E-07, 7.31668E-07, 7.31668E-07, 1.38607E-06, 5.42179E-07, 4.34802E-07
1990,"RH0050","HRVMSE","H3 ","BURDEN","pCi/kg", 1.90977E+01, 1.90977E+01, 1.90977E+01, 1.90977E+01,
1.79798E+04, 2.42002E+04, 3.12386E+04, 3.12386E+04, 5.20661E+04, 2.18047E+04, 1.65240E+04
1990,"RH0050","HRVMSE","H3 ","DOSRAD","rad/day", 5.67125E-09, 5.67125E-09, 5.67125E-09, 5.67125E-09,
5.33928E-06, 7.18650E-06, 9.27663E-06, 9.27663E-06, 1.54616E-05, 6.47513E-06, 4.90697E-06
1990,"RH0050","HRVMSE","H3 ","DOSDER","rad/day", 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00
1990,"RH0050","HRVMSE","H3 ","DOSING","rad/day", 3.09753E+01, 3.09753E+01, 3.09753E+01, 3.09753E+01,
2.85303E+04, 3.52527E+04, 4.67677E+04, 4.67677E+04, 8.33295E+04, 3.45718E+04, 2.57908E+04
1990,"RH0050","HRVMSE","H3 ","DOSINH","rad/day", 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00
1990,"RH0050","RCANGS","CCl4 ","BURDEN","ug/kg", 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00
1990,"RH0050","MAYFLY","CCl4 ","BURDEN","ug/kg", 5.06943E-02, 5.06943E-02, 5.06943E-02, 5.06943E-02,
5.83496E-02, 6.45637E-02, 7.07093E-02, 7.07093E-02, 1.01457E-01, 6.48589E-02, 1.75829E-02
1990,"RH0050","MAYFLY","CCl4 "," BMTISS ","unitless", 5.06943E-02, 5.06943E-02, 5.06943E-02, 5.06943E-02,
5.83496E-02, 6.45637E-02, 7.07093E-02, 7.07093E-02, 1.01457E-01, 6.48589E-02, 1.75829E-02
1990,"RH0050","HRVMSE","CCl4 ","DOSINH","ug/kg/day", 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00
1990,"RH0050","HRVMSE","-Rads-","SUMRAD","rad/day", 6.53884E-08, 6.53884E-08, 6.53884E-08, 6.53884E-08,
5.34093E-06, 7.32354E-06, 9.27913E-06, 9.27913E-06, 1.54730E-05, 6.51136E-06, 4.89722E-06
1990,"RH0050","MAYFLY","-Rads-","SUMRAD","rad/day", 4.00539E-05, 4.00539E-05, 4.00539E-05, 4.00539E-05,
9.29692E-05, 1.36747E-04, 2.07406E-04, 2.07406E-04, 3.78735E-04, 1.40443E-04, 1.19386E-04
1990,"RH0050","RCANGS","-Rads-","SUMRAD","rad/day", 7.54994E-09, 7.54994E-09, 7.54994E-09, 7.54994E-09,
8.12296E-06, 1.00665E-05, 1.33977E-05, 1.33977E-05, 2.38039E-05, 9.87721E-06, 7.37140E-06
1990,"RH0050","SALMJV","-Rads-","SUMRAD","rad/day", 2.13907E-06, 2.13907E-06, 2.13907E-06, 2.13907E-06,
3.69897E-06, 5.16700E-06, 7.70061E-06, 7.70061E-06, 1.60394E-05, 5.71137E-06, 4.94818E-06

This file can have several rows of information for every combination of time, location, specie, and analyte. Therefore, this file can become very large. As an example, a 3,890 KB file was generated for a case involving 14 locations, 10 analytes, 7 realizations, 12 times, and 4 output species. The file size directly scales with the number of analytes, locations, species, and times. The file size grows more

slowly than a direct scaling by the number of realizations. The file size can be reduced by selecting fewer times, locations, output species, or solution types.

7.4 Keyword Descriptions for the ECEM Code

This section defines keywords needed to control the ECEM code directly. Most of these keywords can be entered in any order. The only restriction on keyword order is that the END keyword must be the last keyword in the file. General rules for reading the keyword descriptions are explained in Section 1.4. Section 18.0 presents a more detailed description of the keyword language syntax.

7.4.1 ANALYTE Keyword for the ECEM Code

The ANALYTE keyword is used to define the analytes to be used in calculating ecological risk metrics. The following is this keyword's syntax:

```
ANALYTE [ID="quote 1"] [ELEMENT="quote 1"] [PARTICLE=n1] {OUTPUT}
```

Analytes chosen must be a subset of the analytes used in the fate and transport activities controlled through the ESD keyword file. Multiple analyte keywords can be entered. A separate ANALYTE keyword is required for each desired analyte. The modifiers can be entered in any order. The modifiers associated with the ANALYTE keyword are described in Table 7.8.

Table 7.8 Modifiers Associated with the ANALYTE Keyword in the ECEM Code

Modifier	Description
ID	The entry associated with the ID modifier is an analyte identification string (up to six characters long). The analyte ID entered must be one of the set of analytes identified in the environmental settings definition file.
ELEMENT	The entry associated with the ELEMENT modifier is the nonspeciated chemical name of the analyte. The ELEMENT is used to enter the KOW and BCFVEG parameters which are equal for all analytes of the same element.
OUTPUT	The OUTPUT modifier is necessary for data to be output for this species.
PARTICLE	The numerical entry associated with the PARTICLE modifier is the fraction of the airborne quantity of the analyte that is in particulate form. The numerical value must be in the range [0,1].

The following is an example ANALYTE keyword defining zinc as an analyte that is an animal nutrient:

```
ANALYTE ID="Zn" PARTICLE=0.0 OUTPUT
```

7.4.2 CONSUME Keyword for the ECEM Code

The CONSUME keyword is to define the diet of the species identified by the ID modifier. The following is this keyword's syntax:

```
CONSUME [ID= "Quote1"] [PREY] ["Quote2"=Value1] … {"Quotek"=Valuek+1}
   {SOILING=valuek+2} {SEDING=valuek+3}
```

The diet for a species is defined by entering a series of prey species IDs. Each prey species ID must be immediately followed by the normalized fraction of the diet coming from the prey species. If any prey species are entered, the sum of normalized diet fractions must sum to 1. The optional SEDING modifier can be used to identify incidental sediment ingestion for aquatic animal species while the optional modifier SOILING can be used to identify incidental soil ingestion for terrestrial animal species. The values entered for SOILING or SEDING on the CONSUME keyword replace any values for these two parameters read from the SPECIES keyword in the ESD keyword file. The modifiers associated with the CONSUME keyword are described in Table 7.9. Water ingestion for terrestrial animal species is defined using the SPECIES keyword in the ESD keyword file rather than with the CONSUME keyword. Water consumption of upland terrestrial animal species matches with the soil type for the location (clean water for dry locations, groundwater for locations irrigated with groundwater and surface water for locations irrigated with surface water) for every simulated year irrespective of whether irrigation has already started at that year.

Table 7.9 Modifiers Associated with the CONSUME Keyword in the ECEM Code

Modifier	Description
ID	The entry associated with the ID modifier is an analyte identification string (up to six characters long). The analyte ID entered must be one of the set of analytes identified in the environmental scenario file.
SEDING	Optional sediment ingestion rate entered as a fraction of diet. This option only applies to species that are aquatic animals.
SOILING	Optional soil ingestion rate species entered as a fraction of diet. This option only applies to animal species living in a terrestrial (riparian or upland) environment.
PREY	The list of prey species consumed and consumption rates as a fraction of diet for this predator species.

The following is an example CONSUME keywords for carp and riparian beaver:

```
CONSUME ID="QCARPS" PREY
  "QCPBSN"  0.15000
  "QMAYFL"  0.25000
  "QPERIP"  0.50000
  "QMLFOL"  0.10000
  SEDING    0.16000

CONSUME ID="RBEAVR" PREY
  "RCTWOD"  0.50000
  "RMLBRY"  0.50000
  SOILING   0.09000
```

7.4.3 DEBUG Keyword for the ECEM Code

The DEBUG keyword is used to activate dumping of intermediate calculations to the report file. It should be used sparingly and with only one or two realizations; otherwise, the volume of output could fill the user's hard drive. The following is this keyword's syntax:

```
DEBUG [modifier 1] {modifier 2}…{modifier k}
```

Multiple DEBUG cards can be entered with combinations of modifiers, or a single card can be entered containing all of the modifiers. The modifiers can be entered in any order. Table 7.10 describes the modifiers associated with the DEBUG keyword.

Table 7.10 Modifiers Associated with the DEBUG Keyword in the ECEM Code

Modifier	Description
AIR	Intermediate outputs on calculations for air calculations.
ANALYTES	Intermediate results for analyte information.
CONCENTR	Intermediate outputs for concentration data.
CONSTANT	Intermediate outputs for constant data.
RADSUM	Intermediate results for radioactive doses.
GENERATE	Intermediate results for the stochastic variable generation.
LOOP	Messages on the control looping.
SPECIES	Intermediate results for species information.
VERBOSE	Additional messages to the screen showing simulation progress.
OR_QP	Intermediate results for organic radioactive analytes and aquatic plants.
OR_TP	Intermediate results for organic radioactive analytes and terrestrial plants.
OR_QA	Intermediate results for organic radioactive analytes and aquatic animals.
OR_TA	Intermediate results for organic radioactive analytes and terrestrial animals.
NR_QP	Intermediate results for inorganic radioactive analytes and aquatic plants.
NR_TP	Intermediate results for inorganic radioactive analytes and terrestrial plants.
NR_QA	Intermediate results for inorganic radioactive analytes and aquatic animals.
NR_TA	Intermediate results for inorganic radioactive analytes and terrestrial animals.
OS_QP	Intermediate results for organic stable analytes and aquatic plants.
OS_TP	Intermediate results for organic stable analytes and terrestrial plants.
OS_QA	Intermediate results for organic stable analytes and aquatic animals.
OS_TA	Intermediate results for organic stable analytes and terrestrial animals.
NS_QP	Intermediate results for inorganic stable analytes and aquatic plants.
NS_TP	Intermediate results for inorganic stable analytes and terrestrial plants.
NS_QA	Intermediate results for inorganic stable analytes and aquatic animals.
NS_TA	Intermediate results for inorganic stable analytes and terrestrial animals.

The following entries provide examples of the use of the DEBUG keyword:

```
DEBUG ANALYTES
DEBUG RADSUM
DEBUG OR_TA NR_TA OS_TA NS_TA
```

There are no quote strings associated with the DEBUG keyword.

7.4.4 DETAILS Keyword for the ECEM Code

The DETAILS keyword is used to control writing detailed data to the output details file for a variety of solution types. The following is this keyword's syntax:

```
DETAILS [modifier 1] {modifier 2}…{modifier 10}
```

Multiple DETAILS cards can be entered with combinations of modifiers, or a single card can be entered containing all of the modifiers. The modifiers can be entered in any order. Table 7.11 describes the modifiers associated with the DETAILS keyword.

Table 7.11 Modifiers Associated with the DETAILS Keyword in the ECEM Code

Modifier	Description
BURDEN	Presence of the BURDEN modifier initiates output of the body burden (tissue concentrations) for every species and analyte where the species output flag is used (see the SPECIES keyword).
BMRDOS	Presence of the BMRDOS modifier initiates output of the benchmark comparison for the organism dose for animal and plant species exposed to radioactive analytes where the species output flag is used (see the SPECIES keyword).
BMTISS	Presence of the BMTISS modifier initiates output of the benchmark comparison for the body burden of animal and plant species exposed to nonradioactive analytes where the species output flag is used (see the SPECIES keyword).
CONCEN	Presence of the CONCEN modifier initiates output of the water, sediment, and soil concentration data used in the calculations. The media identifiers are: • SWAT denotes surface water (river) • PWAT denotes pore water (river bottom) • GWAT denotes groundwater • SEEP denotes seep water (river bank) • SOIL denotes soil • SEDI denotes sediment (river bottom)
DOSDER	Presence of the DOSDER modifier initiates output of the dermal dose for terrestrial animal species and all analytes where the species output flag is used (see the SPECIES keyword).
DOSHAZ	Presence of the DOSHAZ modifier initiates output of the hazard values for terrestrial animal species and all analytes where the species output flag is used (see the SPECIES keyword).
DOSING	Presence of the DOSDER modifier initiates output of the ingestion dose for terrestrial animal species and all analytes where the species output flag is used (see the SPECIES keyword).
DOSINH	Presence of the DOSDER modifier initiates output of the inhalation dose for terrestrial animal species and all analytes where the species output flag is used (see the SPECIES keyword).
DOSRAD	Presence of the DOSRAD modifier initiates output of the radioactive dose for animal and plant species and all radioactive analytes where the species output flag is used (see the SPECIES keyword).
SUMRAD	Presence of the DOSRAD modifier initiates output of the radioactive dose summed over all radioactive analytes for animal and plant species when the species output flag is used (see the SPECIES keyword).

The following entries provide examples of the use of the DETAILS keyword:

```
DETAILS DOSRAD SUMRAD
DETAILS SUMRAD
```

```
DETAILS DOSING DOSDER BURDEN
```

There are no quote strings associated with the DETAILS keyword.

7.4.5 END Keyword for the ECEM Code

The END keyword signifies the end of all keyword data. It should be the last keyword in the keyword file. All data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

There are no modifiers or quote strings associated with the END keyword.

7.4.6 EXECUTE Keyword for the ECEM Code

The EXECUTE keyword signifies that the user wishes to perform problem execution. If this keyword is not entered, then the inputs are checked for consistency, but the problem will not be executed. This is useful if the run being set up is expected to take a significant amount of computation time. The following is this keyword's syntax:

```
EXECUTE
```

There are no modifiers or quote strings associated with the EXECUTE keyword.

7.4.7 FILE Keyword for the ECEM Code

The FILE keyword is used to enter the names of input and output files except for the report file. The names of the files providing concentration data are contained in the environmental scenario file rather than in the keyword file. The following is this keyword's syntax:

```
FILE [modifier1 "quote1"] {modifier2 "quote2"} ... {modifier5 "quote5"}
```

The file names are entered in quote strings, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. The file name associated with a modifier must be entered before the next modifier is entered. At least one FILE keyword is required for every run of the code. Table 7.12 describes the modifiers associated with the FILE keyword.

Table 7.12 Modifiers Associated with the FILE Keyword in the ECEM Code

Modifier	Description
DETAILS	Optional output file containing detailed solutions by realization. The file is written in comma separated variables format, so a file name extension of *.csv is recommended.
ESD	Required input keyword file (environmental settings definitions) that contains problem definition information for the release and transport codes and information specific to the ECEM code.
HEADER	Required output file containing header type information associated with all of the other output files identified in this table.

Modifier	Description
THRESHOL	Optional output file containing exceedance probabilities for user-specified thresholds. See the THRESHOLD keyword (Section 7.4.19) for more detailed information.
STATISTI	Optional output file containing summary statistics for all calculations. The file is written in comma separated variables format, so a file name extension of *.csv is recommended.
VALUES	Optional output file containing generated values for all stochastic variables. This file is recommended because it contains data required to support uncertainty analyses.

The following two entries define the file for detailed calculations and the header file:

```
FILE DETAILS "TestCase.det"
FILE HEADER "/home/ANALYSIS/Median2/ecem/TestCase.hdr"
```

7.4.8 FOODS Keyword for the ECEM Code

The FOODS keyword is used to designate the location where the FCDA files are to be written and to identify the name of the map file associated with these FCDA files. The following is this keyword's syntax:

```
FOODS [PATH= "quote1"] [MAP= "quote2"] [SACVIEW= "quote3"]
```

The file names are entered in quote strings, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. The file name associated with a modifier must be entered before the next modifier is entered. At least one FOODS keyword is required for every run of the code. Table 7.13 describes the modifiers associated with the FOODS keyword.

Table 7.13 Modifiers Associated with the FOODS Keyword in the ECEM Code

Modifier	Description
PATH	The complete path name identifying the location to which FOOD files are to be written for use by the HUMAN code.
MAP	The name of the file containing the map of the FOOD file contents.
SACVIEW	The file name of the header file for the FOOD files.

The following entry defines the map file and data directory for food concentrations and the header file:

```
FOODS PATH="D:\SAC\CODES_1\ECEM\FOODS\"
MAP="ECEM_FCDA_Map.Dat"
SACVIEW="ECEM_FCDA.Hdr"
```

7.4.9 GROWTH Keyword for the ECEM Code

The GROWTH keyword is used to define the parameters of the growth rate equation described in Section 7.1.2.1. The following is this keyword's syntax:

```
GROWTH  DELTA=value1  BETA=value2
```

These modifiers can be entered in any order, together with their associated data. The following example illustrates the use of the GROWTH keyword:

```
GROWTH  DELTA=0.002 BETA=0.25
```

7.4.10 KDSOIL Keyword for the ECEM Code

The KDSOIL keyword provides the link to the library file of soil-water partition coefficients (K_d) generated by the ECDA program. A separate KDSOIL keyword is needed for every inorganic analyte that has a Henry's coefficient value greater than zero. This keyword is not needed for other analytes. The following is this keyword's syntax:

```
KDSOIL [ANALYTE="quote 1"] [ID="quote 2"]
```

The quote string associated with the ANALYTE modifier is an analyte identification string (up to six characters long). The analyte identification string entered must be one of the set of analytes identified in the environmental settings definition file by the ANALYTE keyword. The quote string associated with the ID modifier is a K_d identification string up to six characters long. The K_d identification string must be the same as one set of IDs identified in the environmental settings definition file by the KDSOIL keyword.

The values of the soil-water partition coefficients should be assigned on an element level. If multiple isotopes of the same analyte are entered they should all reference the same K_d identification string. The following are example KDSOIL keywords:

```
KDSOIL ANALYTE="I129" ID="KdI"
KDSOIL ANALYTE="I131" ID="KdI"
```

7.4.11 LOCATION Keyword for the ECEM Code

The LOCATION keyword identifies the locations for ecological impact calculations that will be generated. Multiple LOCATION keywords are allowed. The locations must be a subset of the locations at which environmental data were computed and stored by the inventory, release, and transport modules. The list of desired locations builds sequentially with each LOCATION record. Upon program entry, no locations are active. The following is this keyword's syntax:

```
LOCATION [PRIMARY="quote 1"] {SECOND="quote 2"} (OUTPUT}
```

The ecological impacts module is activated at a location by entering the location ID string in association with the PRIMARY modifier. A separate LOCATION keyword is required for every desired location. The function of the SECOND modifier is to supply concentrations from other locations that may not be computed at the primary location. If the SECOND location is not entered, impacts are calculated using only concentrations available at the primary location. Table 7.14 describes the modifiers associated with the LOCATION keyword.

Table 7.14 Modifiers Associated with the LOCATION Keyword in the ECEM Code

Modifier	Description
PRIMARY	The entry associated with the PRIMARY modifier is an ecological location identification string (up to six characters in length). The location ID entered must be one from the suite of locations identified in the environmental scenario file.
SECOND	The entry associated with the SECOND modifier is an ecological location identification string (up to six characters in length). The location ID entered must be one of the suite of locations identified in the environmental scenario file.
OUTPUT	The OUTPUT modifier is necessary for data to be output for the location.

For example, the primary location may be in the riparian zone, but a food chain including river species is being modeled. The primary location would be on land, and the secondary location should be chosen as the nearest river location. The following are example LOCATION keywords:

```
LOCATION PRIMARY="EL #001"
LOCATION PRIMARY="EL #002" SECOND="EL #001"
```

7.4.12 REALIZAT Keyword for the ECEM Code

The REALIZAT (or REALIZATION) keyword defines the number of realizations to generate. The following is this keyword's syntax:

```
REALIZATION value1
```

The integer value1 has a minimum value of 1 and a maximum of the number of realizations defined in the environmental settings definition file. If the number of realizations is less than the number of realizations in the concentration data files, then only the first realizations will be used.

The following keyword record sets the number of realizations to 10:

```
REALIZAT 10
```

7.4.13 REPORT Keyword for the ECEM Code

The REPORT keyword is used to define the name of the output report (log) file. It must be the first keyword entered in the keyword file. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The name of the report file is entered in a quote string. File names up to 72 characters long are supported, and path names can be optionally included. The following is an example REPORT keyword record:

```
REPORT "G:\SAC\SystemCodes\ECEM\Test1.rpt"
```

7.4.14 RESPIRE Keyword for the ECEM Code

The RESPIRE keyword is used to define the parameters of the respiration rate equation described in Section 7.1.2.1. This respiration equation only applies to water-respiring species. The following is this keyword's syntax:

```
RESPIRE  GAMMA=value1  PHI=value2
```

The two modifiers can be entered in any order, together with their associated data. The following example illustrates the use of the RESPIRE keyword:

```
RESPIRE  PHI=0.032 GAMMA=0.2
```

7.4.15 SEED Keyword for the ECEM Code

The SEED keyword sets the value for the seed for the random number generator. The following is this keyword's syntax:

```
SEED Value1
```

The value for Value1 must be an integer or real number in the range 1 to 999999. The following is an example keyword record:

```
SEED 344443
```

There are no quote strings or modifiers associated with the SEED keyword.

7.4.16 SPECIES Keyword for the ECEM Code

The SPECIES keyword is used to select the species to be simulated in the ECEM code. The following is this keyword's syntax:

```
SPECIES [ID="quote1"] {INTERNAL} {OUTPUT}
```

A separate SPECIES keyword must be entered for every species being modeled. The ID modifier must be matched with a quote string containing a unique ID that matches one of the species defined in the ESD file (see the SPECIES keyword in Section 2.1.16). The optional OUTPUT modifier initiates output of all information invoked by the DETAILS and STATISTICS keywords for this specie. If no OUTPUT modifiers are entered for any species, then no summary statistics or detailed data will be output.

When present, the INTERNAL modifier causes internal burdens (concentrations) for terrestrial plants to be written to the food files for use in the HUMAN code. If the INTERNAL modifier is omitted, the plant concentrations written to the food files are the combination of internal burden and external contamination. Foods that are peeled such as tree fruit or some vegetables should use the INTERNAL modifier, as well as grain (hulled during processing). If leafy vegetables are thoroughly washed during preparation the INTERNAL modifier could be used, otherwise it could be omitted. For many irrigated foods crops the external concentrations from irrigation deposition can be much larger than the internal plant concentration.

7.4.17 STATISTIC Keyword for the ECEM Code

The STATISTIC keyword is used to control writing summary statistics to the summary statistics file for a variety of solution types. The following is this keyword's syntax:

```
STATISTIC [modifier 1] {modifier 2}…{modifier 12}
```

Multiple STATISTIC cards can be entered with combinations of modifiers, or a single card can be entered containing all of the desired modifiers. The modifiers can be entered in any order. Table 7.15 describes the modifiers associated with the STATISTIC keyword.

Table 7.15 Modifiers Associated with the STATISTIC Keyword in the ECEM Code

Modifier	Description
DEFINE	The presence of this modifier controls the writing of the definitions of stochastic variables to the report file.
GENERATE	The presence of this modifier controls the writing of statistics for all generated stochastic values to the report file.
BMRDOS	Presence of the BMRDOS modifier initiates output for the benchmark comparison for the organism dose for animal and plant species exposed to radioactive analytes where the species output flag is used (see the SPECIES keyword).
BMTISS	Presence of the BMTISS modifier initiates output of the benchmark comparison for the body burden of animal and plant species exposed to nonradioactive analytes where the species output flag is used (see the SPECIES keyword).
BURDEN	Presence of the BURDEN modifier initiates output of summary statistics of the body burden (tissue concentrations) for every species and analyte where the species output flag is used (see the SPECIES keyword).
CONCEN	Presence of the CONCEN modifier initiates output of summary statistics for the water, sediment, and soil concentration data used in the calculations. The media identifiers are: • SWAT denotes surface water (river) • PWAT denotes pore water (river bottom) • GWAT denotes ground water • SEEP denotes seep water (river bank) • SOIL denotes soil • SEDI denotes sediment (river bottom)
DOSDER	Presence of the DOSDER modifier initiates output of summary statistics of the dermal dose for terrestrial animal species and all analytes where the species output flag is used (see the SPECIES keyword).
DOSHAZ	Presence of the DOSHAZ modifier initiates output of summary statistics of the inhalation dose for terrestrial animal species and all analytes where the species output flag is used (see the SPECIES keyword).
DOSING	Presence of the DOSDER modifier initiates output of summary statistics of the ingestion dose for terrestrial animal species and all analytes where the species output flag is used (see the SPECIES keyword).
DOSINH	Presence of the DOSDER modifier initiates output of summary statistics of the inhalation dose for terrestrial animal species and all analytes where the species output flag is used (see the SPECIES keyword).
DOSRAD	Presence of the DOSRAD modifier initiates output of summary statistics of the radioactive dose for animal and plant species and all radioactive analytes where the species output flag is used (see the SPECIES keyword).
SUMRAD	Presence of the DOSRAD modifier initiates output of summary statistics of the radioactive dose summed over all radioactive analytes for animal and plant species when the species output flag is used (see the SPECIES keyword).

The following entries provide examples of the use of the STATISTIC keyword:

```
STATISTIC DOSRAD
STATISTIC DOSING BMTISS
```

There are no quote strings associated with the STATISTIC keyword.

7.4.18 STOCHASTIC Keyword for the ECEM Code

The STOCHASTIC keyword is used to enter the definition of a statistical distribution for stochastic variables. The following is this keyword's syntax:

```
STOCHASTIC ["Quote1"] [Dist_Index Parameters] {TRUNCATE U1 U2} {"Quote2"}
```

The entry for Quote1 must be a unique character string of up to 20 characters that will be used to identify this stochastic variable in subsequent uses. It is case sensitive and embedded spaces are significant. It is sometimes useful to make the character string some combination of a variable name and other data such that it can be recreated easily when stochastic data are needed. The entry for Quote2 is a description for the stochastic variable that can be up to 64 characters long. An entry for Quote2 is not required.

The entry for Dist_Index must be an integer in the range 1 to 11 that identifies the index of a statistical distribution. The available statistical distributions are defined in Section 19.0, Table 17.3. The word Parameters in the general syntax statement indicates the numerical values of parameters required for defining the statistical distribution. The additional modifier TRUNCATE can be used for all distribution types except 1, 3, and 10 (constant, discrete uniform, and user defined). If TRUNCATE is entered, it must be followed by two values in the interval 0 to 1, inclusive. The lower value must be less than the upper value. These two values specify the tail probabilities at which to impose range truncation for the distribution. Truncation data must be entered after all of the other parameters that define the distribution.

The following is an example stochastic card for a bioconcentration factor that is normally distributed with a mean of 125 and a standard deviation of 5 for a frog exposed to carbon-14:

```
STOCHASTIC "BCFC14Frog" 7  125.0  5.0  "Example number 1"
```

Although this section gives the general form of a STOCHASTIC keyword entry, it does not describe the entire set of STOCHASTIC keywords required to run the ECEM code. Section 7.5 provides a more complete set of example STOCHASTIC keywords. Table 7.16 provides the example keywords grouped by variable type.

Table 7.16 Cross Reference to Example STOCHASTIC Keywords for the ECEM Code

Dependencies	Cross Reference
Analyte, Species	Table 7.19 Example ECEM Keywords for the Growth Model for Terrestrial Animals
Analyte	Table 7.20 Example ECEM Keywords for the Root Uptake Model for Terrestrial Plants
Species	Table 7.21 Example ECEM Keywords for the Time Fraction Aquatic Animals Spend Above Water
Analyte, Species	Table 7.22 Example ECEM Keywords for the Depuration Rate for Animal Species
Analyte, Species	Table 7.23 Example ECEM Keywords for the Chemical Assimilation for Aquatic Animal Species
Analyte, Species	Table 7.24 Example ECEM Keywords for the Bioconcentration Factor for Aquatic Animal Species

Dependencies	Cross Reference
Analyte, Species	Table 7.25 Example ECEM Keywords for the Metabolism Loss Rate for Aquatic Species
Species	Table 7.26 Example ECEM Keywords for Plant-Air Partition Coefficients
Species	Table 7.27 Example ECEM Keywords for the Fraction of Time Aquatic Species Spend in Pore Water

7.4.19 THRESHOLD Keyword for the ECEM Code

As an optional calculation, up to two threshold values can be provided by the user to compare against calculated doses and body burdens. The values of the thresholds are entered using the THRESHOLD keyword. Two types of thresholds can be supplied – at the analyte level or at the sum of radioactive doses level. A "SUMRAD" entry associated with the TYPE modifier is used to define thresholds for total radioactive dose by a species. For all other modifiers, the thresholds apply by analyte and species combination. The following is this keyword's syntax:

```
THRESHOLD [TYPE="quote1"] [SPECIES="quote2"] {ANALYTE="quote3"}
   {LIMIT1=value1} {LIMIT2=value2}
```

Table 7.17 describes the modifiers for the THRESHOLD keyword.

Table 7.17 Modifiers Associated with the THRESHOLD Keyword in the ECEM Code

Modifier	Description
ANALYTE	The quote string associated with the ANALYTE modifier must contain an analyte ID. If the SUMRAD modifier is used, the ANALYTE modifier should be omitted (it is ignored). The analyte ID must match with one of the analytes in the ESD keyword file.
SPECIES	The quote string associated with the SPECIES modifier must contain a plant or animal species ID. This ID identifies the species for which this threshold applies.
TYPE	The quote string associated with the TYPE modifier identifies the type of solution for this threshold calculation. The following are valid entries for the quote string: • BURDEN: Body burden (tissue concentration) • DOSDER: Dermal dose • DOSRAD: Radioactive dose • DOSING: Ingestion dose • DOSINH: Inhalation dose • DOSDER: Dermal dose • SUMRAD: Sum of the radionuclide dose over analytes
LIMIT1	The numerical value associated with the LIMIT1 modifier identifies a user-specified threshold for calculation of an exceedance probability. The limit is applicable to a specific combination of solution type, species, and analyte.

Modifier	Description
LIMIT2	The numerical value associated with the LIMIT2 modifier identifies a user-specified threshold for calculation of an exceedance probability. The limit is applicable to a specific combination of solution type, species, and analyte. Use the LIMIT1 modifier to define a single limit value.

An example of a set of THRESHOLD keywords is given in the following:

```
THRESHOLD TYPE="BURDEN" ANALYTE="C14"  SPECIES="CHCATF"
   LIMIT1=0.005  LIMIT2=0.01
THRESHOLD TYPE="DOSRAD" ANALYTE= "C14"  SPECIES= "CHCATF"
   LIMIT1=0.04  LIMIT2=0.065
THRESHOLD TYPE="SUMRAD" SPECIE="CHCATF" LIMIT1=23.4
```

7.4.20 THROTTLE Keyword for the ECEM Code

The optional THROTTLE keyword allows the user to define a suite of analytes to run and then reduce the number that are being run. The reduction on the set of analytes occurs after all random sampling has been performed but before any species related calculations are performed. In essence, this allows calculations to be separated into a series of runs while maintaining the same statistical sampling sequences for all the runs. The following is this keyword's syntax:

```
THROTTLE ["quote1"] {"quote2"} … {"quoten"n}
```

Each quote string must identify an analyte ID entered using an ANALYTE keyword. If an ID is present on this keyword then calculations for it are deactivated after them statistical sampling is complete.

There are no modifiers or numerical entries associated with the THROTTLE keyword.

7.4.21 TIMES Keyword for the ECEM Code

The TIMES keyword identifies the times at which the calculations are to be performed. The following is this keyword's syntax:

```
TIMES [ [T1] {T2} … {Tn} | {ALL} ]
```

The numerical entries T1, T2, …, Tn are the times (whole number years) when outputs are desired. These times must be a subset of the times at which environmental data were computed and stored by the inventory, release, and transport modules. Multiple TIMES keywords can be entered. If the modifier ALL is used, results will be calculated for every time in the ESD keyword file. If the modifier ALL is used, no numerical values should be entered. The following is an example TIMES keyword that requests output for the three years 2020, 2075, and 3014:

```
TIMES 2020 2075 3014
```

There are no quote strings associated with the TIMES keyword.

7.4.22 TITLE Keyword for the ECEM Code

The TITLE keyword is used to define a single-line problem title. The problem title will be written to output files. If the title is not supplied, then the program will error terminate. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 72 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the Ecological impacts code."
```

There are no modifiers associated with the TITLE keyword.

7.4.23 USER Keyword for the ECEM Code

The USER keyword is used to identify the user of the program. The user name will be written to output files. If the user name is not supplied, then the program will error terminate. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

There are no modifiers associated with the USER keyword.

7.4.24 VARIABLE Keyword for the ECEM Code

The VARIABLE keyword is used to enter values for several variables that are constant rather than stochastic. The following is this keyword's syntax:

```
VARIABLE {COWHDFX=V1} {EXPOSI=V2} {GASCON=V3} {RFRAC=V4}
   {AREA=V5} {LENGTH=V6} {TP_BMR=v7 [TP_UNITS="quote_tp"]}
   {TA_BMR=v8 [TA_UNITS="quote_ta"]} {QP_BMR=v9 [QP_UNITS="quote_qp"]}
   {QA_BMR=v10 [QA_UNITS="quote_qa"]}
```

Table 7.18 describes the modifiers associated with the VARIABLE keyword. Multiple VARIABLE keywords can be entered, each with a portion of the modifiers. If a modifier is entered more than once, the last definition is the one used in the calculations.

Table 7.18 Modifiers Associated with the VARIABLE Keyword in the ECEM Code

Modifier	Description
AREA	The numerical value associated with the AREA modifier defines the area of contamination for terrestrial plants and animals (m^2). This value is used in the equations for computing particulate concentrations in air.
COWHDFX	The numerical value associated with the COWHDFX modifier defines the value of the Cowherd function for terrestrial plants and animals (unitless). This value is used in computing particulate concentrations in air.

Modifier	Description
EXPOSI	The numerical value associated with the EXPOSI modifier defines the exposure interval (seconds) for terrestrial plants and animals exposed to gas-phase contaminants. A typical value is an entire year.
GASCON	The numerical value associated with the GASCON modifier defines the universal gas constant (pascal-m^3/mole-K) used in terrestrial plant calculations.
LENGTH	The numerical value associated with the LENGTH modifier defines the length of side of contaminated area for terrestrial plants and animals (m). This value is used in the equations for computing particulate concentrations in air.
RFRAC	The numerical value associated with the RFRAC modifier defines the respirable fraction of particulates in air for terrestrial plants and animals (gram/m^2-hr). This value is used in the equations for computing particulate concentrations in air.
TA_BMR	The numerical value associated with the TA_BMR modifier gives the value of the benchmark value for radiation dose to terrestrial animals. The typical value is 0.1 rad/day. This numerical value must be paired with the TA_UNITS modifier to identify the units for the radiation dose benchmark.
TA_UNITS	The quote string associated with the TA_UNITS identifies the units associated with the TA_BMR benchmark value. The only valid entry is "rad/day".
TP_BMR	The numerical value associated with the TP_BMR modifier gives the value of the benchmark value for radiation dose to terrestrial plants. The typical value is 1.0 rad/day. This numerical value must be paired with the TP_UNITS modifier to identify the units for the radiation dose benchmark.
TP_UNITS	The quote string associated with the TP_UNITS identifies the units associated with the TP_BMR benchmark value. The only valid entry is "rad/day".
QA_BMR	The numerical value associated with the QA_BMR modifier gives the value of the benchmark value for radiation dose to aquatic animals. The typical value is 1.0 rad/day. This numerical value must be paired with the QA_UNITS modifier to identify the units for the radiation dose benchmark.
QA_UNITS	The quote string associated with the AA_UNITS identifies the units associated with the QA_BMR benchmark value. The only valid entry is "rad/day".
QP_BMR	The numerical value associated with the QP_BMR modifier gives the value of the benchmark value for radiation dose to aquatic plants. The typical value is 1.0 rad/day. This numerical value must be paired with the QP_UNITS modifier to identify the units for the radiation dose benchmark.
QP_UNITS	The quote string associated with the QP_UNITS identifies the units associated with the QP_BMR benchmark value. The only valid entry is "rad/day".

The following are example keywords defining this suite of variables for terrestrial plants:

```
VARIABLE COWHDFX    0.0497 EXPOSI=7.9E+8
VARIABLE GASCON     8.314
```

```
VARIABLE RFRAC      0.036
VARIABLE AREA=500.0  LENGTH=1000.0
```

The following are example keywords defining this suite of variables for radiation dose benchmarks for all plant and animal species. These keywords are only needed if the BMRDOS solution is selected on the DETAILS or STATISTIC keywords.:

```
VARIABLE TP_BMR=1.0 TP_UNITS="rad/day"
VARIABLE TA_BMR=0.1 TA_UNITS="rad/day"
VARIABLE QP_BMR=1.0 QP_UNITS="rad/day"
VARIABLE QA_BMR=1.0 QA_UNITS="rad/day"
```

7.5 Example Stochastic Keywords for the ECEM Code

Typically, a large number of STOCHASTIC keywords are needed for a run of the ECEM code. For example, one run of the code with 10 analytes and 57 species required 4085 STOCHASTIC keywords. The exact number of keywords for a run depends on the number and type of analytes and the number and type of species. The general description of a STOCHASTIC keyword for the ECEM code is provided in Section 7.4.17. Additional information about statistical distributions is provided in Section 19.0.

The general description of the STOCHASTIC keyword uses two quote strings. The first quote string is used to associate a specific statistical distribution to a variable in the code. The second quote string is a descriptive phrase used only for labeling purposes in output files. The first quote string, which must be unique, is a combination of analyte ID, species ID, and variable name. Character case and embedded spaces change the definition of the quote string. Table 7.19 gives example keywords for terrestrial species for a number of variables. In each case, the first quote string is the concatenation of the analyte ID (blank padded to six characters in length if necessary), the species ID (blank padded to six characters in length if necessary), and a variable name.

The first two example keywords in the table define the inhalation absorption factor (ALPHAVAP or α_{vapi}) for terrestrial animals (see Section 7.1.1.2.4). The second set of two example keywords defines the inhalation particulate absorption factor (ALPHAPAR or α_{pari}) for terrestrial animals (see Section 7.1.1.2.5). The third set of two example keywords defines the ingestion absorption factor (ALPHAING or α_{ingi}) for terrestrial animals (see Section 7.1.1.2.7). The fourth set of two example keywords defines the dermal permeability for soil (ALPHADS or α_{dci}) for terrestrial animals (see Section 7.1.1.2.1). The fifth set of two example keywords defines the dermal absorption for water (ALPHADW or K_{pi}) for terrestrial animals (see Section 7.1.1.2.2). If there were 10 analytes and 17 terrestrial animals, then five groups of 170 STOCHASTIC keywords would be required instead of the five groups of two example keywords.

Table 7.19 Example ECEM Keywords for the Growth Model for Terrestrial Animals

Analyte	Species	Variable	Description	Units	Statistical Distribution
CCl4	AMCOOT	ALPHAVAP (α_{vapi})	Inhalation absorption factor for CCl4 and AMCOOT	unitless	Triangular on Lower Limit .36, Mode .4, Upper Limit .44
`STOCHASTIC "CCl4 AMCOOTALPHAVAP" 6 3.600E-01 4.000E-01 4.400E-01 "Inhalation absorption factor for CCl4 and AMCOOT"`					
Cs137	COYOTE	ALPHAVAP (α_{vapi})	Inhalation absorption factor for Cs137 and COYOTE	unitless	Triangular on Lower Limit .421, Mode .468, Upper Limit .515
`STOCHASTIC "Cs137 COYOTEALPHAVAP" 6 4.21E-01 4.68E-01 5.15E-01 "Inhalation absorption factor for Cs137 and COYOTE"`					
CCl4	AMCOOT	ALPHAPAR (α_{pari})	Inhalation particulate absorption factor for CCl4 and AMCOOT	unitless	Triangular on Lower Limit .36, Mode .4, Upper Limit .44
`STOCHASTIC "CCl4 AMCOOTALPHAPAR" 6 3.600E-01 4.000E-01 4.400E-01 "Inhalation particulate absorption factor for CCl4 and AMCOOT"`					
CrVI	CARP	ALPHAPAR (α_{pari})	Inhalation particulate absorption factor for CrVI and CARP	unitless	Triangular on Lower Limit .288, Mode .32, Upper Limit .352
`STOCHASTIC "CrVI CARP ALPHAPAR" 6 2.88E-01 3.20E-01 3.52E-01 "Inhalation particulate absorption factor for CrVI and CARP"`					
AMCOOT		ALPHAING (α_{ingi})	Ingestion absorption factor for CCl4 and AMCOOT	unitless	Triangular on Lower Limit .585, Mode .65, Upper Limit .715
`STOCHASTIC "CCl4 AMCOOTALPHAING" 6 5.850E-01 6.500E-01 7.150E-01 "Ingestion absorption factor for CCl4 and AMCOOT"`					
CrVI	CARP	ALPHAING (α_{ingi})	Ingestion absorption factor for CrVI and CARP	Unitless	Triangular on Lower Limit .027, Mode .03, Upper Limit .033

Analyte	Species	Variable	Description	Units	Statistical Distribution
STOCHASTIC "CrVI CARP ALPHAING" 6 2.70E-02 3.00E-02 3.30E-02 "Ingestion absorption factor for CrVI and CARP"					
CCl4	AMCOOT	ALPHADS (α_{dci})	Dermal permeability (soil) for CCl4 and AMCOOT	unitless	Triangular on Lower Limit .009, Mode .01, Upper Limit .011
STOCHASTIC "CCl4 AMCOOTALPHADS " 6 9.000E-03 1.000E-02 1.100E-02 "Dermal permeability (soil) for CCl4 and AMCOOT"					
CrVI	CARP	ALPHADS (α_{dci})	Dermal permeability (soil) for CrVI and CARP	unitless	Triangular on Lower Limit .0031, Mode .00344, Upper Limit .00378
STOCHASTIC "CrVI CARP ALPHADS " 6 3.10E-03 3.44E-03 3.78E-03 "Dermal permeability (soil) for CrVI and CARP"					
CCl4	AMCOOT	ALPHADW (K_{pi})	Dermal absorption (water) for CCl4 and AMCOOT	cm/hr	Triangular on Lower Limit .0198, Mode .022, Upper Limit .0242
STOCHASTIC "CCl4 AMCOOTALPHADW " 6 1.980E-02 2.200E-02 2.420E-02 "Dermal absorption (water) for CCl4 and AMCOOT"					
Cs137	COYOTE	ALPHADW (K_{pi})	Dermal absorption (water) for Cs137 and COYOTE	cm/hr	Constant 0
STOCHASTIC "Cs137 COYOTEALPHADW " 1 0 "Dermal absorption (water) for Cs137 and COYOTE"					

The model for converting root uptake of analytes to above-ground plant-tissue concentrations requires a value for the log base 10 of the octanol-water partitioning coefficient (KOW or K_{ow}) (see Section 7.1.1.1.2). A STOCHASTIC keyword for the KOW variable is needed for every combination of terrestrial plant species and analyte. Table 7.20 provides example keywords for this variable. The first quote string for the STOCHASTIC keywords would hold the concatenation of the analyte ID (blank padded to six characters long, if necessary) and the variable name KOW. A STOCHASTIC keyword is also needed for every combination of terrestrial plant and analytes for the bioconcentration factor for vegetation (BCFVEG or Bv) (see Section 7.1.1.1.2). The first quote string for the STOCHASTIC keywords for bioconcentration values would hold the concatenation of the analyte ID (blank padded to six characters long, if necessary) and the variable name BCFVEG.

Table 7.20 Example ECEM Keywords for the Root Uptake Model for Terrestrial Plants

Analyte	Variable	Description	Units	Statistical distribution
CCl4	K_{ow}	Log base 10 of the octanol-water partition coefficient for CCl4	Unitless	Normal with a mean of 2.629, Standard deviation of 0.645
`STOCHASTIC "CCl4 KOW" 7 2.627 0.645` `"Log base 10 of the octanol-water partition coefficient for CCl4"`				
CrVI	K_{ow}	Log base 10 of the octanol-water partition coefficient for CrVI	Unitless	Constant 0.0
`STOCHASTIC "CrVI KOW" 1 0.0` `"Log base 10 of the octanol-water partition coefficient for CrVI"`				
Sr90	BCFVEG (Bv)	Bioconcentration factor for Sr90 in vegetation	kg-soil/kg-dry-plant	Triangular on Lower Limit 14.2, Mode 15.8, Upper Limit 17.4
`STOCHASTIC "Sr90 BCFVEG" 6 1.42E+01 1.58E+01 1.74E+01` `"Bioconcentration factor for Sr90 in vegetation"`				
Tc99	BCFVEG (Bv)	Bioconcentration factor for Tc99 in vegetation	kg-soil/kg-dry-plant	Triangular on Lower Limit 19.1, Mode 21.2, Upper Limit 23.3
`STOCHASTIC "Tc99 BCFVEG" 6 1.91E+01 2.12E+01 2.33E+01` `"Bioconcentration factor for Tc99 in vegetation"`				

Calculation of the external dose from contact with sediment for aquatic species requires information about the fraction of time the species spends above water. The equation for this calculation is given in Section 7.1.3.5. A distinct STOCHASTIC keyword is needed for every aquatic species for this variable, and three examples are given in Table 7.21. The first quote string for the STOCHASTIC keywords would hold the concatenation of the species ID (blank padded to six characters long, if necessary) and the variable name FABOVE.

Table 7.21 Example ECEM Keywords for the Time Fraction Aquatic Animals Spend Above Water

Species	Variable	Description	Units	Statistical Distribution
AMCOOT	FABOVE	Fraction of time spent above water for AMCOOT	Unitless	Constant 1.0
`STOCHASTIC "AMCOOTFABOVE" 1 1.0` `"Fraction of time spent above water for AMCOOT"`				
AMKSTL	FABOVE	Fraction of time spent above water for AMKSTL	Unitless	Constant 1.0
`STOCHASTIC "AMKSTLFABOVE" 1 1.0` `"Fraction of time spent above water for AMKSTL"`				

Calculation of doses for animal species from dermal contact with contaminants is dependent on the depuration rate of the species (see Section 7.1.1.2.1). A distinct STOCHASTIC keyword is needed for every animal species for this variable, and three examples are given in Table 7.22. The first quote string for the STOCHASTIC keywords would hold the concatenation of the analyte ID (blank padded to six characters in length, if necessary), the species ID (blank padded to 6 characters in length, if necessary) and the variable name DEPRATE.

Table 7.22 Example ECEM Keywords for the Depuration Rate for Animal Species

Analyte	Species	Variable	Description	Units	Statistical Distribution
CCl4	AMCOOT	DEPRATE (K_{ei})	Depuration rate of AMCOOT for CCl4	1/day	Triangular on Lower Limit .765, Mode .85, Upper Limit .935
`STOCHASTIC "CCl4 AMCOOTDEPRATE" 6 7.650E-01 8.500E-01 9.350E-01 "Depuration rate of AMCOOT for CCl4"`					
CrVI	CARP	DEPRATE (K_{ei})	Depuration rate of CARP for CrVI	1/day	Triangular on Lower Limit .0468, Mode .052, Upper Limit .0572
`STOCHASTIC "CrVI CARP DEPRATE" 6 4.680E-02 5.200E-02 5.720E-02 "Depuration rate of CARP for CrVI"`					
Cs137	COYOTE	DEPRATE (K_{ei})	Depuration rate of COYOTE for Cs137	1/day	Triangular on Lower Limit .072, Mode .08, Upper Limit .088
`STOCHASTIC "Cs137 COYOTEDEPRATE" 6 7.200E-02 8.000E-02 8.800E-02 "Depuration rate of COYOTE for Cs137"`					

Calculation of the body burden for aquatic animal species is dependent on the chemical assimilation of contaminants for the species (see Section 7.1.2.1). A distinct STOCHASTIC keyword is needed for every animal species for this variable, and three examples are given in Table 7.23. The first quote string for the STOCHASTIC keywords would hold the concatenation of the analyte ID (blank padded to six characters long, if necessary), the species ID (blank padded to six characters in length, if necessary), and the variable name ALPHAIJ.

Table 7.23 Example ECEM Keywords for the Chemical Assimilation for Aquatic Animal Species

Analyte	Species	Variable	Description	Units	Statistical Distribution
CCl4	CARP	ALPHAIJ (α_{ij})	Chemical assimilation efficiency of CARP for CCl4	g contaminant assimilated per g contaminant ingested	Constant 1
`STOCHASTIC "CCl4 CARP ALPHAIJ" 1 1 "Chemical assimilation efficiency of CARP for CCl4"`					

Analyte	Species	Variable	Description	Units	Statistical Distribution
CrVI	CHCATF	ALPHAIJ (α_{ij})	Chemical assimilation efficiency of CHCATF for CrVI	g contaminant assimilated per g contaminant ingested	Triangular on Lower Limit .027, Mode .03, Upper Limit .033
`STOCHASTIC "CrVI  CHCATFALPHAIJ" 6  2.700E-02  3.000E-02 3.300E-02 "Chemical assimilation efficiency of CHCATF for CrVI"`					
CrVI	CLAMS	ALPHAIJ (α_{ij})	Chemical assimilation efficiency of CLAMS for CrVI	g contaminant assimilated per g contaminant ingested	Triangular on Lower Limit .0243, Mode .027, Upper Limit .0297
`STOCHASTIC "CrVI  CLAMS ALPHAIJ" 6  2.430E-02  2.700E-02 2.970E-02 "Chemical assimilation efficiency of CLAMS for CrVI"`					

Calculation of the body burden for aquatic animal species is dependent on the bioconcentration factor of contaminants for the species (see Section 7.1.2.1). A distinct STOCHASTIC keyword is needed for every combination of animal species and inorganic analyte for this variable, and three examples are given in Table 7.24. The first quote string for the STOCHASTIC keywords would hold the concatenation of the analyte ID (blank padded to six characters long, if necessary), the species ID (blank padded to six characters long, if necessary), and the variable name BCF.

Table 7.24 Example ECEM Keywords for the Bioconcentration Factor for Aquatic Animal Species

Analyte	Species	Variable	Description	Units	Statistical Distribution
CrVI	CARP	BCF	Bioconcentration factor of CARP for CrVI	L/kg	Triangular on Lower Limit .018, Mode .02, Upper Limit .022
`STOCHASTIC "CrVI  CARP  BCF" 6  1.800E-02  2.000E-02 2.200E-02 "Bioconcentration factor of CARP for CrVI"`					
CrVI	CPBLSN	BCF	Bioconcentration factor of CPBLSN for CrVI	L/kg	Triangular on Lower Limit .09, Mode .1, Upper Limit .11
`STOCHASTIC "CrVI  CPBLSNBCF" 6  9.000E-02  1.000E-01 1.100E-01 "Bioconcentration factor of CPBLSN for CrVI"`					
U238	MAYFLY	BCF	Bioconcentration factor of MAYFLY for U238	L/kg	Triangular on Lower Limit .000279, Mode .00031, Upper Limit .000341
`STOCHASTIC "U238  MAYFLYBCF" 6  2.790E-04  3.100E-04 3.410E-04 "Bioconcentration factor of MAYFLY for U238"`					
CrVI	CPBLSN	BCF	Bioconcentration factor of CPBLSN for CrVI	L/kg	Triangular on Lower Limit .09, Mode .1, Upper Limit .11
`STOCHASTIC "CrVI  CPBLSNBCF" 6  9.000E-02  1.000E-01 1.100E-01 "Bioconcentration factor of CPBLSN for CrVI"`					

Analyte	Species	Variable	Description	Units	Statistical Distribution
U238	MAYFLY	BCF	Bioconcentration factor of MAYFLY for U238	L/kg	Triangular on Lower Limit .000279, Mode .00031, Upper Limit .000341
STOCHASTIC "U238 MAYFLYBCF" 6 2.790E-04 3.100E-04 3.410E-04 "Bioconcentration factor of MAYFLY for U238"					

Calculation of the body burden for aquatic animal species is dependent on the metabolism loss rate of the analyte for the species (see Section 7.1.2.1). A distinct STOCHASTIC keyword is needed for every combination of animal species analyte for this variable, and three examples are given in Table 7.25. The first quote string for the STOCHASTIC keywords would hold the concatenation of the analyte ID (blank padded to six characters long, if necessary), the species ID (blank padded to six characters long, if necessary), and the variable name METBLOSS.

Table 7.25 Example ECEM Keywords for the Metabolism Loss Rate for Aquatic Species

Analyte	Species	Variable	Description	Units	Statistical Distribution
CCl4	CARP	METBLOSS (K_{mi})	Metabolism loss rate for CCl4 in CARP	1/day	Constant 0
STOCHASTIC "CCl4 CARP METBLOSS" 1 0 "Metabolism loss rate for CCl4 in CARP"					
Cs137	MAYFLY	METBLOSS (K_{mi})	Metabolism loss rate for Cs137 in MAYFLY	1/day	Constant 0
STOCHASTIC "Cs137 MAYFLYMETBLOSS" 1 0 "Metabolism loss rate for Cs137 in MAYFLY"					
I129	MAYFLY	METBLOSS (K_{mi})	Metabolism loss rate for I129 in MAYFLY	1/day	Constant 0
STOCHASTIC "I129 MAYFLYMETBLOSS" 1 0 "Metabolism loss rate for I129 in MAYFLY"					

The calculation of body burden for terrestrial plants includes the plant-air partition coefficient for air to above-ground plant parts for particulate-bound contaminants (K_{pa2}) and the plant-soil partition coefficient for rain splash (K_{ps1}). See Section 7.1.1.1.4 for a description of K_{pa2} and Section 7.1.1.1.1 for a description of K_{ps1}. A distinct STOCHASTIC keyword is needed for every terrestrial plant species analyte for this variable, and two examples are given in Table 7.26. The first quote string for the STOCHASTIC keywords would hold the concatenation of the species ID (blank padded to six characters long, if necessary) and the variable name KPS1 or KPA2.

Table 7.26 Example ECEM Keywords for Plant-Air Partition Coefficients

Species	Variable	Description	Units	Statistical Distribution
BLCTWD	KPS1	Plant-soil partition coefficient for BLCTWD	kg soil/kg plant wet wt	Triangular on Lower Limit .00306, Mode .0034, Upper Limit .00374
`STOCHASTIC "BLCTWDKPS1 " 6 3.060E-03 3.400E-03 3.740E-03 "Plant-Soil partition coefficient for BLCTWD"`				
BLCTWD	KPA2	Plant-air partition coefficient for BLCTWD	m^3/kg wet weight	Triangular on Lower Limit 2,970; Mode 3,300; Upper Limit 3,630
`STOCHASTIC "BLCTWDKPA2 " 6 2.970E+03 3.300E+03 3.630E+03 "Plant-Air partition coefficient for BLCTWD"`				

The calculation of body burden for aquatic species depends on the fraction of the time the species spends in pore water (see Section 7.1.2.1). A distinct STOCHASTIC keyword is needed for every aquatic species for this variable, and two examples are given in Table 7.27. The first quote string for the STOCHASTIC keywords would hold the concatenation of the species ID (blank padded to six characters long, if necessary) and the variable name BPORE.

Table 7.27 Example ECEM Keywords for the Fraction of Time Aquatic Species Spend in Pore Water

Species	Variable	Description	Units	Statistical Distribution
CARP	BPORE	Relative exposure time to pore water for CARP	unitless	Triangular on Lower Limit .045, Mode .05, Upper Limit .055
`STOCHASTIC "CARP BPORE " 6 4.500E-02 5.000E-02 5.500E-02 "Relative exposure time to pore water for CARP"`				
CHCATF	BPORE	Relative exposure time to pore water for CHCATF	unitless	Triangular on Lower Limit .09, Mode .1, Upper Limit .11
`STOCHASTIC "CHCATFBPORE " 6 9.000E-02 1.000E-01 1.100E-01 "Relative exposure time to pore water for CHCATF"`				

8.0 FCDA_ASCII – Food Concentration Data File Conversions

8.1 Overview

The FCDA_ASCII program converts binary food concentration files into text format. The sole purpose of the conversion is to create a file that is human readable in a text editor.

8.1.1 Location in the Processing Sequence

The FCDA_ASCII can be executed any time after the ECEM code has created food concentration data files.

8.1.2 How the Code Is Invoked

FCDA_ASCII can run under either the Windows or the Linux operating system. Under the Windows operating system (Releases XP or 7), ECDA_ASCII executes in a DOS box. A run of FCDA_ASCII is initiated by entering the following command line:

```
FCDA_ASCII
```

Under the Linux operating system FCDA_ASCII is executed through any of the following Bourne Shell or C Shell commands:

```
fcda_ascii.exe
```

For these commands, "FCDA_ASCII .EXE" or "fcda_ascii.exe" is the name of the executable program.

8.1.3 Memory Requirements

The FCDA_ASCII code uses dynamic memory allocation. However, only one line of the input file is in memory at any given time, so the memory requirements are minimal. It is expected that most, if not all, of the runs of the FCDA_ASCII code will require less than 2 MB of memory.

8.2 File Definitions

The FCDA_ASCII code reads one file and writes one file.

8.2.1 Input Files

The FCDA_ASCII code reads a food concentration data accumulator (FCDA) file. This file is in binary format and is created by the ECEM program.

8.2.2 Output Files

The FCDA_ASCII code writes one data file. This file is a text translation of the binary FCDA file. An example of the first 20 lines of the output text file for a file is provided in Table 8.1. The numbers in the left column are record numbers that are not in the original data set. The file starts with an analyte

identifier followed by species identifier and the location type identifier. This file only contained one realization of data.

Table 8.1 Excerpts from an FCDA_ASCII Output File

```
File: N:\CA1_median\foods\Food_C14_UUPIGS.fod
      1 C14
      2 UUPIGS
      3 UPLAND
      4    1945 UH0001  1.85791E+00
      5    1945 UH0001  1.85791E+00
      6    1945 UH0001  1.85791E+00
      7    1945 UH0002  1.85791E+00
      8    1945 UH0002  1.85791E+00
      9    1945 UH0002  1.85791E+00
     10    1945 UH0003  1.85791E+00
     11    1945 UH0003  1.85791E+00
     12    1945 UH0003  1.85791E+00
     13    1945 UH0004  1.39627E+00
     14    1945 UH0004  1.39627E+00
     15    1945 UH0004  1.39627E+00
     16    1945 UH0005  1.39627E+00
     17    1945 UH0005  1.39627E+00
     18    1945 UH0005  1.39627E+00
     19    1945 UH0006  1.85791E+00
```

8.3 Code Execution

The FCDA_ASCII program runs in an interactive mode. A screen image from a run of the code on a Windows machine is provided in Figure 8.1. The user must provide answers to five prompts:

1. The name of the binary FCDA file must be provided. A full pathname is required unless the FCDA file is in the same directory where the FCDA_ASCII code was invoked.
2. The name of the output ASCII file must be provided. The user can select any name that is not identical to the input file name. An extension of ".txt" is recommended.
3. The number of realizations for the simulation must be provided.
4. The location ID's to be translated must be identified. Enter ALL to translate data for every location in the simulation. Enter a specific location ID to translate data for just one location.
5. The number of data records to be translated must be provided. Care must be taken when translating a large FCDA file such that the output file does not exceed 2.1 gigabytes in size. If the output file exceeds that size, the program will error terminate.

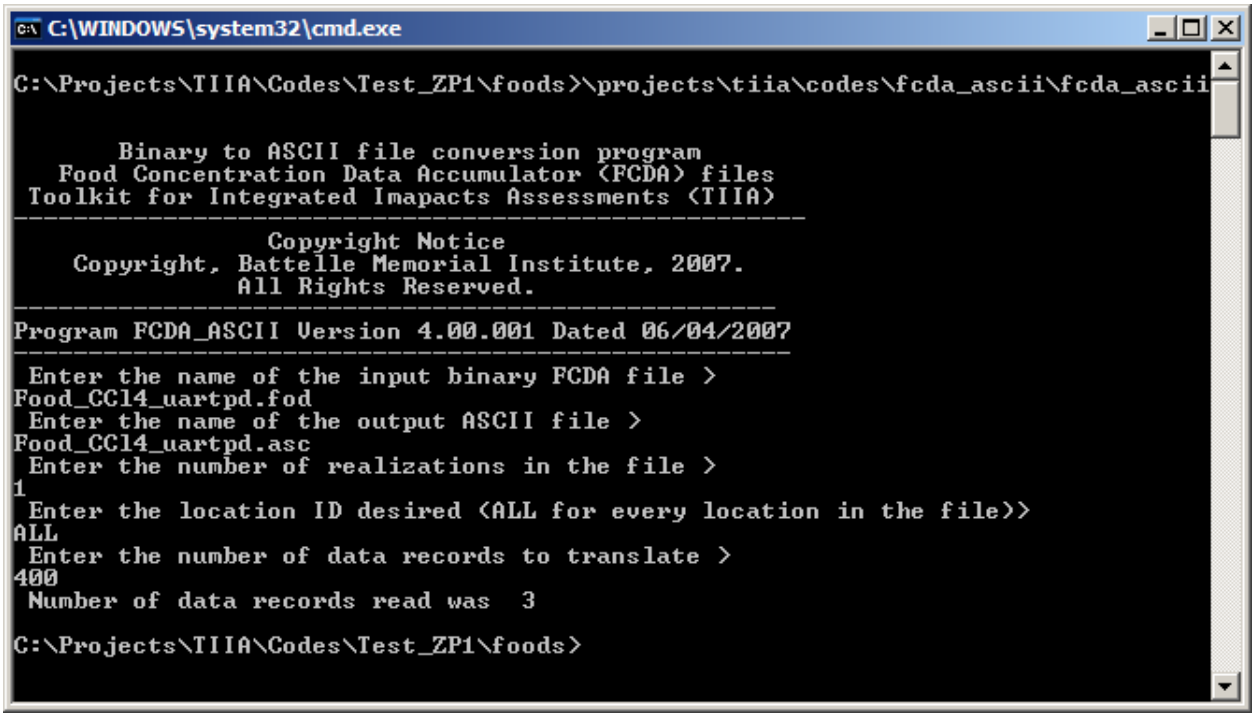

Figure 8.1 Screen Image of an FCDA_ASCII Run

9.0 FILLECDA – Environmental Concentration Data File Modifications

9.1 Overview

The ECDA program creates environmental concentration data accumulator (ECDA) files and initializes the contents. Other programs (RIPSAC, and SOIL) can then fill in the concentration values for different media. The FILLECDA program provides the capability to insert user-specified concentration values into any record in an ECDA file. These values can be entered as explicit deterministic values or they can be defined as statistical distributions.

9.1.1 Location in the Processing Sequence

The FILLECDA program can be used any time after the ECDA files are created by the ECDA program.

9.1.2 How the Code Is Invoked

FILLECDA can run under either the Windows or the Linux operating system. Under the Windows operating system (Releases XP or 7), FILLECDA executes in a DOS box. A run of FILLECDA is initiated by entering the following command line:

```
FILLECDA "Keyfilename"
```

Under the Linux operating system FILLECDA is executed through any of the following Bourne Shell or C Shell commands:

```
fillecda-1.exe "Keyfilename"
```

For these commands, “FILLECDA.EXE” or “fillecda-1.exe” is the name of the executable program, and “Keyfilename” is the name of a control keyword file. Both the name of the executable program and the keyword file may contain path information. If FILLECDA is invoked without entering the name of the keyword file, then the code will prompt the user for the file name. The keyword file, which should be prepared using an editor that can handle ASCII files without leaving embedded control codes, contains text control information describing the run. If FILLECDA cannot open the keyword file, then the code will terminate execution after writing an error message to the standard output device.

9.1.3 Memory Requirements

The FILLECDA program has minimal memory requirements. The memory is small because data for only a single record of an ECDA file is generated and written at any one time.

9.2 File Definitions

The FILLECDA program reads three input files and writes to two or more output files. These files are described in the following paragraphs.

9.2.1 Input Files

9.2.2 FILLECDA Keyword File

The FILLECDA keyword file contains control information and also defines the concentration values to be inserted in the ECDA files. An example file is provided in Table 9.1. Detailed definitions of the keywords are provided in Section 9.3.

Table 9.1 Example Keyword File for the FILLECDA Program

```
REPORT "FillECDA_Test01.Rpt"        ! Report file name (first keyword)
TITLE "Test FillECDA - Case Test01" ! Title for labeling purposes
USER "Paul W. Eslinger"             ! User name for labeling purposes
FILE ESD "ESD_Test01.key"           ! Name of the ESD keyword file
REALIZAT 5                          ! Number of realizations
VERBOSE DEFINITIONS STATISTICS      ! Activate data echo
SEED 5555                           ! Random seed for Stochastic data
!
DATA LOCATION="UH0002" ANALYTE="CCl4"   YEAR=2010 MEDIA="GWAT"
  VALUES=1.4 1.41 1.42 1.43 1.44
DATA LOCATION="UH0072" ANALYTE="CCl4"   YEAR=2010 MEDIA="SOSW"
  VALUES=1.5 1.51 1.52 1.53 1.54
DATA LOCATION="UH0072" ANALYTE="CCl4"   YEAR=2000 MEDIA="GWAT"
  VALUES=2.3 2.31 2.32 2.33 2.34
DATA LOCATION="UH0154" ANALYTE="CCl4"   YEAR=2010 MEDIA="SOGW"
  STOCHASTIC 2 1.6 1.64
DATA LOCATION="UH0154" ANALYTE="NITRAT" YEAR=2000 MEDIA="GWAT"
  VALUES=3.7 3.71 3.72 3.73 3.74
!
END
```

9.2.3 Other Input Files

The FILLECDA program also reads two other input files. These files are the ESD keyword file and the ECDA index file. The ESD keyword file contains the names of the concentration files that are to be modified. The ECDA map file contains index data related to writing to the ECDA concentration files.

9.2.4 Output Files

The code writes to two or more output files. These files are a report file and one or more ECDA concentration files.

9.2.4.1 FILLECDA Report File

The report file contains summary information from the run of the FILLECDA code. This file contains a record of the code version, time and date of run execution, input and output file names, run information, and a summary table of results. This file also contains any error messages generated by the FILLECDA code.

9.2.4.2 Concentration Files

The FILLECDA program writes some data to an ECDA file for every analyte identified on a DATA keyword in the FILLECDA keyword file.

9.3 Keyword Definitions for the FILLECDA Code

In general, the keywords for FILLECDA can be entered in any order. The only restriction is that the END keyword must be the last entry in the file.

9.3.1 DATA Keyword for FILLECDA

The DATA keyword is used to define the data values to be inserted into one or more ECDA files. Data values can be deterministic (all values entered explicitly) or they can be generated from a specified statistical distribution. The syntax for this keyword when deterministic data are entered is:

```
DATA [LOCATION="quote"] [MEDIA="quote"] [ANALYTE="quote"] [YEAR=number]
   [VALUES=number, …, number]
```

The syntax for this keyword when stochastic data are entered is:

```
DATA [LOCATION="quote"] [MEDIA="quote"] [ANALYTE="quote"] [YEAR=number]
   [STOCHASTIC=number, …, number]
```

This keyword identifies the data for all realizations of concentration for a specific analyte, location, media, and time combination. More than one DATA keyword can be entered. The modifiers for the DATA keyword are defined in Table 9.2.

Table 9.2 Modifiers Associated with the DATA Keyword in FILLECDA

Modifier	Description
ANALYTE	The quote string associated with the ANALYTE modifier contains the analyte ID for the concentration data values. The analyte ID must be one of the set of analytes defined in the ESD keyword file.
LOCATION	The quote string associated with the LOCATION modifier contains the location ID for the concentration data values. The location ID must be one of the set of locations defined in the ESD keyword file.
MEDIA	The quote string associated with the MEDIA modifier contains the media ID for the concentration data values. The media ID must be one of the following: GWAT, SEEP, SWAT, PWAT, SEDI, SORP, SODR, SOGW, SOSW, AIRC, or AIRD.
YEAR	The numerical value associated with the YEAR modifier identifies the calendar year at which the concentration data apply. The year entered must be one of the years defined on the TIMES keyword in the ESD keyword file.
VALUES	The numerical values associated with the VALUES modifier contain the data values to be entered in the ECDA file. There must be as many values entered as there are realizations defined in the ESD keyword file. Only one of the VALUES and STOCHASTIC modifiers can be used on a single keyword entry.

Modifier	Description
STOCHASTIC	The numerical values associated with the STOCHASTIC modifier contain information to define a statistical distribution.. The entries for defining a statistical distribution are explained in Section 19.1. Only one of the VALUES or STOCHASTIC modifiers can be used on a single DATA keyword entry.

If a DATA keyword does not identify a valid analyte, location, media, and time combination in the ECDA data file, then the information on that DATA keyword is discarded and an error message is written to the report file. Example entries for the DATA keyword for a case of two realizations are the following:

```
DATA LOCATION="EL01" ANALYTE="I129" YEAR=10000 MEDIA="SEEP" VALUES=1.1 1.3
DATA LOCATION="EL01" ANALYTE="U236" YEAR=10000 MEDIA="SORP" VALUES=1.2 1.4
DATA LOCATION="EL02" ANALYTE="U238" YEAR=10000 MEDIA="SWAT" VALUES=11 12
DATA LOCATION="EL02" ANALYTE="Tc99" YEAR=10000 MEDIA="SWAT" VALUES=11.1 10
DATA LOCATION="EL02" ANALYTE="Tc99" YEAR=10000
   MEDIA="PWAT" STOCHASTIC 2 23.0 27.5
```

9.3.2 END Keyword for FILLECDA

The END keyword signifies the end of all keyword data. Nominally it will be the last keyword in the keyword file. All data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

9.3.3 FILE Keyword for FILLECDA

The FILE keyword is used to enter the name of the ESD keyword file. The following is this keyword's syntax:

```
FILE [ESD="quote 1"]
```

The file name is entered in a quote string, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. An example of the use of this keyword follows:

```
FILE ESD="/home/ANALYSIS/practice-median/ESD_practice-median.key"
```

9.3.4 REALIZAT Keyword for FILLECDA

The REALIZ (or REALIZATION) keyword defines the number of realizations to process. The following is this keyword's syntax:

```
REALIZATION value1
```

This keyword gives the number of realizations of data that will be entered on each DATA record. The number must match exactly with the number of realizations in the ESD keyword file. The following keyword record sets the number of realizations to 10:

```
REALIZAT 10
```

9.3.5 REPORT Keyword for FILLECDA

The REPORT keyword is used to define the name of the output report (log) file. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The name of the report file is entered in a quote string. File names up to 200 characters long are supported, and path names can be included. The following is an example REPORT keyword record:

```
REPORT "/SAC/SystemCodes/Cultural/Test1.rpt"
```

9.3.6 SEED Keyword for FILLECDA

The SEED keyword sets the value for the seed for the random number generator. This keyword is required only if one or more DATA keywords define stochastic data. The following is this keyword's syntax:

```
SEED Value1
```

The value for Value1 must be an integer or real number in the range 1 to 999999. The following is an example keyword record:

```
SEED 344443
```

There are no modifiers or quote strings associated with the SEED keyword.

9.3.7 TITLE Keyword for FILLECDA

The TITLE keyword is used to define a single-line problem title. The problem title will be written to output files. If the title is not supplied, then the program will terminate with an error. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 200 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the FILLECDA code."
```

9.3.8 USER Keyword for FILLECDA

The USER keyword is used to identify the user of the program. The user name will be written to output files. If the user name is not supplied, then the program will error terminate. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

9.3.9 VERBOSE Keyword for FILLECDA

The presence of the optional VERBOSE keyword initiates additional output to the report file. The following is this keyword's syntax:

```
VERBOSE {DEFINITIONS} {STATISTICS}
```

Entry of the VERBOSE keyword without any modifiers causes the data inserted into the ECDA files to be written to the report file. If the DEFINITI modifier is used, the definitions of the statistical distributions are also written to the report file. If the STATISTICS modifier is used, summary statistics for the generated statistical distributions are also written to the report file.

10.0 FILLFCDA – Food Concentration Data File Modifications

10.1 Overview

The ECEM program creates food concentration data accumulator (FCDA) files containing concentrations in food products that are utilized in the HUMAN code. The FILLFCDA program provides the capability to insert user-specified concentration values into any record in an FCDA file. These values can be entered as explicit deterministic values or they can be defined as statistical distributions.

10.1.1 Location in the Processing Sequence

The FILLFCDA program can be used any time after the FCDA files are created by the ECEM program.

10.1.2 How the Code Is Invoked

FILLFCDA can run under either the Windows or the Linux operating system. Under the Windows operating system (Releases XP or 7), FILLFCDA executes in a DOS box. A run of FILLFCDA is initiated by entering the following command line:

```
FILLFCDA "Keyfilename"
```

Under the Linux operating system FILLFCDA is executed through any of the following Bourne Shell or C Shell commands:

```
fillfcda-1.exe "Keyfilename"
```

For these commands, “FILLFCDA.EXE” or “fillfcda-1.exe” is the name of the executable program, and “Keyfilename” is the name of a control keyword file. Both the name of the executable program and the keyword file may contain path information. If FILLFCDA is invoked without entering the name of the keyword file, then the code will prompt the user for the file name. The keyword file, which should be prepared using an editor that can handle ASCII files without leaving embedded control codes, contains text control information describing the run. If FILLFCDA cannot open the keyword file, then the code will terminate execution after writing an error message to the standard output device.

10.1.3 Memory Requirements

The FILLFCDA program has moderate memory requirements. The major memory driver is storing the information from all DATA keywords before any outputs are processed. If memory requirements become excessive, the problem can be subdivided into multiple runs, each using a subset of the data.

10.2 File Definitions

The FILLFCDA program reads three input files and writes to two or more output files. These files are described in the following paragraphs.

10.2.1 Input Files

10.2.1.1 FILLFCDA Keyword File

The FILLFCDA keyword file contains control information and also defines the concentration values to be inserted in the FCDA files. An example file is provided in Table 10.1. Detailed definitions of the keywords are provided in Section 10.3.

Table 10.1 Example Keyword File for the FILLFCDA Program

```
! Keyword file for the FillFCDA program
REPORT "Test.Rpt"                ! Report file name (first keyword)
TITLE "Test the FillFCDA Code"   ! Title for labeling purposes
USER "Paul W. Eslinger"          ! User name for labeling purposes
FILE ESD "ESD.Key"               ! Name of the ESD keyword file
REALIZAT 1                       ! Number of realizations
! Upland locations
DATA LOCATION="UH0002" ANALYTE="H3" YEAR=2150  SOIL="SOSW"
  SPECIES="UCATMT" VALUES=0.83482
DATA LOCATION="UH0002" ANALYTE="H3" YEAR=2150  SOIL="SOGW"
  SPECIES="UCATMT" VALUES=0.93036
DATA LOCATION="UH0002" ANALYTE="H3" YEAR=2150  SOIL="SODR"
  SPECIES="UCATMT" VALUES=0.98167
!
! Riparian Locations
DATA LOCATION="RHP001" ANALYTE="H3" YEAR=2100  SPECIES="RMLBRY"
  VALUES=0.63039
DATA LOCATION="RHP001" ANALYTE="H3" YEAR=2100  SPECIES="RMDEER"
  VALUES=0.01514
DATA LOCATION="RHP001" ANALYTE="H3" YEAR=2100  SPECIES="RMALRD"
  VALUES=0.76302
!
! Aquatic locations
DATA LOCATION="QHP001" ANALYTE="H3" YEAR=2100  SPECIES="QCARPS"
  VALUES=0.61637
DATA LOCATION="QHP001" ANALYTE="H3" YEAR=2100  SPECIES="QSBASS"
  VALUES=0.29431
DATA LOCATION="QHP001" ANALYTE="H3" YEAR=2100  SPECIES="QMWTFS"
  VALUES=0.86436
!
END
```

10.2.1.2 Other Input Files

The FILLFCDA program also reads two other input files. These files are the ESD keyword file and the FCDA index file. The ESD keyword file contains the names of the concentration files that are to be modified. The FCDA map file contains index data related to writing to the FCDA concentration files.

10.2.2 Output Files

The code writes to two or more output files. These files are a report file and one or more FCDA concentration files.

10.2.2.1 FILLFCDA Report File

The report file contains summary information from the run of the FILLFCDA code. This file contains a record of the code version, time and date of run execution, input and output file names, run information, and a summary table of results. This file also contains any error messages generated by the FILLFCDA code.

10.2.2.2 Concentration Files

The FILLFCDA program writes some data to an FCDA file for every combination of analyte and SPECIES identified on DATA keywords in the FILLFCDA keyword file.

10.3 Keyword Definitions for the FILLFCDA Code

In general, the keywords for FILLFCDA can be entered in any order. The only restriction is that the END keyword must be the last keyword in the file.

10.3.1 DATA Keyword for FILLFCDA

The DATA keyword is used to define the data values to be inserted into one or more FCDA files. Data values can be deterministic (all values entered explicitly) or they can be generated from a specified statistical distribution. The syntax for this keyword when deterministic data are entered is:

```
DATA [LOCATION="quote"] [SPECIES="quote"] [ANALYTE="quote"] [YEAR=number]
   {SOIL="quote"} [VALUES=number, …, number]
```

The syntax for this keyword when stochastic data are entered is:

```
DATA [LOCATION="quote"] [SPECIES="quote"] [ANALYTE="quote"] [YEAR=number]
   {SOIL="quote"} [STOCHASTIC=number, …, number]
```

This keyword identifies the data for all realizations of concentration for a specific analyte, location, soil type, species, and time combination. More than one DATA keyword can be entered. The modifiers for the DATA keyword are defined in Table 10.2.

Table 10.2 Modifiers Associated with the DATA Keyword in FILLFCDA

Modifier	Description
ANALYTE	The quote string associated with the ANALYTE modifier contains the analyte ID for the concentration data values. The analyte ID must be one of the set of analytes defined in the ESD keyword file.
LOCATION	The quote string associated with the LOCATION modifier contains the location ID for the concentration data values. The location ID must be one of the set of locations defined in the ESD keyword file.

Modifier	Description
SOIL	The quote string associated with the optional SOIL modifier contains the ID for a soil type. This modifier is not used if an aquatic or riparian species species is specified. If a terrestrial species living in the upland zone is defined, then one of the values "SODR", "SOGW", or "SOSW" must be used. These values define, respectively, soil with no irrigation, soil with groundwater used for irrigation, and soil with surface water used for irrigation.
SPECIES	The quote string associated with the SPECIES modifier contains the ID for an ecological species. The species ID must be one of the ecological speciues defined in the ESD keyword file.
YEAR	The numerical value associated with the YEAR modifier identifies the calendar year at which the concentration data apply. The year entered must be one of the years defined on the TIMES keyword in the ESD keyword file.
VALUES	The numerical values associated with the VALUES modifier contain the concentration values to be entered in the FCDA file. As many values must be entered as there are realizations defined in the ESD keyword file. Only one of the VALUES and STOCHASTIC modifiers can be used on a single keyword entry.
STOCHASTIC	The numerical values associated with the STOCHASTIC modifier contain information to define a statistical distribution.. The entries for defining a statistical distribution are explained in Section 19.1. Only one of the VALUES or STOCHASTIC modifiers can be used on a single DATA keyword entry.

If a DATA keyword does not identify a valid analyte, location, species, soil, and time combination in the FCDA data file, then the information on that DATA keyword is discarded and an error message is written to the report file. Example entries for the DATA keyword for a case of one realization are the following:

```
! Upland locations
DATA LOCATION="UH0002" ANALYTE="H3" YEAR=2150  SOIL="SOSW"
   SPECIES="UCATMT" VALUES=0.83482
DATA LOCATION="UH0002" ANALYTE="H3" YEAR=2150  SOIL="SOGW"
   SPECIES="UCATMT" VALUES=0.93036

! Riparian Locations
DATA LOCATION="RHP001" ANALYTE="H3" YEAR=2100  SPECIES="RMLBRY"
   VALUES=0.63039
DATA LOCATION="RHP001" ANALYTE="H3" YEAR=2100  SPECIES="RMDEER"
   VALUES=0.01514

! Aquatic locations
DATA LOCATION="QHP001" ANALYTE="H3" YEAR=2100  SPECIES="QCARPS"
   VALUES=0.61637
DATA LOCATION="QHP001" ANALYTE="H3" YEAR=2100  SPECIES="QSBASS"
   STOCHASTIC 2 0.6 0.8
```

10.3.2 END Keyword for FILLFCDA

The END keyword signifies the end of all keyword data. Nominally it will be the last keyword in the keyword file. All data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

10.3.3 FILE Keyword for FILLFCDA

The FILE keyword is used to enter the name of the ESD keyword file. The following is this keyword's syntax:

```
FILE [ESD="quote 1"]
```

The file name is entered in a quote string, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. An example of the use of this keyword follows:

```
FILE ESD="/home/ANALYSIS/practice-median/ESD_practice-median.key"
```

10.3.4 FOODS Keyword for FILLFCDA

The FOODS keyword is used to designate the location where the FCDA files are to be written and to identify the name of the map file associated with these FCDA files. The following is this keyword's syntax:

```
FOODS [PATH= "quote1"] [MAP= "quote2"]
```

The file names are entered in quote strings, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. The file name associated with a modifier must be entered before the next modifier is entered. At least one FOODS keyword is required for every run of the code. Table 10.3 describes the modifiers associated with the FOODS keyword.

Table 10.3 Modifiers Associated with the FOODS Keyword in FILLECDA

Modifier	Description
PATH	The complete path name identifying the location of the directory where FOOD files already exist.
MAP	The name of the file containing the map of the FOOD file contents.

The following entry defines the map file and data directory for food concentrations and the header file:

```
FOODS PATH="D:\SAC\CODES_1\ECEM\FOODS\"
MAP="ECEM_FCDA_Map.Dat"
```

10.3.5 REALIZAT Keyword for FILLFCDA

The REALIZ (or REALIZATION) keyword defines the number of realizations to process. The following is this keyword's syntax:

```
REALIZAT value1
```

This keyword gives the number of realizations of data that will be entered on each DATA record. The number must match exactly with the number of realizations in the ESD keyword file. The following keyword record sets the number of realizations to 10:

```
REALIZAT 10
```

10.3.6 REPORT Keyword for FILLFCDA

The REPORT keyword is used to define the name of the output report (log) file. It must be the first keyword entered in the keyword file. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The name of the report file is entered in a quote string. File names up to 200 characters long are supported, and path names can be included. The following is an example REPORT keyword record:

```
REPORT "/SAC/SystemCodes/Cultural/Test1.rpt"
```

1.1.1 TITLE Keyword for FILLFCDA

The TITLE keyword is used to define a single-line problem title. The problem title will be written to output files. If the title is not supplied, then the program will error terminate. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 200 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the FILLFCDA code."
```

10.3.7 USER Keyword for FILLFCDA

The USER keyword is used to identify the user of the program. The user name will be written to output files. If the user name is not supplied, then the program will error terminate. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

10.3.8 VERBOSE Keyword for FILLFCDA

The presence of the optional VERBOSE keyword initiates additional output to the report file. The following is this keyword's syntax:

```
VERBOSE {DEFINITIONS} {STATISTICS}
```

Entry of the VERBOSE keyword without any modifiers causes the data inserted into the FCDA files to be written to the report file. If the DEFINITI modifier is used, the definitions of the statistical distributions are also written to the report file. If the STATISTICS modifier is used, summary statistics for the generated statistical distributions are also written to the report file.

11.0 HIGHDOSE – Dose Extraction for ECEM

11.1 Overview

The HIGHDOSE code is designed to extract the largest impact calculated by the ECEM (see Eslinger et al. [2006b], Volume 2, Section 4.0) code over a suite of locations at each of several time steps. For example, it can determine the species with the highest dose along the riparian zone at a set of times.

11.1.1 Location in the Processing Sequence

The HIGHDOSE code must follow a run of the ECEM code.

11.1.2 How the Code Is Invoked

HIGHDOSE can run under either the Windows or the Linux operating system. Under the Windows operating system (Releases XP or 7), HIGHDOSE executes in a DOS box. A run of HIGHDOSE is initiated by entering the following command line:

```
HIGHDOSE "Keyfilename"
```

Under the Linux operating system HIGHDOSE is executed through any of the following Bourne Shell or C Shell commands:

```
highdose-1.exe "Keyfilename"
```

For these commands, “HIGHDOSE.EXE” or “highdose.exe” is the name of the executable program, and “Keyfilename” is the name of a control keyword file. Both the name of the executable program and the keyword file may contain path information. If HIGHDOSE is invoked without entering the name of the keyword file, then the code will prompt the user for the file name. The keyword file, which should be prepared using an editor that can handle ASCII files without leaving embedded control codes, contains text control information describing the run. If HIGHDOSE cannot open the keyword file, then the code will terminate execution after writing an error message to the standard output device.

11.1.3 Memory Requirements

The HIGHDOSE program has minimal memory requirements. A run of the code to extract values for all upland locations required less than 2 MB of memory.

11.2 File Definitions

The HIGHDOSE program reads three input files and writes to two output files. These files are described in the following paragraphs.

11.2.1 Input Files

The input files for the HIGHDOSE program are a control keyword file, a species definition file, and a details result file output by the ECEM code.

11.2.1.1 HIGHDOSE Keyword File

The HIGHDOSE keyword file contains control information. An example file is provided in Table 11.1. Detailed definitions of the keywords are provided in Section 11.3.

Table 11.1 Example Keyword File for HIGHDOSE

```
! Keyword file for the FillECDA program
REPORT "Test.Rpt"
TITLE "Testing of the HighDose Code Using a ECEM Rev. 1 run"
USER "Paul W. Eslinger"
FILE SPECIES "Species.csv"
FILE ECEM "Ecem_Det.Csv"
FILE RESULTS "Test.Csv"
REALIZATION 2
MEMORY TABLEROW=3 REALIZATION=25 RECORDS=1000
!VERBOSE
SOLUTION "SUMRAD"
ANALYTE "-Rads-"
SOIL "SOSW"
! The following keywords allow multiple choices
LOCATION "TH0001" "TH0003" "TH0015" "TH0017"
         "TH0002" "TH0005" "TH0006"
TIME 1950  1955  1960  1965
END
```

11.2.1.2 Species Definition File

The HIGHDOSE program requires a species definition file. This file contains the species type, species ID, and species name for every species for which data are provided in the ECEM results file. This information is required, but is used mainly for labeling purposes. This file is a text file written using a comma-separated format. An example file is provided in Table 11.2.

Table 11.2 Example Species Definition File for HIGHDOSE

```
"TA","AMCOOT","American coot"
"TA","AMCOUP","American coot - upland"
"TA","EGGS","Chicken eggs - upland"
"TA","BEAVER","Beaver"
"QA","CARP","Carp"
"TA","COYOTE","Coyote"
"QA","DAPMAG","Daphnia magna"
"TP","DENSDG","Dense sedge"
"TP","DENSUP","Dense sedge - upland"
"TP","FUNGI","Fungi"
"TP","MULBRY","Mulberry"
"TP","MULBUP","Mulberry - upland"
"TA","MULDER","Mule deer"
"TP","GRAIN","Generic grain species"
"TP","POTATO","Potato"
"TA","MILKCW","Milk cow"
"QP","PERPHY","Periphyton"
"QP","PHYPLK","Phytoplankton"
```

11.2.1.3 ECEM Results File

The third input file for the HIGHDOSE program is nominally generated with a run of the ECEM code. This file contains data output from ECEM under the control of the DETAILS keyword in ECEM.

11.2.2 Output Files

The HIGHDOSE program writes two output files. One file is a report file that contains text information about the run of the code. It is not described further here. The other output file is the results file containing the extracted information. The first few lines from an example results file is provided in Table 11.3.

Table 11.3 Example Results File from the HIGHDOSE Code

```
"Code Name:","HighDose"
"Code Version:","4.00.001"
"Code Date:"," 5 Jun 2007"
"Run ID:","20070605130624"
"Run Title:","Testing of the HighDose Code Using a ECEM Rev. 1 run"
"User Name:","Paul W. Eslinger"

"Realization 2 is requested."

"Results for location ID = TH0010 year = 1965 solution = SUMRAD soil type = SOSW and
analyte type = -Rads-"
"No matching data were found"

"Results for location ID = TH0011 year = 1950 solution = SUMRAD soil type = SOSW and
analyte type = -Rads-"
"Terrestrial Plants"," ","Terrestrial Animals"," ","Aquatic Plants"," ","Aquatic
Animals"
"Specie","Dose","Specie","Dose","Specie","Dose","Specie","Dose"
"MULBUP", 7.445E+04,"AMCOUP", 1.592E+05,"      ", 0.000E+00,"      ", 0.000E+00
"POTATO", 1.806E+04,"COYOTE", 1.390E+05,"      ", 0.000E+00,"      ", 0.000E+00
"DENSUP", 1.806E+04,"MILKCW", 1.354E+05,"      ", 0.000E+00,"      ", 0.000E+00

"Results for location ID = TH0011 year = 1955 solution = SUMRAD soil type = SOSW and
analyte type = -Rads-"
"Terrestrial Plants"," ","Terrestrial Animals"," ","Aquatic Plants"," ","Aquatic
Animals"
"Specie","Dose","Specie","Dose","Specie","Dose","Specie","Dose"
"MULBUP", 8.090E+04,"AMCOUP", 5.339E+04,"      ", 0.000E+00,"      ", 0.000E+00
"DENSUP", 1.950E+04,"MILKCW", 4.703E+04,"      ", 0.000E+00,"      ", 0.000E+00
"POTATO", 1.950E+04,"MULDER", 2.893E+04,"      ", 0.000E+00,"      ", 0.000E+00
```

The most typical method for looking at the results of the HIGHDOSE code is to reformat the comma-separated results into a table. An example of such a result is provided in Table 11.4.

Table 11.4 Reformatted Output From the HIGHDOSE Code

Results for location ID = NAPLSH year = 2500 solution = SUMRAD and analyte type = -Rads-							
Terrestrial Plants		**Terrestrial Animals**		**Aquatic Plants**		**Aquatic Animals**	
Specie	**Dose**	**Specie**	**Dose**	**Specie**	**Dose**	**Specie**	**Dose**
TULE	9.75E-11	CLFSWL	1.75E-08	PERPHY	7.72E-09	MAYFLY	3.57E-08
BLCTWD	8.81E-11	AMCOOT	7.94E-09	WMLFOL	5.74E-09	CRYFSH	1.17E-08
MULBRY	8.81E-11	BUFLHD	5.32E-09	PHYPLK	6.43E-12	CPBLSN	7.99E-09
CYLCRS	4.67E-11	COMSNP	5.01E-09			SALMJV	5.53E-09
RCANGS	3.36E-11	RACOON	3.20E-09			RTRTJV	5.53E-09

11.3 Keyword Definitions for the HIGHDOSE Code

In general, the keywords for the HIGHDOSE code can be entered in any order. The only restriction is that the END keyword must be the last keyword in the file.

11.3.1 ANALYTE Keyword for HIGHDOSE

The ANALYTE keyword is used to define the analyte (or analytes) for which data will be processed. The following is this keyword's syntax:

```
ANALYTE ["quote 1"]
```

The single quote string must either be a single analyte ID from the set of the analytes in the ESD keyword file, or the string "-Rads-" if the combined dose over multiple radioactive analytes is desired. Two examples of this keyword are the following:

```
ANALYTE "C14"
ANALYTE "-Rads-"
```

11.3.2 END Keyword for HIGHDOSE

The END keyword signifies the end of all keyword data. All data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

11.3.3 FILE Keyword for HIGHDOSE

The FILE keyword is used to enter the names of all input and output files except for the report file. The following is this keyword's syntax:

```
FILE [modifier1="quote1"] {modifier2="quote2"} {modifier3="quote3"}
```

The file names are entered in quote strings, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. The file name associated with a modifier must be entered before the next modifier is entered. At least one FILE keyword is required for every run of the code.

The name of the ECEM details file is associated with the modifier ECEM. The name of the input file defining ecological species is associated with the modifier SPECIES. The name of the output file from

HIGHDOSE is associated with the modifier RESULTS. Example file keywords that define these three files are the following:

```
FILE SPECIES "Species.csv"
FILE ECEM "ECEM_SWEIS_det_Bg.Csv"
FILE RESULTS "High_Rads_Bg.Csv"
```

11.3.4 LOCATION Keyword for HIGHDOSE

The LOCATION keyword is used to define the set of locations for which data will be processed. The following is this keyword's syntax:

```
LOCATION ["quote 1"] {"quote2" … "quoten"]
```

One or more quote strings must contain valid location IDs from locations specified in the ESD keyword file. Data for a given time step is scanned over the entire set of specified locations. An example LOCATION keyword defining ten locations is the following:

```
LOCATION
   "UH0001" "UH0002" "UH0003" "UH0004" "UH0005"
   "UH0006" "UH0007" "UH0008" "UH0009" "UH0010"
```

11.3.5 MEMORY Keyword for HIGHDOSE

The MEMORY keyword is used to define some variables that determine the amount of memory used in the code. The following is this keyword's syntax:

```
MEMORY [TABLEROW=N1] [REALIZAT=N2] [RECORDS=N3]
```

The modifiers associated with the MEMORY keyword are described in Table 11.5.

Table 11.5 Modifiers Associated with the MEMORY Keyword in HIGHDOSE

Modifier	Description
TABLEROW	The numerical value associated with the TABLEROW modifier defines the number of rows to use in the output table. A value of 3 to 5 is suggested.
REALIZAT	The numerical value associated with the REALIZAT modifier defines the number of realizations used in the run of ECEM that produced the detailed data file being analyzed.
RECORDS	The numerical value associated with the RECORDS modifier defines the number of records that may be matched in the detailed data file for a single year and location combination. Typically this value can be set to the number of species.

An example keyword where the user specifies five rows for the output table for a deterministic run of ECEM that utilized 100 species is the following:

```
MEMORY TABLEROW=5 REALIZATION=1 RECORDS=100
```

11.3.6 REALIZAT Keyword for HIGHDOSE

The REALIZAT (or REALIZATION) keyword defines the single realization for which data are to be extracted. The following is this keyword's syntax:

```
REALIZATION value1
```

The integer value1 has a minimum value of 1 and a maximum of the number of realizations performed by the ECEM code. The following keyword record extracts data for realization number 10:

```
REALIZAT 10
```

11.3.7 REPORT Keyword for HIGHDOSE

The REPORT keyword is used to define the name of the output report (log) file. It must be the first keyword entered in the keyword file. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The name of the report file is entered in a quote string. File names up to 200 characters long are supported, and path names can be included. The following is an example REPORT keyword record:

```
REPORT "/SAC/C/Test.rpt"
```

11.3.8 SOIL Keyword for HIGHDOSE

The SOIL keyword is used to define the solution type for which data will be processed. The following is this keyword's syntax:

```
SOIL ["quote 1"]
```

The single quote string is case sensitive and six characters in length. The modifiers associated with the SOILTYPE keyword are given in Table 11.6.

Table 11.6 Modifiers Associated with the SOIL Keyword in HIGHDOSE

Modifier	Description
NONE	Applies to all aquatic locations
SORP	Riparian locations
SODR	Dry (non irrigated) upland locations
SOGW	Groundwater irrigated upland locations
SOSW	Surface water irrigated upland locations

An example of this keyword is the following:

```
SOIL "SOGW"
```

11.3.9 SOLUTION Keyword for HIGHDOSE

The SOLUTION keyword is used to define the solution type for which data will be processed. The following is this keyword's syntax:

```
SOLUTION ["quote 1"]
```

The single quote string is case sensitive and six characters in length. The modifiers associated with the SOIL keyword are given in Table 11.7.

Table 11.7 Modifiers Associated with the SOLUTION Keyword in HIGHDOSE

Modifier	**Description**
BURDEN	Body burdens (pCi or µg/kg wet wt)
DOSRAD	Radioactive dose (rem)

BMTISS	Ratios to tissue benchmarks (unitless)
SUMRAD	Sum of radioactive dose (rem)
CONCEN	Media concentrations (see MEDIA keyword modifiers for units)

An example of this keyword is the following:

```
SOLUTION "BURDEN"
```

11.3.10 TIME Keyword for HIGHDOSE

The TIME keyword identifies the times at which the calculations are to be performed. The following is this keyword's syntax:

```
TIME [T1] {T2} … {Tn}
```

The numerical entries T1, T2, …, Tn are the times (whole number years) when outputs are desired. These times must be a subset of the times at which environmental data were computed and stored by the inventory, release, and transport modules. Only one TIME keyword should be entered. The following is an example TIME keyword that requests output for the three years 2020, 2075, and 3014:

```
TIME 2020 2075 3014
```

11.3.11 TITLE Keyword for HIGHDOSE

The TITLE keyword is used to define a single-line problem title. The problem title will be written to output files. The program will error terminate if the title is not supplied. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 200 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the HIGHDOSE code."
```

11.3.12 USER Keyword for HIGHDOSE

The USER keyword is used to identify the user of the program. The user name will be written to output files. The program will error terminate if the user name is not supplied. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

11.3.13 VERBOSE Keyword for HIGHDOSE

The presence of the optional VERBOSE keyword initiates additional output to the report file. The following is this keyword's syntax:

```
VERBOSE
```

12.0 HIGHIMPACT – Maximum Impact Extraction for HUMAN

12.1 Overview

The HIGHIMPACT code is designed to extract the largest impact result calculated by the HUMAN code over a suite of locations at each of several time steps. For example, it can provide the largest dose to an individual outside the Hanford core zone as a function of time.

12.1.1 Location in the Processing Sequence

The HIGHIMPACT code must follow a run of the HUMAN code.

12.1.2 How the Code Is Invoked

HIGHIMPACT can run under either the Windows or the Linux operating system. Under the Windows operating system (Releases XP or 7), HIGHIMPACT executes in a DOS box. A run of HIGHIMPACT is initiated by entering the following command line:

```
HIGHIMPACT "Keyfilename"
```

Under the Linux operating system HIGHIMPACT is executed through any of the following Bourne Shell or C Shell commands:

```
highimpact-1.exe "Keyfilename"
```

For these commands, “HIGHIMPACT .EXE” or “highimpact-1.exe” is the name of the executable program, and “Keyfilename” is the name of a control keyword file. Both the name of the executable program and the keyword file may contain path information. If HIGHIMPACT is invoked without entering the name of the keyword file, then the code will prompt the user for the file name. The keyword file, which should be prepared using an editor that can handle ASCII files without leaving embedded control codes, contains text control information describing the run. If HIGHIMPACT cannot open the keyword file, then the code will terminate execution after writing an error message to the standard output device.

12.1.3 Memory Requirements

The HIGHIMPACT program has minimal memory requirements. A run of the code to extract values for all upland locations required less than 2 MB of memory.

12.2 File Definitions

The HIGHIMPACT program reads two input files and writes two output files. These files are described in the following sections.

12.2.1 Input Files

The HIGHIMPACT program reads a control keyword file and an impact details file written by the HUMAN code. The HIGHIMPACT keyword file contains control information. An example file is provided in Table 12.1. Detailed definitions of the keywords are provided in Section 12.3.

Table 12.1 Example Keyword File for the HIGHIMPACT Program

```
! Keyword file for HIGHIMPACT
REPORT "Test.Rpt"
TITLE "Testing of the HighImpact Code Using a HUMAN Rev. 1 run"
USER "Paul W. Eslinger"
FILE HUMAN "Farmer_CA1_median_Dtl.csv"
FILE RESULTS "Test.Csv"
REALIZAT HUMAN=1 SINGLE=1
! Locations can be multiply defined
LOC_ID "UH1082" "UH1083"
! Times can be multiply defined
TIME 1990  1992
! The following solutions must be uniquely defined
S_TYPE "GWAT"
ANA_ID "C14"
R_TYPE "CON"
VERBOSE
END
```

12.2.2 Output Files

The HIGHIMPACT program writes two output files. One file is a report file that contains text information about the run of the code. It is not described further here. The other output file is the results file containing the information about the highest impact over a set of locations for every year. An example results file is provided in Table 12.2.

Table 12.2 Example Results File from the HIGHIMPACT Code

```
"Code Name:","HighImpact"
"Code Version:","1.00.005"
"Code Date:","22 MAr 2006"
"Run ID:","20060515152050"
"Run Title:","Maximum dose for the upland Residential Farmer scenario"
"User Name:","Paul W. Eslinger"
"Solution type:","SINGLE = 1","COMBIN","RAD","SUMDOSE"
1945,"UH2709", 8.29183E-03
1950,"UH2709", 1.85205E-02
1955,"UH0858", 1.50036E+00
1960,"UH1642", 9.24540E-01
1965,"UH1643", 3.96217E+00
1970,"UH1643", 4.82087E+00
1975,"UH1644", 3.36062E+00
1980,"UH1644", 1.90950E+00
1985,"UH1643", 1.12953E+00
1990,"UH1642", 6.65234E-01
1991,"UH1642", 5.95870E-01
1992,"UH1642", 5.27415E-01
```

```
1993,"UH1642", 4.52947E-01
1994,"UH1643", 3.87738E-01
1995,"UH1643", 3.63506E-01
1996,"UH1643", 3.40908E-01
1997,"UH1643", 3.18804E-01
1998,"UH1709", 2.94928E-01
1999,"UH1709", 2.77404E-01
2000,"UH1709", 2.60285E-01
```

12.3 Keyword Definitions for the HIGHIMPACT Code

In general, the keywords for the HIGHIMPACT code can be entered in any order. The only restriction is that the END keyword must be the last keyword in the file.

The keyword selections require the user to specify a set of possible values for the first five data values on each line in the details file written by the HUMAN code. The relative position of the values in the details file and the associated keyword is the following:

1. TIME – Multiple time definitions are allowed on a single TIME keyword.
2. LOCATION – Multiple location definitions are allowed on a single LOCATION keyword.
3. ANA_ID – A single solution is required for this keyword.
4. R_TYPE – A single solution is required for this keyword.
5. S_TYPE – A single solution is required for this keyword.

Values for the data in positions 3, 4, and 5 depend on the specified solutions. An easy way to choose the correct combination is to examine the results data file that is to be processed.

12.3.1 ANA_ID Keyword for HIGHIMPACT

The ANA_ID keyword is used to define the analyte (or analytes) for which data will be processed. The following is this keyword's syntax

```
ANA_ID ["quote 1"]
```

The single quote string must either be a single analyte ID from the set of the analytes in the ESD keyword file, or the string "-Rads-" if the combined dose over multiple radioactive analytes is desired. Two examples of this keyword are the following:

```
ANA_ID "C14"
ANA_ID "-Rads-"
```

12.3.2 END Keyword for HIGHIMPACT

The END keyword signifies the end of all keyword data. All data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

12.3.3 FILE Keyword for HIGHIMPACT

The FILE keyword is used to enter the names of all input and output files except for the report file. The following is this keyword's syntax:

```
FILE [modifier1="quote1"] {modifier2="quote2"}
```

The file names are entered in quote strings, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. The file name associated with a modifier must be entered before the next modifier is entered. At least one FILE keyword is required for every run of the code.

The name of the human details file is associated with the modifier HUMAN. The name of the output file from HIGHIMPACT is associated with the modifier RESULTS. Example file keywords that define these two files are the following:

```
FILE HUMAN "Farmer_CA1_median_Dtl.csv"
FILE RESULTS "Farmer_High.csv"
```

12.3.4 LOC_ID Keyword for HIGHIMPACT

The LOC_ID keyword is used to define the set of locations for which data will be processed. The following is this keyword's syntax:

```
LOC_ID ["quote 1"] {"quote2" … "quoten"]
```

One or more quote strings must contain valid location IDs from locations specified in the ESD keyword file. Data for a given time step is scanned over the entire set of specified locations. An example LOC_ID keyword defining ten locations is the following:

```
LOC_ID
   "UH0001" "UH0002" "UH0003" "UH0004" "UH0005"
   "UH0006" "UH0007" "UH0008" "UH0009" "UH0010"
```

12.3.5 REALIZAT Keyword for HIGHIMPACT

The REALIZAT (or REALIZATION) keyword is used to define the realizations for which data will be processed. The following is this keyword's syntax:

```
REALIZAT [HUMAN=N1] [MAXIMUM|MEAN|SINGLE=N2]
```

The modifiers associated with the REALIZAT keyword are described in Table 12.3. Only one of the MAXIMUM, MEAN, or SINGLE modifiers is allowed during a run of the code.

Table 12.3 Modifiers Associated with the REALIZAT Keyword in HIGHIMPACT

Modifier	Description
HUMAN	The numerical value associated with the HUMAN modifier defines the number of realizations contained in the details file written by the HUMAN code.
MAXIMUM	This modifier indicates that the maximum over all realizations will be used in determining the highest impact at each location.
MEAN	This modifier indicates that the arithmetic mean over all realizations will be used in determining the highest impact at each location.
SINGLE	This modifier indicates that data from a single realization will be used in determining the highest impact at each location. The realization number to use is provided in the numerical value associated with the SINGLE modifier.

An example keyword where the user specifies using the arithmetic mean for a data file containing 100 realizations of data is the following:

```
REALIZAT HUMAN=100 MEAN
```

An example keyword where the user specifies using the data for realization 23 from a data file containing 100 realizations of data is the following:

```
REALIZAT HUMAN=100 SINGLE=23
```

12.3.6 REPORT Keyword for HIGHIMPACT

The REPORT keyword is used to define the name of the output report (log) file. It must be the first keyword entered in the keyword file. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The name of the report file is entered in a quote string. File names up to 200 characters long are supported, and path names can be included. The following is an example REPORT keyword record:

```
REPORT "/SAC/C/Test.rpt"
```

12.3.7 R_TYPE Keyword for HIGHIMPACT

The R_TYPE keyword is used to partially define the solution type for which data will be processed. The following is this keyword's syntax:

```
R_TYPE ["quote 1"]
```

The single quote string is case sensitive and six characters in length. The modifiers associated with the analyte type for the R_TYPE keyword are given in Table 12.4.

Table 12.4 Modifiers Associated with the R_TYPE Keyword in HIGHIMPACT

Modifier	Description
ALL	The analyte field is used for a quantity that is a sum over analytes.
CAR	The analyte is a carcinogenic chemical.
CONMEDIA	The analyte field is used to select an environmental medium.
CONFOODS	The analyte field is used to select a food species.
HAZ	The analyte is a hazardous chemical.
RAD	The analyte is a radionuclide.

An example of this keyword is the following:

```
R_TYPE "RAD"
```

12.3.8 S_TYPE Keyword for HIGHIMPACT

The S_TYPE keyword is also used to define the solution type for which data will be processed. The following is this keyword's syntax:

```
S_TYPE ["quote 1"]
```

The single quote string is case sensitiveand is two to seven characters in length. The modifiers associated with the S_TYPE keyword are given in Table 12.5.

Table 12.5 Modifiers Associated with the S_TYPE Keyword in HIGHIMPACT

Modifier	Description
S_TYPE Modifiers Associated with R_TYPE CONMEDIA	
AIRC	Air concentrations
GWAT	Groundwater concentrations
SEDI	Sediment concentrations
SEEP	Seep water concentrations
SODR	Soil concentrations, no irrigation
SOGW	Soil concentrations, groundwater irrigated
SORP	Riparian soil concentrations
SOSW	Soil concentrations, surface water irrigated
SWAT	Surface water concentrations
S_TYPE Modifiers Associated with R_TYPE CONFOODS	
BIRD	Food concentration, birds
EGGS	Food concentration, eggs
FISH	Food concentration, fish
FISH_2	Food concentration, 2nd fish type
FISH_3	Food concentration, 3rd fish type
FRUIT	Food concentration, fruit
GRAIN	Food concentration, grain
LEAFVEG	Food concentration, leafy vegetables
MEAT	Food concentration, meat
MILK	Food concentration, milk
ROOTVEG	Food concentration, root vegetables
S_TYPE Modifiers Associated with R_TYPE CAR, HAZ, RAD	
ANADOSE	Analyte dose
ANARISK	Analyte risk (CAR and RAD)
ANAHQ	Analyte hazard quotient (HAZ)
DOSEING	Ingestion dose (CAR, HAZ and RAD)
DOSEINH	Inhalation dose (CAR, HAZ and RAD)
DOSEEXT	External dose (RAD)
DOSEDER	Dermal dose (CAR and HAZ)
HQING	Ingestion hazard quotient (HAZ)
HQINH	Inhalation hazard quotient (HAZ)
HQDER	Dermal hazard quotient (HAZ)
POPDOSE	Population dose (RAD)
POPRISK	Population risk (RAD)
RISKING	Ingestion risk (CAR and RAD)
RISKINH	Inhalation risk (CAR and RAD)
RISKEXT	External risk (RAD)
RISKDER	Dermal risk (CAR)
SUMDOSE	Dose summed over analytes (CAR and HAZ)
SUMHQ	Hazard quotient summed over analytes (HAZ)
S_TYPE Modifiers Associated with R_TYPE ALL	
SUMRISK	Risk summed over carcinogenic chemicals and radionuclides

An example of this keyword is the following:

```
S_TYPE "ANADOSE"
```

12.3.9 TIME Keyword for HIGHIMPACT

The TIME keyword identifies the times at which the calculations are to be performed. The following is this keyword's syntax:

```
TIME [T1] {T2} … {Tn}
```

The numerical entries T1, T2, …, Tn are the times (whole number years) when outputs are desired. These times must be a subset of the times at which environmental data were computed and stored by the inventory, release, and transport modules. Only one TIME keyword should be entered. The following is an example TIME keyword that requests output for the three years 2020, 2075, and 3014:

```
TIME 2020 2075 3014
```

12.3.10 TITLE Keyword for HIGHIMPACT

The TITLE keyword is used to define a single-line problem title. The problem title will be written to output files. The program will error terminate if the title is not supplied. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 200 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the HIGHIMPACT code."
```

12.3.11 USER Keyword for HIGHIMPACT

The USER keyword is used to identify the user of the program. The user name will be written to output files. The program will error terminate if the user name is not supplied. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

12.3.12 VERBOSE Keyword for HIGHIMPACT

The presence of the optional VERBOSE keyword initiates additional output to the report file. The following is this keyword's syntax:

```
VERBOSE
```

13.0 HIGHMEDIA – Extraction of Maximum Media Concentrations

13.1 Overview

The HIGHMEDIA code is designed to extract the maximum media concentrations over a set of specified locations and times for data contained in an ECDA file. For example, it can provide the highest groundwater concentration for a single analyte outside the Hanford core zone as a function of time.

13.1.1 Location in the Processing Sequence

The HIGHMEDIA code reads data from an ECDA file. Thus, the transport codes must have been executed and the media entered in the ECDA files before HIGHMEDIA can be used.

13.1.2 How the Code Is Invoked

HIGHMEDIA can run under either the Windows or the Linux operating system. Under the Windows operating system (Releases XP or 7), HIGHMEDIA executes in a DOS box. A run of HIGHMEDIA is initiated by entering the following command line:

```
HIGHMEDIA "Keyfilename"
```

Under the Linux operating system HIGHMEDIA is executed through any of the following Bourne Shell or C Shell commands:

```
highmedia-1.exe "Keyfilename"
```

For these commands, “HIGHMEDIA.EXE” or “highmedia-1.exe” is the name of the executable program, and “Keyfilename” is the name of a control keyword file. Both the name of the executable program and the keyword file may contain path information. If HIGHMEDIA is invoked without entering the name of the keyword file, then the code will prompt the user for the file name. The keyword file, which should be prepared using an editor that can handle ASCII files without leaving embedded control codes, contains text control information describing the run. If HIGHMEDIA cannot open the keyword file, then the code will terminate execution after writing an error message to the standard output device.

13.1.3 Memory Requirements

The HIGHMEDIA program has minimal memory requirements. A run of the code to extract values for all upland locations required less than 2 MB of memory.

13.2 File Definitions

The HIGHMEDIA program reads two input files and writes two output files. These files are described in the following sections.

13.2.1 Input Files

The HIGHMEDIA program reads a control keyword file and an ECDA file. The HIGHMEDIA keyword file contains control information. An example file is provided in Table 13.1. Detailed definitions of the keywords are provided in Section 13.3.

Table 13.1 Example Keyword File for the HIGHMEDIA Program

```
REPORT "CPO_Alternate_High_GWAT.Rpt"
USER "Paul W. Eslinger"
FILE ESD "\SAC\ANALYSES\CPO_Alternate\ESD_CPO_Alternate.key"
!VERBOSE
ENDINIT

CASE
TITLE "Maximum Concentrations Tc99 at Core Zone Boundary"
FILE RESULTS "CPO_Alternate_GWAT_Tc99_CORE.csv"
ANALYTE "Tc99"
REALIZAT SINGLE=1
MEDIA "GWAT"
UNITS OUTPUT="pCi/L" FACTOR = 1.0E9
TIMES ALL
LOCATION LIST ! Boundary locations for Core Zone
 "UH0722" "UH0724" "UH0725" "UH0736" "UH0739" "UH0748" "UH0749"
 "UH0752" "UH0754" "UH0755" "UH0756" "UH0757" "UH0758" "UH0759"
 "UH0762" "UH0764" "UH0765" "UH0766" "UH0767" "UH0768" "UH0769"
ENDCASE

CASE
TITLE "Maximum Concentrations Tc99 at River Shore Boundary"
FILE RESULTS "CA1_median_GWAT_Tc99_CORE_RIVER.csv"
ANALYTE "Tc99"
REALIZAT SINGLE=1
MEDIA "GWAT"
UNITS OUTPUT="pCi/L" FACTOR = 1.0E9
TIMES ALL
LOCATION LIST ! Boundary locations for the river shore (Hanford Side)
 "RHP001","RHP003","RHP004","RHP005","RHP006","RHP007","RHP008"
 "RHP011","RHP013","RHP014","RHP015","RHP016","RHP017","RHP018"
 "RHP021","RHP023","RHP024","RHP025","RHP026","RHP027","RHP028"
ENDCASE

END
```

13.2.2 Output Files

The HIGHMEDIA program writes two or more output files. One file is a text report file that contains information about the run of the code, including any error messages. The other output file (or files) is the results file containing the information about the highest result over a set of locations for every year. A separate output file is written for every case definition. An example results file is provided in Table 13.2.

Table 13.2 Example Results File from the HIGHMEDIA Code

```
"Code Name:","HighMedia"
"Code Version:","2.00.A.1"
"Code Date:","16 Aug 2004"
"Run ID:","20040817110129"
"Run Title:","HighMedia Using a ECDA Files Rev. 1 run"
"User Name:","Paul W. Eslinger"
"File Name:","H:\CA1_median\ecda_save\Tc99_CA1_median.dat"
"Solution type:","MEDIAN"
"Analyte ID:","Tc99"
"Media ID:","GWAT"
"Year","Solution","Location ID","Easting","Northing"
1990, 4.52490E-07,"UH1230", 5.74522E+05, 1.35992E+05
1991, 3.61323E-07,"UH1230", 5.74522E+05, 1.35992E+05
1992, 2.89056E-07,"UH1230", 5.74522E+05, 1.35992E+05
```

13.3 Keyword Definitions for the HIGHMEDIA Code

The keywords for the HIGHMEDIA code are grouped into an initial section and one or more case groups. The initial section must begin with the REPORT keyword and must end with an ENDINIT keyword. Each analysis case must start with a CASE keyword and end with an ENDCASE keyword. The END keyword must be the last keyword in the file.

13.3.1 Keywords in the Initial Section for HIGHMEDIA

The initial section of keywords starts with the REPORT keyword and ends with the ENDINIT keyword. The run will error terminate if these conditions are not met.

13.3.1.1 ENDINIT Keyword for HIGHMEDIA

The ENDINIT keyword signifies the end of the initial section of the keyword data. The following is this keyword's syntax:

```
ENDINIT
```

13.3.1.2 FILE Keyword for HIGHMEDIA

The FILE keyword is used to enter the names of all input and output files except for the report file. The following is this keyword's syntax in the initial keyword section:

```
FILE [ESD="quote1"]
```

The file name is entered in a quote string, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. The name of the ESD control keyword file is associated with the modifier ESD. An example keyword is the following:

```
FILE ESD "C:\SAC\SAC_1\Analysis_2004\CA1_Median\ESD_CA1_median.key"
```

13.3.1.3 REPORT Keyword for HIGHMEDIA

The REPORT keyword is used to define the name of the output report (log) file. It must be the first keyword entered in the keyword file. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The name of the report file is entered in a quote string. File names up to 200 characters long are supported, and path names can be included. An example keyword is the following:

```
REPORT "/SAC/C/Test.rpt"
```

13.3.1.4 USER Keyword for HIGHMEDIA

The USER keyword is used to identify the user of the program. The user name will be written to output files. The program will error terminate if the user name is not supplied. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

13.3.1.5 VERBOSE Keyword for HIGHMEDIA

The presence of the optional VERBOSE keyword initiates additional output to the report file. The following is this keyword's syntax:

```
VERBOSE
```

13.3.2 Keywords for Specific Cases for HIGHMEDIA

The definition of an extraction case starts with the CASE keyword and ends with the ENDCASE keyword. Multiple extraction cases can be defined.

13.3.2.1 ANALYTE Keyword for HIGHMEDIA

The ANAYTE keyword is used to define the analyte for which data will be processed for a single case. The following is this keyword's syntax:

```
ANALYTE ["quote 1"]
```

The single quote string must be a single analyte ID from the set of the analytes in the ESD keyword file. An example of this keyword using the analyte technetium-99 is the following:

```
ANALYTE "Tc99"
```

13.3.2.2 CASE Keyword for HIGHMEDIA

The CASE keyword signifies the beginning of the definition of a specific case of keyword data. The following is this keyword's syntax:

```
CASE
```

13.3.2.3 ENDCASE Keyword for HIGHMEDIA

The ENDCASE keyword signifies the end of the definition of a specific case of keyword data. The following is this keyword's syntax:

```
ENDCASE
```

13.3.2.4 FILE Keyword for HIGHMEDIA

The FILE keyword is used to enter the names of all input and output files except for the report file. The following is this keyword's syntax in a case definition:

```
FILE [RESULTS="quote1"]
```

File names are entered in quote strings, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. Exactly one FILE keyword is required for every case in the keyword file. The name of the output file from HIGHMEDIA is associated with the modifier RESULTS. An example keyword that defines a results file is the following:

```
FILE RESULTS "Test.Csv"
```

13.3.2.5 LOCATION Keyword for HIGHMEDIA

The LOCATION keyword is used to define the set of locations for which data will be processed for a single case. The following is this keyword's syntax:

```
LOCATION [ALL| LIST ["quote 1"] {"quote2" … "quoten"}]
```

All locations in the ESD keyword file are used when the modifier ALL is present. A list of specific sites can be defined by entering the modifier LIST and a set of quote strings identifying the site IDs of interest. The specific locations entered must be defined in the ESD keyword file. All locations are included in the first example shown below. The second example defines a list of six specific sites.

```
LOCATION ALL
LOCATION LIST "UH1000" "UH1001" "UH1003" "UH1004" "UH1005" "UH1230"
```

13.3.2.6 MEDIA Keyword for HIGHMEDIA

The MEDIA keyword is used to define the media for which data will be processed for a single case. The following is this keyword's syntax:

```
MEDIA ["quote 1"]
```

The single quote string is case sensitive and four characters in length. The modifiers associated with the FILE keyword are given in Table 13.3.

Table 13.3 Modifiers Associated with the MEDIA Keyword in HIGHMEDIA

Modifier	Description
GWAT	concentrations in groundwater (Ci/m^3 or kg/m^3)
SEEP	concentrations in seep water (Ci/m^3 or kg/m^3)
SWAT	concentrations in surface water (river) (Ci/m^3 or kg/m^3)
PWAT	concentrations in river bottom pore water (Ci/m^3 or kg/m^3)
SEDI	concentrations in river bottom sediment ($Ci/kg_{sediment}$ or $kg_{analyte}/kg_{sediment}$)
SORP	concentrations in riparian zone soil (land surface) (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)

SODR	concentrations in upland soil (land surface) with no irrigation (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)
SOGW	concentrations in upland soil (land surface) with groundwater irrigation (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)
SOSW	concentrations in upland soil (land surface) with surface water irrigation (Ci/kg_{soil} or $kg_{analyte}/kg_{soil}$)
AIRC	concentrations in air (Ci/m^3 or kg/m^3)
AIRD	air deposition rates ($Ci/m^2/yr$ or $kg/m^2/yr$)

An example of this keyword that uses concentrations in upland soil with surface water irrigation is the following:

```
MEDIA "SOSW"
```

13.3.2.7 REALIZATION Keyword for HIGHMEDIA

The REALIZAT keyword is used to define the realizations for which data will be processed and the summary technique to be used for a single case. The following is this keyword's syntax:

```
REALIZAT [MAXIMUM | MEAN | MEDIAN | SINGLE=N1]
```

The modifiers associated with the REALIZAT keyword are described in Table 13.4. Only one of the MAXIMUM, MEAN, MEDIAN or SINGLE modifiers are allowed during a run of the code.

Table 13.4 Modifiers Associated with the REALIZAT Keyword in HIGHMEDIA

Modifier	Description
MAXIMUM	This modifier indicates that the maximum over all realizations will be used in determining the highest impact at each location.
MEDIAN	This modifier indicates that the median over all realizations will be used in determining the highest impact at each location.
MEAN	This modifier indicates that the arithmetic mean over all realizations will be used in determining the highest result at each location.
SINGLE	This modifier indicates that data from a single realization will be used in determining the highest result at each location. The realization number to use is provided in the numerical value associated with the SINGLE modifier.

Example keywords where the user specifies using the single realization number 5, the arithmetic mean of all realizations, and the median of all realizations are the following:

```
REALIZAT SINGLE=5
REALIZAT MEAN
REALIZAT MEDIAN
```

13.3.2.8 TIMES Keyword for HIGHMEDIA

The TIMES keyword identifies the times (years) at which the calculations are to be performed for a single case. The following is this keyword's syntax:

```
TIMES [ALL | LIST [T1] {T2} … {Tn}]
```

All times in the ESD keyword file are used when the modifier ALL is present. A list of specific times can be defined by entering the modifier LIST and a set of numerical values identifying the years of interest.

The specific years entered must be defined in the ESD keyword file. All times are included in the first example shown below. The second example defines a list of six years.

```
TIMES ALL
TIMES LIST 2020 2075 3014 3050 4000 12050
```

13.3.2.9 TITLE Keyword for HIGHMEDIA

The TITLE keyword is used to define a single-line problem title for a single case. The problem title will be written to output files. The program will error terminate if the title is not supplied. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 200 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the HIGHMEDIA code."
```

13.3.2.10 UNITS Keyword for HIGHMEDIA

The UNITS keyword is used to define the data units for the analyte to be processed. The following is this keyword's syntax:

```
UNITS [OUTPUT="quote 1"] [FACTOR=N1]
```

The media data in the ECDA files have a predefined set of units (see the MEDIA keyword in Section 13.3.2.6). This keyword allows the user to change the units upon output. The single quote string associated with the modifier OUTPUT contains the units label for the output data (limit of 10 characters). The numerical value associated with the modifier FACTOR is the multiplicative factor required to change from input units to output units. Use a value of 1 if the input units are to be preserved. Example keywords that use groundwater concentrations of technetium-99 and convert the units from Ci/m^3 to pCi/L upon output are the following:

```
ANALYTE "Tc99"
MEDIA "GWAT"
UNITS OUTPUT="pCi/L" FACTOR = 1.0E9
```

13.3.3 Concluding (END) Keyword for HIGHMEDIA

The END keyword signifies the end of all keyword data. All data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

14.0 HUMAN – Human Impact Model

This section contains instructions for the use of the human exposure and risk models and provides the mathematical formulation for the model is provided.

14.1 Mathematical Formulation for the Human Risk Model

The human risk model is a screening-level chronic exposure model. It is intended for use in situations where the environmental contamination conditions are static or only slowly varying. The models are not appropriate for estimating risks from short-term accidental releases.

The HUMAN code addresses pathways related to long-term contamination from sources in air, surface water, and groundwater, with the associated contaminated media of seeps, springs, soils, and sediments. With these as starting points, the code estimates the exposures from contaminant concentrations in surface soil from irrigation, air from resuspension and volatilization, aquatic foods, terrestrial crops, and animal products. Both domestic animals and wild animals may be included. Exposure pathways explicitly modeled include external irradiation, dermal contact, inhalation, and ingestion.

The HUMAN code provides flexibility in combining the various pathways into exposure scenarios. Scenarios are defined through the use of representative sets of input parameters to simulate annual average or lifetime average exposure conditions. The scenarios are focused on individual exposures. Individuals are assumed to spend the amounts of time specified in the scenario at the location of analysis; individual mobility throughout the analysis domain is not supported. Population risks are addressed for radionuclides.

The HUMAN code provides results for radioactive contaminants; non-radioactive but carcinogenic contaminants; and non-radioactive, non-carcinogenic, but still hazardous contaminants. Radiation impacts to people may be calculated as either radiation dose or risk; carcinogenic chemical risks are provided in terms of risk of fatal cancer; risks from hazardous chemicals are provided as Hazard Quotients – the dimensionless ratio of the estimated intake to a standard Reference Dose.

The HUMAN code is designed to accept multiple realizations of concentration of contaminants in the environment. It allows the definition of stochastic exposure parameters, which combine with the uncertainty in the input media concentrations to provide a full range of uncertainty on the final dose or risk to the hypothetical exposed individual.

The following sections provide the mathematical formulations for the human risk model. Concentrations in terrestrial foods are calculated as described in Sections 7.1.1 and 7.1.1.2.

14.1.1 Human Exposure Equations Derived by Pathway

The following equations represent the total exposure of a person to radionuclides and chemicals. These equations describe the exposure or intake and the risk or hazard resulting from those exposures. Note that the user may substitute groundwater for seep/spring water in some scenario definitions.

14.1.1.1 Dermal Exposure (Non-Carcinogenic, Non-Radioactive)

The dose from dermal contact with non-carcinogenic, non-radioactive materials is computed for a number of activities using the following equation:

$$
\begin{aligned}
DH_{der}(c) = {} & C_{soil}(c) \times AF_{soil} \times ABS(c) \times SA_{soil} \times EF_{soil} \times CF1 \times ED \times CF7 / (BW_{adult} \times AT) + \\
& C_{sed}(c) \times AF_{sed} \times ABS(c) \times SA_{sed} \times EF_{sed} \times CF1 \times ED \times CF7 / (BW_{adult} \times AT) + \\
& C_{seep}(c) \times K_p(c) \times SA_{seep} \times ET_{seep} \times EF_{seep} \times CF3 \times ED \times CF7 / (BW_{adult} \times AT) + \\
& C_{surface}(c) \times K_p(c) \times SA_{swim} \times ET_{swim} \times EF_{swim} \times CF3 \times ED \times CF7 / (BW_{adult} \times AT) + \\
& C_{sweat}(c) \times K_p(c) \times SA_{sweat} \times ET_{sweat} \times EF_{sweat} \times CF3 \times ED \times CF7 / (BW_{adult} \times AT) + \\
& C_{shower}(c) \times K_p(c) \times SA_{shower} \times ET_{shower} \times EF_{shower} \times CF3 \times ED \times CF7 / (BW_{adult} \times AT)
\end{aligned}
\qquad (14.1)
$$

where
$DH_{der}(c)$ = dose from dermal absorption of hazardous chemical c (mg/kg/d)
$C_{soil}(c)$ = concentration of contaminant c in soil (μg/kg)
AF_{soil} = adherence factor for soil (mg/cm^2/d)
$ABS(c)$ = material-specific factor to convert administered to absorbed dose for contaminant c (unitless)
SA_{soil} = body surface area exposed to soil (cm^2)
EF_{soil} = exposure frequency to soil (d/yr)
CF1 = unit conversion factor (lE-6 kg/mg)
ED = exposure duration (yr)
CF7 = conversion factor (1E-3 mg/μg)
BW_{adult} = body weight factor of an adult (kg)
AT = averaging time (yr × 365.25 d/yr)
$C_{sed}(c)$ = concentration of contaminant c in sediment (μg/kg)
AF_{sed} = adherence factor for sediment (mg/cm^2/d)
SA_{sed} = body surface area exposed to sediment (cm^2)
EF_{sed} = exposure frequency to sediment (d/yr)
$C_{seep}(c)$ = concentration of contaminant c in seep/spring water (μg/L)
$K_p(c)$ = permeability coefficient for contaminant c in water through skin (cm/hr)
SA_{seep} = body surface area exposed to seep/spring water (cm^2)
ET_{seep} = exposure time to seep/spring water (hr/d)
EF_{seep} = exposure frequency to seep/spring water (d/yr)
CF3 = unit conversion factor (1E-3 L/cm^3)
$C_{surface}(c)$ = concentration of contaminant c in surface water (μg/L)
SA_{swim} = body surface area exposed while swimming (cm^2)
ET_{swim} = exposure time to swimming in surface water (hr/d)
EF_{swim} = exposure frequency to swimming in surface water (d/yr)
$C_{sweat}(c)$ = concentration of contaminant c in sweat lodge water (μg/L)
SA_{sweat} = body surface area exposed to sweat lodge water (cm^2)
ET_{sweat} = exposure time to sweat lodge water (hr/d)
EF_{sweat} = exposure frequency to sweat lodge water (d/yr)
$C_{shower}(c)$ = concentration of contaminant c in shower water (μg/L)
SA_{shower} = body surface area exposed to shower water (cm^2)
ET_{shower} = exposure time to shower water (hr/d)
EF_{shower} = exposure frequency to shower water (d/yr)

The noncancer hazard quotient from dermal contact with non-carcinogenic, non-radioactive materials is computed from dose using the following equation:

$$HQ_{der}(c) = DH_{der}(c) / RfD_{ing}(c) \quad (14.2)$$

where $HQ_{der}(c)$ = hazard quotient from dermal absorption of hazardous chemical c (unitless)
$DH_{der}(c)$ = dose from dermal absorption of hazardous chemical c (mg/kg/d)
$RfD_{ing}(c)$ = reference dose for ingestion of hazardous chemical c (mg/kg/d)

14.1.1.2 Dermal Exposure (Carcinogenic, Non-Radioactive)

The dose from dermal contact with carcinogenic, non-radioactive materials is computed for a number of activities using the following equation:

$$\begin{aligned} DC_{der}(c) = {} & C_{soil}(c) \times AF_{soil} \times ABS(c) \times SA_{soil} \times EF_{soil} \times CF1 \times ED \times CF7 / (BW_{adult} \times AT) + \\ & C_{sed}(c) \times AF_{sed} \times ABS(c) \times SA_{sed} \times EF_{sed} \times CF1 \times ED \times CF7 / (BW_{adult} \times AT) + \\ & C_{seep}(c) \times K_p(c) \times SA_{seep} \times ET_{seep} \times EF_{seep} \times CF3 \times ED \times CF7 / (BW_{adult} \times AT) + \\ & C_{surface}(c) \times K_p(c) \times SA_{swim} \times ET_{swim} \times EF_{swim} \times CF3 \times ED \times CF7 / (BW_{adult} \times AT) + \\ & C_{sweat}(c) \times K_p(c) \times SA_{sweat} \times ET_{sweat} \times EF_{sweat} \times CF3 \times ED \times CF7 / (BW_{adult} \times AT) + \\ & C_{shower}(c) \times K_p(c) \times SA_{shower} \times ET_{shower} \times EF_{shower} \times CF3 \times ED \times CF7 / (BW_{adult} \times AT) \end{aligned} \quad (14.3)$$

where $DC_{der}(c)$ = dose from dermal absorption of carcinogenic contaminant c (mg/kg/d)
$C_{soil}(c)$ = concentration of contaminant c in soil (μg/kg)
AF_{soil} = adherence factor for soil ($mg/cm^2/d$)
$ABS(c)$ = material-specific factor to convert administered to absorbed dose for contaminant c (unitless)
SA_{soil} = body surface area exposed to soil (cm^2)
EF_{soil} = exposure frequency to soil (d/yr)
CF1 = unit conversion factor (lE-6 kg/mg)
ED = exposure duration (yr)
CF7 = conversion factor (1E-3 mg/μg)
BW_{adult} = body weight factor of an adult (kg)
AT = averaging time (yr × 365.25 d/yr)
$C_{sed}(c)$ = concentration of contaminant c in sediment (μg/kg)
AF_{sed} = adherence factor for sediment ($mg/cm^2/d$)
SA_{sed} = body surface area exposed to sediment (cm^2)
EF_{sed} = exposure frequency to sediment (d/yr)
$C_{seep}(c)$ = concentration of contaminant c in seep/spring water (μg/L)
$K_p(c)$ = permeability coefficient for contaminant c in water through skin (cm/hr)
SA_{seep} = body surface area exposed to seep/spring water (cm^2)
ET_{seep} = exposure time to seep/spring water (hr/d)
EF_{seep} = exposure frequency to seep/spring water (d/yr)
CF3 = unit conversion factor (1E-3 L/cm^3)
$C_{surface}(c)$ = concentration of contaminant c in surface water for swimming (μg/L)
SA_{swim} = body surface area exposed while swimming (cm^2)
ET_{swim} = exposure time to swimming in surface water (hr/d)
EF_{swim} = exposure frequency to swimming in surface water (d/yr)
$C_{sweat}(c)$ = concentration of contaminant c in sweat lodge water (μg/L)
SA_{sweat} = body surface area exposed to sweat lodge water (cm^2)
ET_{sweat} = exposure time to sweat lodge water (hr/d)
EF_{sweat} = exposure frequency to sweat lodge water (d/yr)
$C_{shower}(c)$ = concentration of contaminant c in shower water (μg/L)

SA_{shower} = body surface area exposed to shower water (cm^2)
ET_{shower} = exposure time to shower water (hr/d)
EF_{shower} = exposure frequency to shower water (d/yr)

The risk from dermal contact with carcinogenic, non-radioactive materials is computed from dose using the following equation:

$$RC_{der}(c) = DC_{der}(c) \times SF_{ing}(c) \quad (14.4)$$

where $RC_{der}(c)$= risk from dermal absorption of carcinogenic chemical c (risk)
$DC_{der}(c)$ = dose from dermal absorption of carcinogenic chemical c (mg/kg/d)
$SF_{ing}(c)$ = slope factor for ingestion of carcinogenic chemical c (risk per mg/kg/d)

14.1.1.3 External Radiation Exposure

The radiation dose from external radiation sources is computed for a number of activities using the following equation:

$$\begin{aligned} R_{ext}(c) = {} & C_{surface}(c) \times ET_{swim} \times EF_{swim} \times ED \times RCF_{swim}(c) + \\ & C_{surface}(c) \times ET_{boat} \times EF_{boat} \times ED \times RCF_{boat}(c) + \\ & C_{soil}(c) \times SH_{soil} \times ET_{soil} \times EF_{soil} \times ED \times RCF_{soil}(c) + \\ & C_{sed}(c) \times SH_{sed} \times ET_{sed} \times EF_{sed} \times ED \times RCF_{soil}(c) \end{aligned} \quad (14.5)$$

where $R_{ext}(c)$ = dose or risk from external radionuclide c (rem or risk)
$C_{surface}(c)$ = concentration of radionuclide c in surface water (pCi/L)
ET_{swim} = exposure time for swimming (hr/d)
EF_{swim} = exposure frequency for swimming (d/yr)
ED = exposure duration (yr)
$RCF_{swim}(c)$ = dose or risk conversion factor for swimming for radionuclide c (rem/hr per pCi/L or risk/hr per pCi/L)
ET_{boat} = exposure time for boating (hr/d)
EF_{boat} = exposure frequency for boating (d/yr)
$RCF_{boat}(c)$ = dose or risk conversion factor for boating for radionuclide c (rem/hr per pCi/L or risk/hr per pCi/L)
$C_{soil}(c)$ = concentration of radionuclide c in soil (pCi/kg)
SH_{soil} = shielding factor for soil (unitless)
ET_{soil} = exposure time for soil (hr/d)
EF_{soil} = exposure frequency for soil (d/yr)
$RCF_{soil}(c)$ = dose or risk conversion factor for soil and sediment for radionuclide c (rem/hr per pCi/kg or risk/hr per pCi/kg)
$C_{sed}(c)$ = concentration of radionuclide c in sediment (pCi/kg)
SH_{sed} = shielding factor for sediment (unitless)
ET_{sed} = exposure time for sediment (hr/d)
EF_{sed} = exposure frequency for sediment (d/yr)

14.1.1.4 Inhalation Exposure (Hazardous)

The dose from inhalation of non-carcinogenic, non-radioactive, materials is computed for a number of activities using the following equation:

$$DH_{inh}(c) = C_{soil}(c) \times ML \times ET_{soil} \times EF_{soil} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4) +$$
$$C_{seep}(c) \times VF(c) \times ET_{seep} \times EF_{seep} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4) +$$
$$C_{surface}(c) \times VF(c) \times ET_{surface} \times EF_{surface} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4) +$$
$$C_{air}(c) \times ET_{air} \times EF_{air} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4) + \quad (14.6)$$
$$C_{sweat}(c) \times CF_{sweat} \times ET_{sweat} \times EF_{sweat} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4) +$$
$$C_{shower}(c) \times CF_{shower} \times ET_{shower} \times EF_{shower} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4)$$

where $DH_{inh}(c)$ = dose from chronic inhalation of hazardous chemical c (mg/kg/d)
$C_{soil}(c)$ = concentration of contaminant c in soil (µg/kg)
ML = mass loading of soil in the air (kg/m^3)
ET_{soil} = exposure time for breathing soil (hr/d)
EF_{soil} = exposure frequency to soil (d/yr)
ED = exposure duration (yr)
IRATE = inhalation rate (m^3/d)
CF7 = conversion factor (1E-3 mg/µg)
AT = averaging time (yr × 365.25 d/yr)
BW_{adult} = body weight (kg)
CF4 = unit conversion factor (24 hr/d)
$C_{seep}(c)$ = concentration of contaminant c in seep/spring water (µg/L)
VF(c) = volatilization factor for contaminant c (L/m^3)
ET_{seep} = exposure time for breathing volatilized seep/spring water (hr/d)
EF_{seep} = exposure frequency to volatilized seep/spring water (d/yr)
$C_{surface}(c)$ = concentration of contaminant c in surface water (µg/L)
$ET_{surface}$ = exposure time for breathing volatilized surface water (hr/d)
$EF_{surface}$ = exposure frequency to volatilized surface water (d/yr)
$C_{air}(c)$ = concentration of contaminant c in air ($\mu g/m^3$)
ET_{air} = exposure time for breathing contaminated air (hr/d)
EF_{air} = exposure frequency to contaminated air (d/yr)
$C_{sweat}(c)$ = concentration of contaminant c in sweat lodge water (µg/L)
CF_{sweat} = volatilization factor for water used in Native American sweat lodges (L/m^3)
ET_{sweat} = exposure time for breathing in a sweat lodge (hr/d)
EF_{sweat} = exposure frequency to a sweat lodge (d/yr)
$C_{shower}(c)$ = concentration of contaminant c in shower water (µg/L)
CF_{shower} = volatilization factor for water used in an enclosed shower (L/m^3)
ET_{shower} = exposure time for breathing volatilized shower water (hr/d)
EF_{shower} = exposure frequency to volatilized shower water (d/yr)

The noncancer hazard quotient from inhalation of non-carcinogenic, non-radioactive materials is computed from dose using the following equation:

$$HQ_{inh}(c) = DH_{inh}(c) / RfD_{inh}(c) \quad (14.7)$$

where $HQ_{inh}(c)$ = hazard quotient from inhalation of hazardous chemical c (unitless)
$DH_{inh}(c)$ = dose from inhalation of hazardous chemical c (mg/kg/d)
$RfD_{inh}(c)$ = reference dose for inhalation of hazardous chemical c (mg/kg/d)

14.1.1.5 Inhalation Exposure (Carcinogenic)

The dose from inhalation of carcinogenic materials is computed for a number of activities using the following equation:

$$\begin{aligned} DC_{inh}(c) = {} & C_{soil}(c) \times ML \times ET_{soil} \times EF_{soil} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4) + \\ & C_{seep}(c) \times VF(c) \times ET_{seep} \times EF_{seep} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4) + \\ & C_{surface}(c) \times VF(c) \times ET_{surface} \times EF_{surface} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4) + \\ & C_{air}(c) \times ET_{air} \times EF_{air} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4) + \\ & C_{sweat}(c) \times CF_{sweat} \times ET_{sweat} \times EF_{sweat} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4) + \\ & C_{shower}(c) \times CF_{shower} \times ET_{shower} \times EF_{shower} \times ED \times IRATE \times CF7/(AT \times BW_{adult} \times CF4) \end{aligned} \quad (14.8)$$

where $DC_{inh}(c)$ = dose from chronic inhalation of carcinogenic chemical c (mg/kg/d)
$C_{soil}(c)$ = concentration of contaminant c in soil (µg/kg)
ML = mass loading of soil in the air (kg/m^3)
ET_{soil} = exposure time for breathing soil (hr/d)
EF_{soil} = exposure frequency to soil (d/yr)
ED = exposure duration (yr)
IRATE = inhalation (breathing) rate (m^3/d)
CF7 = conversion factor (1E-3 mg/µg)
AT = averaging time (yr × 365.25 d/yr)
BW_{adult} = body weight (kg)
CF4 = unit conversion factor (24 hr/d)
$C_{seep}(c)$ = concentration of contaminant c in seep/spring water (µg/L)
VF(c) = volatilization factor for contaminant c (L/m^3)
ET_{seep} = exposure time for breathing volatilized seep/spring water (hr/d)
EF_{seep} = exposure frequency to volatilized seep/spring water (d/yr)
$C_{surface}(c)$ = concentration of contaminant c in surface water (µg/L)
$ET_{surface}$ = exposure time for breathing volatilized surface water (hr/d)
$EF_{surface}$ = exposure frequency to volatilized surface water (d/yr)
$C_{air}(c)$ = concentration of contaminant c in air ($\mu g/m^3$)
ET_{air} = exposure time for breathing contaminated air (hr/d)
EF_{air} = exposure frequency to volatilized air (d/yr)
$C_{sweat}(c)$ = concentration of contaminant c in sweat lodge water (µg/L)
CF_{sweat} = volatilization factor for water used in Native American sweat lodges (L/m^3)
ET_{sweat} = exposure time for breathing in a sweat lodge (hr/d)
EF_{sweat} = exposure frequency to a sweat lodge (d/yr)
$C_{shower}(c)$ = concentration of contaminant c in shower water (µg/L)
CF_{shower} = volatilization factor for water used in an enclosed shower (L/m^3)
ET_{shower} = exposure time for breathing volatilized shower water (hr/d)
EF_{shower} = exposure frequency to volatilized shower water (d/yr)

The risk from inhalation of carcinogenic, non-radioactive materials is computed from dose using the following equation:

$$RC_{inh}(c) = DC_{inh}(c) \times SF_{inh}(c) \quad (14.9)$$

where $RC_{inh}(c)$ = risk from inhalation of carcinogenic chemical c (risk)
$DC_{inh}(c)$ = dose from inhalation of carcinogenic chemical c (mg/kg/d)

$SF_{inh}(c)$ = slope factor for inhalation of carcinogenic chemical c (risk per mg/kg/d)

14.1.1.6 Inhalation Exposure (Radioactive)

The radiation dose from inhalation of radioactive materials is computed for a number of activities using the following equation:

$$\begin{aligned} R_{inh}(c) = {} & C_{soil}(c) \times ML \times ET_{soil} \times EF_{soil} \times ED \times IRATE \times RCF_{inh}(c) / CF4 + \\ & C_{seep}(c) \times VF(c) \times ET_{seep} \times EF_{seep} \times ED \times IRATE \times RCF_{inh}(c) / CF4 + \\ & C_{surface}(c) \times VF(c) \times ET_{surface} \times EF_{surface} \times ED \times IRATE \times RCF_{inh}(c) / CF4 + \\ & C_{air}(c) \times ET_{air} \times EF_{air} \times ED \times IRATE \times RCF_{inh}(c) / CF4 + \\ & C_{sweat}(c) \times CF_{sweat} \times ET_{sweat} \times EF_{sweat} \times ED \times IRATE \times RCF_{inh}(c) / CF4 + \\ & C_{shower}(c) \times CF_{shower} \times ET_{shower} \times EF_{shower} \times ED \times IRATE \times RCF_{inh}(c) / CF4 \end{aligned} \quad (14.10)$$

where $R_{inh}(c)$ = dose from inhalation of radionuclide c (rem)
$C_{soil}(c)$ = concentration of radionuclide c in soil (pCi/kg)
ML = mass loading of soil in the air (kg/m^3)
ET_{soil} = exposure time for breathing volatilized soil (hr/d)
EF_{soil} = exposure frequency to volatilized soil (d/yr)
ED = exposure duration (yr)
$IRATE$ = inhalation rate (m^3/d)
$RCF_{inh}(c)$ = dose or risk conversion factor for inhalation of radionuclide c (rem/pCi or risk/pCi)
$CF4$ = unit conversion factor (24 hr/d)
$C_{seep}(c)$ = concentration of radionuclide c in seep/spring water (pCi/L)
$VF(c)$ = volatilization factor for radionuclide c (L/m^3)
ET_{seep} = exposure time for breathing volatilized seep/spring water (hr/d)
EF_{seep} = exposure frequency to volatilized seep/spring water (d/yr)
$C_{surface}(c)$ = concentration of radionuclide c in surface water (pCi/L)
$ET_{surface}$ = exposure time for breathing volatilized surface water (hr/d)
$EF_{surface}$ = exposure frequency to volatilized surface water (d/yr)
$C_{air}(c)$ = concentration of radionuclide c in air (pCi/m^3)
ET_{air} = exposure time for breathing contaminated air (hr/d)
EF_{air} = exposure frequency to contaminated air (d/yr)
$C_{sweat}(c)$ = concentration of radionuclide c in sweat lodge water (pCi/L)
CF_{sweat} = volatilization factor for water used in Native American sweat lodges (L/m^3)
ET_{sweat} = exposure time for breathing materials suspended during cultural activities (hr/d)
EF_{sweat} = exposure frequency to materials resuspended during cultural activities (d/yr)
$C_{shower}(c)$ = concentration of radionuclide c in shower water (pCi /L)
CF_{shower} = volatilization factor for water used in showering (L/m^3)
ET_{shower} = exposure time for breathing volatilized shower water (hr/d)
EF_{shower} = exposure frequency to volatilized shower water (d/yr)

14.1.1.7 Ingestion Exposure (Hazardous)

The dose from ingestion of non-carcinogenic, non-radioactive materials is computed for a number of activities using the following equation:

$$\begin{aligned} DH_{ing}(c) = {} & C_{surface}(c) \times IR_{surface} \times ED \times EF_{surface} \times CF7 / (AT \times BW_{adult}) + \\ & C_{ground}(c) \times IR_{ground} \times ED \times EF_{ground} \times CF7 / (AT \times BW_{adult}) + \end{aligned}$$

$$
\begin{aligned}
&C_{seep}(c) \times IR_{seep} \times ED \times EF_{seep} \times CF7 / (AT \times BW_{adult}) + \\
&C_{soil}(c) \times IR_{soilchild} \times ED_{child} \times EF_{soil} \times CF7 / (AT \times BW_{child}) + \\
&C_{soil}(c) \times IR_{soiladult} \times ED_{adult} \times EF_{soil} \times CF7 / (AT \times BW_{adult}) + \\
&C_{sed}(c) \times IR_{sedchild} \times ED_{child} \times EF_{sed} \times CF7 / (AT \times BW_{child}) + \\
&C_{sed}(c) \times IR_{sedadult} \times ED_{adult} \times EF_{sed} \times CF7 / (AT \times BW_{adult}) + \\
&C_{leafy}(c) \times IR_{leafy} \times ED \times EF_{leafy} \times CF7 / (AT \times BW_{adult}) + \\
&C_{root}(c) \times IR_{root} \times ED \times EF_{root} \times CF7 / (AT \times BW_{adult}) + \\
&C_{fruit}(c) \times IR_{fruit} \times ED \times EF_{fruit} \times CF7 / (AT \times BW_{adult}) + \\
&C_{grain}(c) \times IR_{grain} \times ED \times EF_{grain} \times CF7 / (AT \times BW_{adult}) + \\
&C_{meat}(c) \times IR_{meat} \times ED \times EF_{meat} \times CF7 / (AT \times BW_{adult}) + \\
&C_{milk}(c) \times IR_{milk} \times ED \times EF_{milk} \times CF7 / (AT \times BW_{adult}) + \\
&C_{bird}(c) \times IR_{bird} \times ED \times EF_{bird} \times CF7 / (AT \times BW_{adult}) + \\
&C_{eggs}(c) \times IR_{eggs} \times ED \times EF_{eggs} \times CF7 / (AT \times BW_{adult}) + \\
&C_{fish}(c) \times IR_{fish} \times ED \times EF_{fish} \times CF7 / (AT \times BW_{adult}) + \\
&C_{fish\_2}(c) \times IR_{fish\_2} \times ED \times EF_{fish\_2} \times CF7 / (AT \times BW_{adult}) + \\
&C_{fish\_3}(c) \times IR_{fish\_3} \times ED \times EF_{fish\_3} \times CF7 / (AT \times BW_{adult})
\end{aligned}
\qquad (14.11)
$$

where $DH_{ing}(c)$ = dose from chronic ingestion of hazardous chemical c (mg/kg/d)

$C_{surface}(c)$ = concentration of contaminant c in surface water (μg/L)

$IR_{surface}$ = ingestion rate of surface water (L/d)

ED = lifetime exposure duration (yr)

$EF_{surface}$ = exposure frequency for surface (d/yr)

$CF7$ = conversion factor (1E-3 mg/μg)

AT = averaging time (yr × 365 d/yr)

BW_{adult} = body weight for adult (kg)

$C_{ground}(c)$ = concentration of contaminant c in groundwater (μg/L)

IR_{ground} = ingestion rate of groundwater (L/d)

EF_{ground} = exposure frequency for ground (d/yr)

$C_{seep}(c)$ = concentration of contaminant c in seep/spring water (μg/L)

IR_{seep} = ingestion rate of seep/spring water (L/d)

EF_{seep} = exposure frequency for seep (d/yr)

$C_{soil}(c)$ = concentration of contaminant c in soil (μg/kg)

$IR_{soilchild}$ = ingestion rate of soil by a child (kg/d)

ED_{child} = exposure duration for a child (yr)

EF_{soil} = exposure frequency for a bird (d/yr)

BW_{child} = body weight for adult (kg)

$IR_{soiladult}$ = ingestion rate of soil by an adult (kg/d)

ED_{adult} = exposure duration for an adult (yr)

$C_{sed}(c)$ = concentration of contaminant c in sediment (μg/kg)

$IR_{sedchild}$ = ingestion rate of sediment by a child (kg/d)

EF_{sed} = exposure frequency for sediment (d/yr)

$IR_{sedadult}$ = ingestion rate of sediment by an adult (kg/d)

$C_{leafy}(c)$ = concentration of contaminant c in above-ground vegetation (μg/kg)

IR_{leafy} = ingestion rate of above-ground vegetation (kg/d)

EF_{leafy} = exposure frequency for above-ground vegetation (d/yr)

$C_{root}(c)$ = concentration of contaminant c in root vegetables (μg/kg)

IR_{root} = ingestion rate of root vegetables (kg/d)

EF_{root} = exposure frequency for a root (d/yr)

$C_{fruit}(c)$ = concentration of contaminant c in fruit (μg/kg)

IR_{fruit} = ingestion rate of fruit (kg/d)
EF_{fruit} = exposure frequency for a fruit (d/yr)
$C_{grain}(c)$ = concentration of contaminant c in grain (μg/kg)
IR_{grain} = ingestion rate of grain (kg/d)
EF_{grain} = exposure frequency for a grain (d/yr)
$C_{meat}(c)$ = concentration of contaminant c in meat (μg/kg)
IR_{meat} = ingestion rate of meat (kg/d)
EF_{meat} = exposure frequency for meat (d/yr)
$C_{milk}(c)$ = concentration of contaminant c in milk (μg/L)
IR_{milk} = ingestion rate of milk (L/d)
EF_{milk} = exposure frequency for milk (d/yr)
$C_{bird}(c)$ = concentration of contaminant c in domestic and wild birds (μg/kg)
IR_{bird} = ingestion rate of domestic and wild birds (kg/d)
EF_{bird} = exposure frequency for a bird (d/yr)
$C_{eggs}(c)$ = concentration of contaminant c in eggs (μg/kg)
IR_{eggs} = ingestion rate of eggs (kg/d)
EF_{eggs} = exposure frequency for a eggs (d/yr)
$C_{fish}(c)$ = concentration of contaminant c in fish (μg/kg)
IR_{fish} = ingestion rate of fish (kg/d)
EF_{fish} = exposure frequency for a fish (d/yr)
$C_{fish\_2}(c)$ = concentration of contaminant c in second variety of fish (μg/kg)
IR_{fish_2} = ingestion rate of second variety of fish (kg/d)
EF_{fish_2} = exposure frequency for second variety of fish (d/yr)
$C_{fish\_3}(c)$ = concentration of contaminant c in third variety of fish (μg/kg)
IR_{fish_3} = ingestion rate of third variety of fish (kg/d)
EF_{fish_3} = exposure frequency for third variety of fish (d/yr)

The noncancer hazard quotient from ingestion of non-carcinogenic, non-radioactive materials is computed from the ingestion dose using the following equation:

$$HQ_{ing}(c) = DH_{ing}(c) / RfD_{ing}(c) \quad (14.12)$$

Where $HQ_{ing}(c)$ = hazard quotient from ingestion of hazardous chemical c (unitless)
$DH_{ing}(c)$ = dose from ingestion of hazardous chemical c (mg/kg/d)
$RfD_{ing}(c)$ = reference dose for ingestion of hazardous chemical c (mg/kg/d)

14.1.1.8 Ingestion Exposure (Carcinogenic)

The dose from ingestion of carcinogenic, non-radioactive materials is computed for a number of activities using the following equation:

$$\begin{aligned} DC_{ing}(c) = {} & C_{surface}(c) \times IR_{surface} \times ED \times EF_{surface} \times CF7 / (AT \times BW_{adult}) + \\ & C_{ground}(c) \times IR_{ground} \times ED \times EF_{ground} \times CF7 / (AT \times BW_{adult}) + \\ & C_{seep}(c) \times IR_{seep} \times ED \times EF_{seep} \times CF7 / (AT \times BW_{adult}) + \\ & C_{soil}(c) \times IR_{soilchild} \times ED_{child} \times EF_{soil} \times CF7 / (AT \times BW_{child}) + \\ & C_{soil}(c) \times IR_{soiladult} \times ED_{adult} \times EF_{soil} \times CF7 / (AT \times BW_{adult}) + \\ & C_{sed}(c) \times IR_{sedchild} \times ED_{child} \times EF_{sed} \times CF7 / (AT \times BW_{child}) + \\ & C_{sed}(c) \times IR_{sedadult} \times ED_{adult} \times EF_{sed} \times CF7 / (AT \times BW_{adult}) + \\ & C_{leafy}(c) \times IR_{leafy} \times ED \times EF_{leafy} \times CF7 / (AT \times BW_{adult}) + \end{aligned}$$

$$C_{root}(c) \times IR_{root} \times ED \times EF_{root} \times CF7 / (AT \times BW_{adult}) + \quad (14.13)$$
$$C_{fruit}(c) \times IR_{fruit} \times ED \times EF_{fruit} \times CF7 / (AT \times BW_{adult}) +$$
$$C_{grain}(c) \times IR_{grain} \times ED \times EF_{grain} \times CF7 / (AT \times BW_{adult}) +$$
$$C_{meat}(c) \times IR_{meat} \times ED \times EF_{meat} \times CF7 / (AT \times BW_{adult}) +$$
$$C_{milk}(c) \times IR_{milk} \times ED \times EF_{milk} \times CF7 / (AT \times BW_{adult}) +$$
$$C_{bird}(c) \times IR_{bird} \times ED \times EF_{bird} \times CF7 / (AT \times BW_{adult}) +$$
$$C_{eggs}(c) \times IR_{eggs} \times ED \times EF_{eggs} \times CF7 / (AT \times BW_{adult}) +$$
$$C_{fish}(c) \times IR_{fish} \times ED \times EF_{fish} \times CF7 / (AT \times BW_{adult}) +$$
$$C_{fish\_2}(c) \times IR_{fish\_2} \times ED \times EF_{fish\_2} \times CF7 / (AT \times BW_{adult}) +$$
$$C_{fish\_3}(c) \times IR_{fish\_3} \times ED \times EF_{fish\_3} \times CF7 / (AT \times BW_{adult})$$

where $DC_{ing}(c)$ = dose from chronic ingestion of carcinogenic chemical c (mg/kg/d)

$C_{surface}(c)$ = concentration of contaminant c in surface water (μg/L)
$IR_{surface}$ = ingestion rate of surface water (L/d)
ED = lifetime exposure duration (yr)
$EF_{surface}$ = exposure frequency for surface water (d/yr)
$CF7$ = conversion factor (1E-3 mg/μg)
AT = averaging time (yr × 365 d/yr)
BW_{adult} = body weight for adult (kg)
$C_{ground}(c)$ = concentration of contaminant c in groundwater (μg/L)
IR_{ground} = ingestion rate of groundwater (L/d)
EF_{ground} = exposure frequency for ground (d/yr)
$C_{seep}(c)$ = concentration of contaminant c in seep/spring water (μg/L)
IR_{seep} = ingestion rate of seep/spring water (L/d)
EF_{seep} = exposure frequency for seep (d/yr)
$C_{soil}(c)$ = concentration of contaminant c in soil (μg/kg)
$IR_{soilchild}$ = ingestion rate of soil by a child (kg/d)
ED_{child} = exposure duration for a child (yr)
EF_{soil} = exposure frequency for a bird (d/yr)
BW_{child} = body weight for adult (kg)
$IR_{soiladult}$ = ingestion rate of soil by an adult (kg/d)
ED_{adult} = exposure duration for an adult (yr)
$C_{sed}(c)$ = concentration of contaminant c in sediment (μg/kg)
$IR_{sedchild}$ = ingestion rate of sediment by a child (kg/d)
EF_{sed} = exposure frequency for sediment (d/yr)
$IR_{sedadult}$ = ingestion rate of sediment by an adult (kg/d)
$C_{leafy}(c)$ = concentration of contaminant c in above-ground vegetation (μg/kg)
IR_{leafy} = ingestion rate of above-ground vegetation (kg/d)
EF_{leafy} = exposure frequency for above-ground vegetation (d/yr)
$C_{root}(c)$ = concentration of contaminant c in root vegetables (μg/kg)
IR_{root} = ingestion rate of root vegetables (kg/d)
EF_{root} = exposure frequency for a root (d/yr)
$C_{fruit}(c)$ = concentration of contaminant c in fruit (μg/kg)
IR_{fruit} = ingestion rate of fruit (kg/d)
EF_{fruit} = exposure frequency for a fruit (d/yr)
$C_{grain}(c)$ = concentration of contaminant c in grain (μg/kg)
IR_{grain} = ingestion rate of grain (kg/d)
EF_{grain} = exposure frequency for a grain (d/yr)
$C_{meat}(c)$ = concentration of contaminant c in meat (μg/kg)

IR_{meat} = ingestion rate of meat (kg/d)
EF_{meat} = exposure frequency for meat (d/yr)
$C_{milk}(c)$ = concentration of contaminant c in milk (μg/L)
IR_{milk} = ingestion rate of milk (L/d)
EF_{milk} = exposure frequency for milk (d/yr)
$C_{bird}(c)$ = concentration of contaminant c in domestic and wild birds (μg/kg)
IR_{bird} = ingestion rate of domestic and wild birds (kg/d)
EF_{bird} = exposure frequency for a bird (d/yr)
$C_{eggs}(c)$ = concentration of contaminant c in eggs (μg/kg)
IR_{eggs} = ingestion rate of eggs (kg/d)
EF_{eggs} = exposure frequency for a eggs (d/yr)
$C_{fish}(c)$ = concentration of contaminant c in fish (μg/kg)
IR_{fish} = ingestion rate of fish (kg/d)
EF_{fish} = exposure frequency for a fish (d/yr)
$C_{fish\_2}(c)$ = concentration of contaminant c in second variety of fish (μg/kg)
IR_{fish_2} = ingestion rate of second variety of fish (kg/d)
EF_{fish_2} = exposure frequency for second variety of fish (d/yr)
$C_{fish\_3}(c)$ = concentration of contaminant c in third variety of fish (μg/kg)
IR_{fish_3} = ingestion rate of third variety of fish (kg/d)
EF_{fish_3} = exposure frequency for third variety of fish (d/yr)

The risk from ingestion of carcinogenic, non-radioactive materials is computed from dose using the following equation:

$$RC_{ing}(c) = DC_{ing}(c) \times SF_{ing}(c) \tag{14.14}$$

where $RC_{ing}(c)$= risk from chronic ingestion of carcinogenic chemical c (risk)
$DC_{ing}(c)$ = dose from chronic ingestion of carcinogenic chemical c (mg/kg/d)
$SF_{ing}(c)$ = slope factor for chronic ingestion of carcinogenic chemical c (risk per mg/kg/d)

14.1.1.9 Ingestion Exposure (Radioactive)

The dose from ingestion of radioactive materials is computed for a number of activities using the following equation:

$$\begin{aligned} R_{ing}(c) = {} & C_{surface}(c) \times IR_{surface} \times ED \times EF_{surface} \times RCF_{ing}(c) + \\ & C_{ground}(c) \times IR_{ground} \times ED \times EF_{ground} \times RCF_{ing}(c) + \\ & C_{seep}(c) \times IR_{seep} \times ED \times EF_{seep} \times RCF_{ing}(c) + \\ & C_{soil}(c) \times (IR_{soilchild} \times ED_{child} + IR_{soiladult} \times ED_{adult}) \times EF_{soil} \times RCF_{ing}(c) + \\ & C_{sed}(c) \times (IR_{sedchild} \times ED_{child} + IR_{sedadult} \times ED_{adult}) \times EF_{sed} \times RCF_{ing}(c) + \\ & C_{leafy}(c) \times IR_{leafy} \times ED \times EF_{leafy} \times RCF_{ing}(c) + \\ & C_{root}(c) \times IR_{root} \times ED \times EF_{root} \times RCF_{ing}(c) + \\ & C_{fruit}(c) \times IR_{fruit} \times ED \times EF_{fruit} \times RCF_{ing}(c) + \\ & C_{grain}(c) \times IR_{grain} \times ED \times EF_{grain} \times RCF_{ing}(c) + \\ & C_{meat}(c) \times IR_{meat} \times ED \times EF_{meat} \times RCF_{ing}(c) + \\ & C_{milk}(c) \times IR_{milk} \times ED \times EF_{milk} \times RCF_{ing}(c) + \\ & C_{bird}(c) \times IR_{bird} \times ED \times EF_{bird} \times RCF_{ing}(c) + \\ & C_{eggs}(c) \times IR_{eggs} \times ED \times EF_{eggs} \times RCF_{ing}(c) + \\ & C_{fish}(c) \times IR_{fish} \times ED \times EF_{fish} \times RCF_{ing}(c) + \end{aligned} \tag{14.15}$$

$$C_{fish\_2}(c) \times IR_{fish\_2} \times ED \times EF_{fish\_2} \times RCF_{ing}(c) +$$
$$C_{fish\_3}(c) \times IR_{fish\_3} \times ED \times EF_{fish\_3} \times RCF_{ing}(c)$$

where
$R_{ing}(c)$ = dose from chronic ingestion of radionuclide c (rem)
$C_{surface}(c)$ = concentration of radionuclide c in surface water (pCi/L)
$IR_{surface}$ = ingestion rate of surface water (L/d)
$EF_{surface}$ = exposure frequency of an adult to surface water (d/yr)
ED = exposure duration (yr)
$RCF_{ing}(c)$ = dose or risk conversion factor for ingestion of radionuclide c (rem/pCi or risk/pCi)
$C_{ground}(c)$ = concentration of radionuclide c in groundwater (pCi/L)
IR_{ground} = ingestion rate of groundwater (L/d)
EF_{ground} = exposure frequency of an adult to groundwater (d/yr)
$C_{seep}(c)$ = concentration of radionuclide c in seep/spring water (pCi/L)
IR_{seep} = ingestion rate of seep/spring water (L/d)
EF_{seep} = exposure frequency of an adult to seep/spring water (d/yr)
$C_{soil}(c)$ = concentration of radionuclide c in soil (pCi/kg)
$IR_{soilchild}$ = ingestion rate of soil by a child (kg/d)
ED_{child} = exposure duration for a child (yr)
$IR_{soiladult}$ = ingestion rate of sediment by a child (kg/d)
ED_{adult} = exposure duration for an adult (yr)
EF_{soil} = exposure frequency of an adult to soil (d/yr)
$C_{sed}(c)$ = concentration of radionuclide c in sediment (pCi/kg)
$IR_{sedchild}$ = ingestion rate of sediment by a child (kg/d)
$IR_{sedadult}$ = ingestion rate of sediment by a child (kg/d)
EF_{sed} = exposure frequency of an adult to sediment (d/yr)
$C_{leafy}(c)$ = concentration of radionuclide c in above-ground vegetation (pCi/kg)
IR_{leafy} = ingestion rate of above-ground vegetation (kg/d)
EF_{leafy} = exposure frequency of an adult to leafy vegetables (d/yr)
$C_{root}(c)$ = concentration of radionuclide c in root vegetables (pCi/kg)
IR_{root} = ingestion rate of root vegetables (kg/d)
EF_{root} = exposure frequency of an adult to root vegetables (d/yr)
$C_{fruit}(c)$ = concentration of radionuclide c in fruit (pCi/kg)
IR_{fruit} = ingestion rate of fruit (kg/d)
EF_{fruit} = exposure frequency of an adult to fruit (d/yr)
$C_{grain}(c)$ = concentration of radionuclide c in grain (pCi/kg)
IR_{grain} = ingestion rate of grain (kg/d)
EF_{grain} = exposure frequency of an adult to grain (d/yr)
$C_{meat}(c)$ = concentration of radionuclide c in meat (pCi/kg)
IR_{meat} = ingestion rate of meat (kg/d)
EF_{meat} = exposure frequency of an adult to meat (d/yr)
$C_{milk}(c)$ = concentration of radionuclide c in milk (pCi/L)
IR_{milk} = ingestion rate of milk (L/d)
EF_{milk} = exposure frequency of an adult to milk (d/yr)
$C_{bird}(c)$ = concentration of radionuclide c in domestic and wild birds (pCi/kg)
IR_{bird} = ingestion rate of domestic and wild birds (kg/d)
EF_{bird} = exposure frequency of an adult to birds (d/yr)
$C_{eggs}(c)$ = concentration of radionuclide c in eggs (pCi/kg)
IR_{eggs} = ingestion rate of eggs (kg/d)
EF_{eggs} = exposure frequency of an adult to eggs (d/yr)
$C_{fish}(c)$ = concentration of radionuclide c in fish (pCi/kg)
IR_{fish} = ingestion rate of fish (kg/d)

EF_{fish} = exposure frequency of an adult to fish (d/yr)
$C_{fish\_2}(c)$ = concentration of radionuclide c in second variety of fish (pCi/kg)
IR_{fish_2} = ingestion rate of second variety of fish (kg/d)
EF_{fish_2} = exposure frequency of an adult to second variety of fish (d/yr)
$C_{fish\_3}(c)$ = concentration of radionuclide c in third variety of fish (pCi/kg)
IR_{fish_3} = ingestion rate of third variety of fish (kg/d)
EF_{fish_3} = exposure frequency of an adult to third variety of fish (d/yr)

14.1.1.10 Concentrations for Special Native American Activities

A unique Native American pathway involves use of a sweat lodge. The assumption for the sweat lodge was that water would be collected and poured over hot rocks to create steam. The concentration in the sweat lodge water comes from the following expression:

$$C_{sweat}(c) = C_{water}(c) \tag{14.16}$$

where $C_{sweat}(c)$ = concentration of contaminant c in sweat lodge water (pCi/L or µg/L)
$C_{water}(c)$ = concentration of contaminant c in the water source (pCi/L or µg/L)

The code implementation allows the choice of groundwater, seep water, or surface water for this calculation.

14.1.1.11 Water Concentration for Showering

The assumption for showering was that hot water would create steam in the enclosed shower stall. The concentration in the shower water comes from the following expression:

$$C_{shower}(c) = C_{water}(c) \tag{14.17}$$

where

$C_{shower}(c)$ = concentration of contaminant c in shower water (pCi/L or µg/L)
$C_{water}(c)$ = concentration of contaminant c in the water source (pCi/L or µg/L)

The code implementation allows the choice of groundwater, seep water, or surface water for this calculation.

14.1.2 Total Dose, Hazard, and Risk Calculations

Dose, hazard, and risk can be summed to provide an estimate of total effects across analytes and pathways. The following sections describe how results are summed to provide estimates of total dose, hazard, and risk.

14.1.2.1 Total Dose from Hazardous Chemicals

The total dose for all hazardous chemicals across all pathways comes from the following equation:

$$DH_{tot} = \sum_{c} DH_{der}(c) + \sum_{c} DH_{inh}(c) + \sum_{c} DH_{ing}(c) \quad (14.18)$$

where DH_{tot} = total dose from hazardous chemicals (mg/kg/d)
$DH_{der}(c)$ = dose from dermal absorption of hazardous chemical c (mg/kg/d)
$DH_{inh}(c)$ = dose from chronic inhalation of hazardous chemical c (mg/kg/d)
$DH_{ing}(c)$ = dose from ingestion of hazardous chemical c (mg/kg/d)

14.1.2.2 Total Dose from Carcinogenic Chemicals

The total dose for all carcinogenic chemicals across all pathways comes from the following equation:

$$DC_{tot} = \sum_{c} DC_{der}(c) + \sum_{c} DC_{inh}(c) + \sum_{c} DC_{ing}(c) \quad (14.19)$$

Where DC_{tot} = total dose from carcinogenic chemicals (mg/kg/d)
$DC_{der}(c)$ = dose from dermal absorption of carcinogenic chemical c (mg/kg/d)
$DC_{inh}(c)$ = dose from inhalation of carcinogenic chemical c (mg/kg/d)
$DC_{ing}(c)$ = dose from chronic ingestion of carcinogenic chemical c (mg/kg/d)

14.1.2.3 Total Dose from Radionuclides

The total dose for all radioactive analytes across all pathways comes from the following equation:

$$DR_{tot} = \sum_{c} R_{ext}(c) + \sum_{c} R_{inh}(c) + \sum_{c} R_{ing}(c) \quad (14.20)$$

where DR_{tot} = total dose from radionuclides (rem)
$R_{ext}(c)$ = dose from external exposure to radionuclide c (rem)
$R_{inh}(c)$ = dose from inhalation of radionuclide c (rem)
$R_{ing}(c)$ = dose from ingestion of radionuclide c (rem)

14.1.2.4 Total Hazard Index

The hazard index (HI) is the sum of the individual pathway hazard quotients. The hazard index is calculated using the following equation:

$$HI = \sum_{c} HQ_{der}(c) + \sum_{c} HQ_{inh}(c) + \sum_{c} HQ_{ing}(c) \quad (14.21)$$

where HI = total hazard index (unitless)
$HQ_{der}(c)$ = hazard quotient from dermal absorption of hazardous chemical c (unitless)
$HQ_{inh}(c)$ = hazard quotient from inhalation of hazardous chemical c (unitless)
$HQ_{ing}(c)$ = hazard quotient from ingestion of hazardous chemical c (unitless)

14.1.2.5 Total Risk from Carcinogenic Chemicals

The total lifetime risk of cancer incidence from exposure to carcinogenic chemicals is the sum of the individual pathway risks. The total carcinogenic risk is calculated using the following equation:

$$RC_{tot} = \sum_{c} RC_{der}(c) + \sum_{c} RC_{inh}(c) + \sum_{c} RC_{ing}(c) \quad (14.22)$$

where RC_{tot} = total cancer risk from carcinogenic chemicals (risk)
$RC_{der}(c)$ = cancer risk from dermal absorption of carcinogenic chemical c (risk)
$RC_{inh}(c)$ = cancer risk from inhalation of carcinogenic chemical c (risk)
$RC_{ing}(c)$ = cancer risk from ingestion of carcinogenic chemical c (risk)

14.1.2.6 Total Risk from Radionuclides

The total lifetime risk of cancer from exposure to radionuclides is the sum of the individual pathway risks. This risk is either a risk of cancer incidence or cancer fatality depending on the risk factor chosen when estimating pathway risks. The total radionuclide risk is calculated using the following equation:

$$RR_{tot} = \sum_{c} R_{ext}(c) + \sum_{c} R_{inh}(c) + \sum_{c} R_{ing}(c) \quad (14.23)$$

where RR_{tot} = total cancer risk from radionuclides (risk)
$R_{ext}(c)$ = cancer risk from external exposure to radionuclide c (risk)
$R_{inh}(c)$ = cancer risk from inhalation of radionuclide c (risk)
$R_{ing}(c)$ = cancer risk from ingestion of radionuclide c (risk)

14.1.2.7 Total Risk

The total lifetime risk of cancer incidence to an exposed individual is the sum of the incidence risk from carcinogenic chemicals the incidence risk from radionuclides. If fatality risk was estimated for radionuclides, then it is not appropriate to sum the radionuclide and chemical risks. Total risk is calculated using the following equation:

$$Risk = RC_{tot} + RR_{tot} \quad (14.24)$$

where

Risk = total cancer incidence risk from all analytes (risk)
RC_{tot} = total cancer incidence risk from carcinogenic chemicals (risk)
RR_{tot} = total cancer incidence risk from radionuclides (risk)

14.1.3 Population Dose and Risk for Radioactive Contaminants

The population radiation dose is calculated as the sum of doses to individuals for a set of locations. With the limitation that the code only runs a single exposure scenario at a time, the activities of the people at the different locations can be different. For example, some could be drinking groundwater, and some could be drinking surface water; however, they all would be drinking the same amount of water. The equation for this calculation is:

$$Dose_{pop} = \sum_{loc} \left(Dose_{ind} \times Pop_{loc} \right) \quad (14.25)$$

where

$Dose_{pop}$ = population dose (person-rem)

$Dose_{ind}$ = radioactive dose (rem) to an individual at a location
Pop_{loc} = number of people living at the location (persons)

The sum goes over all locations identified for the specific run of the HUMAN code.

The population risk from radioactive materials is calculated using the following equation:

$$Risk_{pop} = \sum_{loc} \left(Risk_{ind} \times Pop_{loc} \right) \tag{14.26}$$

where
$Risk_{pop}$ = number of people in the population that are expected to develop or die from cancer
$Risk_{ind}$ = cancer incidence or fatality risk (risk)
Pop_{loc} = number of people living at the location (persons)

14.2 Code Execution Environment

14.2.1 Location in the Processing Sequence

The HUMAN code requires access to a number of data files developed by other computer codes. In particular, the ECDA and FCDA files shown on Figure 1.1 must have defined and filled with concentration data before the HUMAN code can be used to calculate impacts. These concentration data files must have been developed under the control of the same ESD keyword file that the HUMAN code reads to determine processing options.

14.2.2 How the Code Is Invoked

HUMAN can run under either the Windows or the Linux operating system. Under the Windows operating system (Releases XP or 7), HUMAN executes in a DOS box. A run of HUMAN is initiated by entering the following command line:

```
HUMAN "Keyfilename"
```

Under the Linux operating system HUMAN is executed through any of the following Bourne Shell or C Shell commands:

```
human-1.exe "Keyfilename"
```

For these commands, HUMAN or “human.exe” is the name of the executable program, and “Keyfilename” is the name of a human scenario keyword file. Both the name of the executable program and the keyword file may contain path information. If HUMAN is invoked without entering the name of the keyword file, then the code will prompt the user for the file name. The keyword file, which should be prepared using an editor that can handle ASCII files without leaving embedded control codes, contains text control information describing the run. If HUMAN cannot open the keyword file, then the code will terminate execution after writing an error message to the standard output device.

If the string “-help” is entered instead of the keyword file name a few help lines are written to the standard output. The help lines identify the correct command line options for the code. Code execution terminates after the help message has been displayed when the “-help” option is used.

14.2.3 Memory Requirements

The HUMAN code uses dynamic memory allocation, so the memory requirements depend on the problem being analyzed. A reasonably large example run where the HUMAN code required 3.84 MB of memory (on a Windows 2000 machine) used 7 analytes, 35 times steps, 25 realizations, and 1618 locations. It is expected that most, if not all, of the runs of the HUMAN code will require fewer than 5 MB of memory.

14.3 Data Files

The HUMAN code reads four or more input files and writes up to seven output files. The number of input files depends on the number of contaminants being analyzed. The number of output files depends on the options selected in the HUMAN code. These files are described in the following sections.

14.3.1 Input Files

The input files for the HUMAN code are keyword files and a suite of concentration-data-related files. One keyword file controls the case the HUMAN code will execute, and it points to the ESD keyword file. The suite of concentration data files are all identified in the ESD keyword file – the user of the HUMAN code only needs to identify the ESD keyword file. The following are the input files:

- **ESD Keyword File.** The ESD keyword file contains the control information the inventory and environmental transport codes use to generate concentration data files. Section 2.1 provides definitions for these keywords.
- **HUMAN Keyword File.** The HUMAN Keyword file controls the scenario to be analyzed by the HUMAN code. The options and data available are constrained by the case defined in the ESD Keyword file. Section 14.4 describes the contents of the HUMAN keyword file. Table 14.1 provides excerpted records from a keyword file for the HUMAN code.
- **ECDA Concentration Files.** The ECDA concentration files contain all the concentration data available for the impact codes. The concentrations for all analytes are based on the same time and location data. There is a "map" file for the ECDA files containing indexing information for each of the concentration data files. In addition, there is a separate concentration data file for every analyte used in the impacts scenario. For example, when running a scenario with seven analytes, there will be one map file and seven concentration data files.
- **FCDA Concentration Files.** The FCDA concentration files contain all the food concentrations that are computed and written by the ECEM ecological impacts. The concentrations for all foods are based on the same time and location data. There is a "map" file for the FCDA files containing indexing information for each of the food concentration data files. In addition, there is a separate concentration data file for every food used in the impacts scenario. For example, when running a scenario with nine foods, there will be one map file and nine food concentration data files.

14.3.1.1 ESD Keyword File

The HUMAN code also reads keywords from the environmental settings file. These keywords are read from a different file and can have a different definition from a keyword defined for internal use in the HUMAN code. The environmental settings keywords are defined in Section 2.1. The following keywords are required:

- ANALYTE – definition of analytes in the environmental simulations
- END – end of the environmental settings keywords
- FILE – file names for the concentration file for each analyte
- LOCATION – locations at which concentrations were generated
- REALIZAT – number of realizations that were simulated
- SPECIES – species for which body burdens were generated
- TIMES – times at which concentrations were generated
- TITLE – environmental simulation title

14.3.1.2 HUMAN Keyword File

The HUMAN keyword definition file contains control information for the desired impact simulation. Individual keywords are defined in Section 14.4. Table 14.1 contains excerpted keywords from a keyword file for the HUMAN code. The complete file is 2925 lines long.

Table 14.1 Excerpted Records from a Keyword File for the HUMAN Code

```
! Report File (Must be first Entry)
REPORT "Human_CA_Ref_A_ResFarmer.Rpt"
! Other identification information
TITLE "Updated Composite Analysis - Residential Farmer Scenario - Hanford + Background Run"
USER  "AC"
EXECUTE
! Random Seed for Stochastics
SEED STOCHASTIC 421468
! Number of Realizations
REALIZATIONS 1
FILE DETAIL   "Human_CA_Ref_A_ResFarmer_Dtl.csv"     ! Risk detailed data
FILE VALUES   "Human_CA_Ref_A_ResFarmer_Val.csv"     ! Generated stochastic variables
FILE HEADER   "Human_CA_Ref_A_ResFarmer_SACVIEW.Hdr" ! Header file
! Environmental keyword file
FILE ESD "/home/ANALYSIS5/CA_Ref_A/ESD_CA_Ref_A.key"
FOOD PATH="/home/ANALYSIS5/CA_Ref_A/foods/"
    MAP ="Ecem_CA_Ref_A_map_foods.dat
INGESTION
  FISH =    "None"
 ...
  EGGS =    "UCHKEG"
!
FOODSOIL SOGW
SWEAT None
SHOWER GROUND
DETAILS SUMDOSE ! Dose summed over analytes
DETAILS ANADOSE ! Dose for every analyte
!  Analyte definitions
ANALYTE ID="H3" RADIOACT OUTPUT
...
ANALYTE ID="U238" RADIOACT OUTPUT
!-------------------------------| ECDA Concentration Solution Times  |-------------------------------!
TIMES
  1945  1950  1955  1960  1965  1970  1975  1980  1985  1990  !
 11200 11250                          !
 !
```

```
LOCATION PRIMARY="UH0002" SECOND="QHP025" POP=0 BIRD="UH0002" MEAT="UH0002"
FISH="QHP215" OUTPUT
...
LOCATION PRIMARY="UHR123" SECOND="QHRWI1" POP=0 BIRD="UHR123" MEAT="UHR123"
FISH="QHP215" OUTPUT
!------------------------------| Start of scenario-specific values |---------------------------------!
STOCHASTIC "EFBOAT" 1 0 "Exposure frequency for boating  (d/yr)"
...
STOCHASTIC "EFFISH" 1 0 "Exposure frequency for fish  (d/yr)"
! Exposure times
STOCHASTIC "ETBOAT" 1 0 "Exposure time for boating  (hr/d)"
...
STOCHASTIC "EDADULT" 1 1 "Exposure duration for an adult (yr)"
! Inhalation and ingestion
STOCHASTIC "IRATE" 1 20 "Inhalation rate (m^3/d)"
...
STOCHASTIC "IRGRAIN" 1 0 "Ingestion rate, grain (kg/d)"
! Soil parameters
STOCHASTIC "ML" 1 0.00000005 "Mass loading of soil in air (kg/m^3)"
STOCHASTIC "AFSOIL" 1 0.275 "Adherance factor for soil (mg/cm^2/d)"
STOCHASTIC "AFSED" 1 0.275 "Adherance factor for sediment (mg/cm^2/d)"
! Individual definition
STOCHASTIC "BWCHILD" 1 16 "Body weight for a child (kg)"
STOCHASTIC "BWADULT" 1 70 "Body weight for an adult (kg)"
STOCHASTIC "SASOIL" 1 5000 "Body surface area - soils (cm^2)"
STOCHASTIC "SASED" 1 5000 "Body surface area - sediments (cm^2)"
STOCHASTIC "SASEEP" 1 20000 "Body surface area - seep water (cm^2)"
STOCHASTIC "SASWIM" 1 20000 "Body surface area - surface water (cm^2)"
STOCHASTIC "SASWEAT" 1 20000 "Body surface area - sweat lodge (cm^2)"
STOCHASTIC "SASHOWER" 1 20000 "Body surface area - showering (cm^2)"
STOCHASTIC "CFSWEAT" 1 0.2 "Air concentration factor for sweat lodge (L/m^3)"
STOCHASTIC "CFSHOWER" 1 0.1 "Air concentration factor for showering (L/m^3)"
STOCHASTIC "SHIELDSOIL" 1 0.8 "Soil shielding factor (unitless)"
STOCHASTIC "SHIELDSED" 1 0.2 "Sediment shielding factor (unitless)"
!-----------------------------------------| Dose Conversion Factors |-----------------------------------------!
! Best estimate dose factor keywords (Data Directly From Referenced Tables)
STOCHASTIC "H3    DFSOIL"  1  0 "(Reference) H3 dose factor for soil (rem/hr per pCi/kg)"
STOCHASTIC "H3    DFSWIM"  1  0 "(Reference) H3 dose factor for swimming (rem/hr per pCi/L)"
STOCHASTIC "H3    DFBOAT"  1  0 "(Reference) H3 dose factor for boating (rem/hr per pCi/L)"
STOCHASTIC "H3    DFING"  1  6.401000E-11 "(Reference) H3 dose factor for ingestion (rem/pCi)"
STOCHASTIC "H3    DFINH"  1  6.401000E-11 "(Reference) H3 dose factor for inhalation (rem/pCi)"
!-----------------------------------------| Risk Conversion Factors |-----------------------------------------!
! Best estimate risk keywords (Data Directly From Referenced Tables) for the dietary scenario
STOCHASTIC "H3    RFSOIL"  1  0 "Deterministic (Reference) H3 risk factor for soil (risk/hr per pCi/kg)"
STOCHASTIC "H3    RFSWIM"  1  0 "Deterministic (Reference) H3 risk factor for swimming (risk/hr per pCi/L)"
STOCHASTIC "H3    RFBOAT"  1  0 "Deterministic (Reference) H3 risk factor for boating (risk/hr per pCi/L)"
STOCHASTIC "H3    RFING"  1  6.512000E-14 "Deterministic (Reference) H3 risk factor for ingestion (risk/pCi)"
STOCHASTIC "H3    RFINH"  1  5.624000E-14 "Deterministic (Reference) H3 risk factor for inhalation (risk/pCi)"
!---------------------------| Radionuclide Volatilization Factors |-----------------------------!
STOCHASTIC "H3    VF" 1 0.002 "Deterministic (reference) H3 Volatilization Factor [L/m3]"
! End of Inputs
END
```

14.3.1.3 ECDA Concentration Files

The ECDA provides a central storage location for concentration data for all analytes at the environmental locations and times needed to perform social-cultural analyses. The ECDA files are described in Section 2.2.

14.3.1.4 FCDA Concentration Files

The FCDA provides a central storage location for food concentration data for all food species at the environmental locations and times needed to perform HUMAN impacts analyses. The FCDA files are described in Section 2.3.

14.3.2 Output Files

Up to seven output files can be written by the HUMAN code. The number of files depends on the options selected in the scenario being analyzed. The following are the output files:

- **Report File**: This required file contains a summary of the scenario being analyzed and contains any error messages. An example report file for the HUMAN code is provided in Table 14.2.
- **Header File**: This required file contains information used by post-processor programs to allow easy extraction of subsets of the results computed by the HUMAN code. An example of this file is given in Table 14.3.
- **Stochastic Values File**: This optional file contains the values for every stochastic variable generated in the HUMAN code. The description of the VALUES modifier on the FILE keyword (see Section 14.4.7) explains how to activate writing this file. A subset of the data written to this file for a run using five realizations is provided in Table 14.4.
- **Risk Detailed Data**: This optional file contains the detailed values for the dose and risk values generated in the HUMAN code. The description of the DETAIL modifier on the FILE keyword (see Section 14.4.7) explains how to activate writing this file. A subset of the data written to this file for a run using five realizations is provided in Table 14.5.
- **Risk Summary Statistics**: This optional file contains the summary statistics for the dose and risk values generated in the HUMAN code. The description of the STATS modifier on the FILE keyword (see Section 14.4.7) explains how to activate writing this file. A subset of the data written to this file for a run using five realizations is provided in Table 14.6.

14.3.2.1 HUMAN Report File

Table 14.2 provides excerpted records from an example report file for the HUMAN code. This file contains information for a run of the HUMAN code using 4 analytes, 1 realization, 2873 locations, and 77 solution times. This example file is a typical size for the report file, provided that no debug options are selected. The size of this file grows rapidly when debug options are selected. For example, this file is about 12 KB in size. If the debug options are turned on, the file grows to 6.3 MB. A run using all debug options having a large number of locations, analytes, solution times, and realizations could generate a report file larger than 2 GB. Some of the lines in the table are wrapped in the word processing but they are not wrapped in the file.

Table 14.2 Excerpted Records from an Example Report File for the HUMAN Code

```
                  H     H  U     U  M     M   AAAAA   N     N
                  H     H  U     U  MM   MM  A     A  NN    N
                  H     H  U     U  M M M M  A     A  N N   N
                  HHHHHHH  U     U  M  M  M  AAAAAAA  N  N  N
                  H     H  U     U  M     M  A     A  N   N N
                  H     H  U     U  M     M  A     A  N    NN
                  H     H   UUUUU   M     M  A     A  N     N

                              Human    3.05.004
                         Last Modified on 13 Apr 2006

                         Stochastic Human Risk Analysis
               Systems Assessment Capability (SAC), Revision 1
               ------------------------------------------------
                           Developed By Battelle
                     Pacific Northwest National Laboratory
                           Richland, Washington
               ------------------------------------------------
        Current Run ID = 20060503131735   User Name = AC
               System Date = 05-03-2006   System Time = 13:17:35

           The software used to generate this output is experimental
              and has not been formally tested or peer reviewed.

                               Review Signatures
Input Prepared By: _____________________________       Date: _________________
Input Reviewed By: _____________________________       Date: _________________
======================== Echo of the Problem Definition ======================
Title: Updated Composite Analysis - Residential Farmer Scenario - Hanford + Bac
User:  AC
   1 Realizations requested in this run
   1 Realizations available in the concentration files
File Name for Input Keyword Data
File: Human_CA_Ref_A_ResFarmer.key
File Name for use in SACVIEW
File: Human_CA_Ref_A_ResFarmer_SACVIEW.Hdr
File Name for Detailed Risk Data
File: Human_CA_Ref_A_ResFarmer_Dtl.csv
...
File Name for Media Concentrations for analyte with ID="H3"
File: /home/ANALYSIS5/CA_Ref_A/ecda/CA_Ref_A_H3.bin
...
File Name for Media Concentrations for analyte with ID="Np237"
File: /home/ANALYSIS5/CA_Ref_A/ecda/CA_Ref_A_Np237.bin

Debug Flag Information
   No  : Concentration Data
...
   Yes : Stochastic Calculations
   No  : Food concentrations

Output Data Options Information
   Yes : Dose details summed over analytes of similar type
...
   No  : Media Level Concentrations

Averaging time for risk calculations (not used for rad dose)
   Value =  25567.50   Units are days

Sweat lodge option is not used
Shower water selection is used : Water source is Ground water
```

```
Analye Information based on 15 possible analytes.
     1 : H3     : NR : Carcinogen F : Hazardous F : Radioactive T : Tritium
     2 : C14    : NR : Carcinogen F : Hazardous F : Radioactive T : Carbon-14
     3 : Sr90   : NR : Carcinogen F : Hazardous F : Radioactive T : Strontium-90
     4 : U238   : NR : Carcinogen F : Hazardous F : Radioactive T : Uranium-238
A total of 14 analytes have been requested.

Soil type selection for for upland food
 SOGW   : Groundwater irrigation
FOOD Information
   MILK    : Species "UCATMK"  "cattle (milk)"
...
   ROOTVEG : Species "URTVEG"  "root vegetables"
Time Slices Requested: (Index, Calendar Year) based on 308 possible times.
      1 :  1945 : Included in this scenario
...
      308: 12050 : Included in this scenario
A total of 308 times have been requested.

Locations Requested: based on 4317 possible locations.
  Index   Location    Second     Third       Pop     Bird Concen.    Meat Concen.
Fish Concen.    Fish_2 Concen     Fish_3 Concen
  -----   --------   --------   --------   -------   -------------   -------------   -
------------   ---------------   ---------------
      1 : "UH0002" : "QHP025" : "      " :       0 : BIRD="UH0002" : MEAT="UH0002" :
FISH="None  " : FISH_2="None  " : FISH_3="None  "
...
      2828 : "UHR123" : "QHRWI1" : "      " :       0 : BIRD="UHR123" : MEAT="UHR123"
: FISH="None  " : FISH_2="None  " : FISH_3="None  "
A total of 2828 locations have been requested.
======================== End of the Problem Definition ========================
Starting Problem Execution
    Date: 05/03/2006
    Time: 13:18:07.824
Information on food files used in this run
Food: LEAFVEG   Unit:  24  Analyte: "H3    "  Species: "ULFVEG"  File:
"/home/ANALYSIS5/CA_Ref_A/foods/Food_H3_ULFVEG.fod"
...
Food: BIRD      Unit: 120  Analyte: "Np237 "  Species: "UCHKAD"  File:
"/home/ANALYSIS5/CA_Ref_A/foods/Food_Np237_UCHKAD.fod"
Food: EGGS      Unit: 121  Analyte: "Np237 "  Species: "UCHKEG"  File:
"/home/ANALYSIS5/CA_Ref_A/foods/Food_Np237_UCHKEG.fod"

Concentration data units conversion factors
    1 : H3     : NR : Ground water  :  1.00000E+09 : From Ci/m^3       to pCi/L
...
    1 : H3     : NR : Air Concen.   :  1.00000E+12 : From Ci/m^3       to pCi/m^3

Ending Problem Execution
    Date: 05/01/2006
    Time: 12:09:31.235
Message originating in routine HUMAN
Message: Normal Termination
```

14.3.2.2 HUMAN Header File

The HUMAN header file is an output file containing information used by post-processor programs to allow easy extraction of subsets of the results computed by the HUMAN code. This file is required for

every run of the HUMAN code. An example of this file is given in Table 14.3. The file contains the following sections of information:

- A header section of basic run information
- Number of realizations processed
- Solution times selected
- Locations used
- Analytes processed
- Solutions selected
- Output file names

The user only specifies the name of this file; users should not modify the file after it is generated by the HUMAN code. Because this file has at most a few hundred entries, the file size is always much smaller than 1 MB. File names for options not selected are set to null.

Table 14.3 Example HUMAN Header File

```
type: "Human"
title: "Updated Composite Analysis - Residential Farmer Scenario - Hanford
+ Bac"
user: "AC"
name: "Human"
version: "3.05.004"
date: "13 Apr 2006"
id: "20060503131735"
envfile: "/home/ANALYSIS5/CA_Ref_A/ESD_CA_Ref_A.key"
realizations: 1
times: 308
 1945
 ...
 12050
locations: 2828
"UH0002","UnsuitableForAgricul"
"UH0003","UnsuitableForAgricul"
"UH0004","AgExclusionBuffer"
...
"UHR121","Richland"
"UHR122","Richland"
"UHR123","Richland"
analytes: 17
"H3    ","F","F","T","Tritium"
"C14   ","F","F","T","Carbon-14"
"Sr90  ","F","F","T","Strontium-90"
"U238  ","F","F","T","Uranium-238"
"COMBIN","CAR","Summed over carcinogenic analytes"
"COMBIN","HAZ","Summed over hazardous analytes"
"COMBIN","RAD","Summed over radioactive analytes"
solutions: 2
"ANADOSE","Analyte dose"
"SUMDOSE","Dose summed over analyes"
statistics_impacts: "NULL"
detail_impacts: "Human_CA_Ref_A_ResFarmer_Dtl.csv"
```

14.3.2.3 HUMAN Stochastic Values File

The stochastic values file is an optional output file that contains the values for every stochastic variable generated in the HUMAN code. The description of the VALUES modifier on the FILE keyword (see Section 14.4.7) explains how to activate writing this file. The values are written as text in comma-separated format so they can be imported easily into a spreadsheet or other software. Each line of the file consists of the ID of the stochastic variable followed by a value for every generated realization. A subset of the data written to this file for a run using five realizations is provided in Table 14.4. Because this file has at most a few hundred entries, the file size is always much smaller than 1 MB.

Table 14.4 Excerpted Records from the Stochastic Values File

```
"DOSE2RISK", 6.63298E-04, 8.95216E-04, 4.28789E-04, 7.61322E-04, 3.24067E-04
"Sr90  DFSOIL", 3.90004E-10, 7.28447E-10, 2.60232E-10, 5.63547E-10, 5.15688E-10
"Sr90  DFINH", 3.00188E-07, 2.71429E-07, 6.30467E-07, 1.09017E-07, 1.41680E-07
"U     HQINH", 1.00014E+00, 9.98158E-01, 9.94201E-01, 1.00092E+00, 1.00480E+00
"CCl4  SFING", 4.34638E-01, 8.02780E-02, 1.85404E-01, 1.43329E-01, 2.62328E-02
"CCl4  SFINH", 1.75551E-02, 3.65071E-01, 2.56433E-02, 7.24165E-02, 5.14025E-02
"EFBOAT", 2.44306E+01, 1.12904E+01, 1.78827E+01, 5.08665E+00, 2.99136E+01
"ETRIVER", 1.75214E+01, 1.53131E+01, 1.31528E+01, 1.10683E+01, 1.87175E+01
"ED", 1.44600E+01, 1.60701E+01, 6.21335E+01, 4.98780E+01, 2.99073E+01
"EFLEAFY", 3.60858E+02, 3.34866E+02, 2.94225E+02, 3.25261E+02, 2.76094E+02
"QPBIRD", 4.90110E-01, 4.32282E-01, 5.87973E-01, 5.38815E-01, 4.58023E-01
"QWBIRD", 2.22780E-01, 3.69238E-01, 2.49782E-01, 1.42156E-01, 2.92976E-01
"BWADULT", 6.21404E+01, 7.29195E+01, 8.22975E+01, 6.95193E+01, 8.40544E+01
"SASOIL", 5.00000E+03, 5.00000E+03, 5.00000E+03, 5.00000E+03, 5.00000E+03
"SARIVER", 2.00000E+04, 2.00000E+04, 2.00000E+04, 2.00000E+04, 2.00000E+04
"IRSEDCHILD", 2.47929E-04, 4.71712E-04, 3.42739E-05, 2.08821E-04, 3.33628E-04
"IRMEAT", 1.47307E+00, 2.16214E+00, 1.08884E-01, 2.99069E+00, 7.07404E-01
"IRATE", 3.38178E+01, 2.51633E+01, 2.98956E+01, 2.03503E+01, 2.78600E+01
"Sr90  TFDEER", 7.39602E-02, 4.40583E-02, 3.74697E-02, 1.29689E-02, 1.81908E-02
"Sr90  TFBIRD", 5.63319E-01, 2.14527E+00, 1.47448E+00, 2.64039E+00, 6.26559E-02
"IRGRATE", 9.07806E+02, 8.51027E+02, 6.27562E+02, 5.60488E+02, 7.31329E+02
"SHIELDSOIL", 8.00000E-01, 8.00000E-01, 8.00000E-01, 8.00000E-01, 8.00000E-01
"AFSED", 3.96716E-01, 1.41329E-01, 1.28814E-01, 4.29907E-01, 2.54937E-01
```

14.3.2.4 HUMAN Risk Detailed Data

The risk detailed data file is an optional output file that contains the detailed values for dose and risk generated in the HUMAN code. The description of the DETAIL modifier on the FILE keyword (see Section 14.4.7) explains how to activate writing this file. Section 14.4.4 describes the solution types that can be written to the file. The values are written as text in comma-separated format so they can be imported easily into a spreadsheet or other software. Each line of the file consists of six identifiers followed by a value for every generated realization. Table 14.5 provides a subset of the data written to this file for a run using five realizations. The first two lines in the table actually reside on one line in the data file. The following are the six identifiers on each line:

- Time: Year for which the data are valid
- Location ID: The location identifier where the data are valid
- Analyte ID: The identification of the analyte for which the data were computed
- Analyte Type: A flag for analyte type:
  - RAD – Radioactive analyte
  - CAR – Carcinogenic analyte
  - HAZ – Noncarcinogenic analyte

- ALL – Sum over all analytes
- CONMEDIA – Environmental concentration
- CONFOODS – Food concentration

- Solution type: A flag for solution type that has the following definition:
  - AIRC - Air concentrations
  - ANADOSE - Analyte dose
  - ANARISK - Analyte risk
  - ANAHQ - Analyte hazard quotient
  - BIRD - Food concentration, birds
  - DOSEING - Ingestion dose
  - DOSEINH - Inhalation dose
  - DOSEEXT - External dose
  - DOSEDER - Dermal dose
  - EGGS - Food concentration, eggs
  - FISH - Food concentration. fish
  - FRUIT - Food concentration, fruit
  - GRAIN - Food concentration, grain
  - GWAT - Groundwater concentrations
  - HQING - Ingestion hazard quotient
  - HQINH - Inhalation hazard quotient
  - HQDER - Dermal hazard quotient
  - LEAFVEG - Food concentration, leafy vegetables
  - MEAT - Food concentration, meat
  - MILK - Food concentration, milk
  - POPDOSE - Population dose (radioactive)
  - POPRISK - Population risk (radioactive)
  - RISKING - Ingestion risk
  - RISKINH - Inhalation risk
  - RISKEXT - External risk
  - RISKDER - Dermal risk
  - ROOTVEG - Food concentration, root vegetables
  - SEDI - Sediment concentrations
  - SEEP - Seep water concentrations
  - SODR - Soil concentrations, no irrigation
  - SOGW - Soil concentrations, groundwater irrigated
  - SORP - Riparian soil concentrations
  - SOSW - Soil concentrations, surface water irrigated
  - SUMDOSE - Dose summed over analytes
  - SUMRISK - Risk summed over analytes
  - SUMHQ - Hazard quotient summed over analytes
  - SWAT - Surface water concentrations
- Units: The units associated with the computed data

Table 14.5 Excerpted Records from the Risks Detailed Data File

```
"Time","Location ID","Analyte ID","Analyte Type","Solution
Type","Units","Values by realization"
1945,"UH0002","H3","RAD","ANADOSE","Rem", 6.82940E-16
1945,"UH0002","C14","RAD","ANADOSE","Rem", 3.06619E-07
1945,"UH0002","Cl36","RAD","ANADOSE","Rem", 0.00000E+00
1945,"UH0002","Se79","RAD","ANADOSE","Rem", 3.08574E-24
1945,"UH0002","Sr90","RAD","ANADOSE","Rem", 2.22632E-19
1945,"UH0002","Tc99","RAD","ANADOSE","Rem", 2.81113E-15
1945,"UH0002","I129","RAD","ANADOSE","Rem", 6.89559E-08
...
1945,"UH0002","COMBIN","RAD","SUMDOSE","Rem", 3.75575E-07
1945,"UH0003","H3","RAD","ANADOSE","Rem", 9.57946E-15
1945,"UH0003","C14","RAD","ANADOSE","Rem", 3.06621E-07
1945,"UH0003","Cl36","RAD","ANADOSE","Rem", 0.00000E+00
1945,"UH0003","Se79","RAD","ANADOSE","Rem", 3.12809E-23
1945,"UH0003","Sr90","RAD","ANADOSE","Rem", 2.87494E-17
1945,"UH0003","Tc99","RAD","ANADOSE","Rem", 9.17985E-14
...
1950,"UH1546","Se79","RAD","ANADOSE","Rem", 3.88087E-14
1950,"UH1546","Sr90","RAD","ANADOSE","Rem", 1.01264E-14
1950,"UH1546","Tc99","RAD","ANADOSE","Rem", 3.74360E-11
1950,"UH1546","I129","RAD","ANADOSE","Rem", 5.40670E-09
1950,"UH1546","Cs137","RAD","ANADOSE","Rem", 0.00000E+00
1950,"UH1546","Ra226","RAD","ANADOSE","Rem", 6.04740E-16
1950,"UH1546","Pa231","RAD","ANADOSE","Rem", 4.84173E-23
1950,"UH1546","U233","RAD","ANADOSE","Rem", 1.28079E-11
1950,"UH1546","U235","RAD","ANADOSE","Rem", 3.15323E-21
...
1950,"UH1562","U233","RAD","ANADOSE","Rem", 0.00000E+00
1950,"UH1562","U235","RAD","ANADOSE","Rem", 0.00000E+00
```

This file can have up to nine rows of information for every combination of time, location, and analyte. Therefore, this file can become very large. As an example, a 227 KB file was generated for a case involving 11 locations, 10 analytes, 5 realizations, and 3 times. The file size directly scales with the number of analytes, locations, and times. The file size grows more slowly than a direct scaling by the number of realizations. As another example, a 463 MB file was generated for a case involving 1618 locations, 6 analytes, 11 realizations, and 35 times, using all details output options. The file size can be reduced by selecting fewer detailed solution types.

14.3.2.5 HUMAN Risk Summary Statistics

This optional file contains summary statistics for dose and risk values generated in the HUMAN code. The description of the STATS modifier on the FILE keyword (see Section 14.4.7) tells how to activate writing this file. The solution types that can be written to the file are described in Section 14.4.16. The values are written as text in comma-separated format so they can be imported easily into a spreadsheet or other software. Each line of the file consists of six identifiers followed by summary statistics (nine percentiles, mean value, and standard deviation). Table 14.6 provides a subset of the data written to this file for a run using five realizations. The six identifiers on each line are the following:

- Time: Year for which the data are valid
- Location ID: The location identifier where the data are valid

- Analyte ID: The identification of the analyte for which the data were computed
- Analyte Type: A flag for analyte type:
  - ALL – Sum over all analytes
  - CAR – Carcinogenic analyte
  - CONFOODS – Food concentration
  - CONMEDIA – Environmental concentration
  - HAZ – Noncarcinogenic analyte
  - RAD – Radioactive analyte
- Solution type: A flag for solution type that has the following definition:
  - AIRC - Air concentrations
  - ANADOSE - Analyte dose
  - ANARISK - Analyte risk
  - ANAHQ - Analyte hazard quotient
  - BIRD - Food concentration, birds
  - DOSEING - Ingestion dose
  - DOSEINH - Inhalation dose
  - DOSEEXT - External dose
  - DOSEDER - Dermal dose
  - EGGS - Food concentration, eggs
  - FISH - Food concentration. fish
  - FRUIT - Food concentration, fruit
  - GRAIN - Food concentration, grain
  - GWAT - Groundwater concentrations
  - HQING - Ingestion hazard quotient
  - HQINH - Inhalation hazard quotient
  - HQDER - Dermal hazard quotient
  - LEAFVEG - Food concentration, leafy vegetables
  - MEAT - Food concentration, meat
  - MILK - Food concentration, milk
  - POPDOSE - Population dose (radioactive)
  - POPRISK - Population risk (radioactive)
  - RISKING - Ingestion risk
  - RISKINH - Inhalation risk
  - RISKEXT - External risk
  - RISKDER - Dermal risk
  - ROOTVEG - Food concentration, root vegetables
  - SEDI - Sediment concentrations
  - SEEP - Seep water concentrations
  - SODR - Soil concentrations, no irrigation
  - SOGW - Soil concentrations, groundwater irrigated
  - SORP - Riparian soil concentrations
  - SOSW - Soil concentrations, surface water irrigated
  - SUMDOSE - Dose summed over analytes
  - SUMRISK - Risk summed over analytes
  - SUMHQ - Hazard quotient summed over analytes
  - SWAT - Surface water concentrations

- Units: The units associated with the computed data

The data for each record in this file are too long to present without with line-wrapping in this document. Each record in the file occupies two lines in Table 14.6.

Table 14.6 Excerpted Records from the Risk Summary Statistics File

```
"Time","Location ID","Analyte ID","Analyte Type","Solution
Type","Units","Minimum","5th Percentile","10th Percentile","25th
Percentile","Median","75th Percentile","90th Percentile","95th
Percentile","Maximum","Mean","Standard Deviation"
2000,"UH0413","H3","RAD","DOSEING","Rem", 1.59834E-05, 1.59834E-05, 1.59834E-
05, 1.59834E-05, 5.56380E-05, 5.56380E-05, 6.87785E-05, 6.87785E-05,
1.60365E-04, 7.03381E-05, 5.39783E-05
2000,"UH0413","H3","RAD","DOSEINH","Rem", 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00, 0.00000E+00
2000,"UH0413","H3","RAD","DOSEEXT","Rem", 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00, 0.00000E+00
2000,"UH0413","H3","RAD","POPDOSE","Person-Rem", 3.28856E-02, 3.28856E-02,
3.28856E-02, 3.28856E-02, 5.38282E-02, 5.38282E-02, 7.53793E-02, 7.53793E-02,
1.02619E-01, 6.13590E-02, 2.80091E-02
2100,"UH0414","Tc99","RAD","DOSEING","Rem", 7.90825E-08, 7.90825E-08,
7.90825E-08, 7.90825E-08, 8.38515E-07, 8.38515E-07, 7.16277E-06, 7.16277E-06,
1.32302E-04, 2.81574E-05, 5.82919E-05
2100,"UH0414","Tc99","RAD","DOSEINH","Rem", 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00, 0.00000E+00
2100,"UH0415","U","HAZ","DOSEEXT","Unitless", 2.13679E-07, 2.13679E-07,
2.13679E-07, 2.13679E-07, 6.95310E-07, 6.95310E-07, 1.37764E-06, 1.37764E-06,
1.67892E-05, 3.87023E-06, 7.23683E-06
2100,"UH0415","U","HAZ","ANAHQ","Unitless", 2.48891E-06, 2.48891E-06,
2.48891E-06, 2.48891E-06, 1.75020E-05, 1.75020E-05, 9.33037E-05, 9.33037E-05,
3.77678E-04, 9.97710E-05, 1.59648E-04
2100,"UH0415","ALL","HAZ","SUMHQ","Unitless", 2.48891E-06, 2.48891E-06,
2.48891E-06, 2.48891E-06, 1.75020E-05, 1.75020E-05, 9.33037E-05, 9.33037E-05,
3.77678E-04, 9.97710E-05, 1.59648E-04
2100,"UH3870","ALL","HAZ","SUMHQ","Unitless", 3.05987E-20, 3.05987E-20,
3.05987E-20, 3.05987E-20, 9.17589E-07, 9.17589E-07, 3.95330E-06, 3.95330E-06,
4.92935E-04, 9.95633E-05, 2.19907E-04
2100,"POPDOS","ALL","RAD","SUMDOSE","Person-Rem", 6.13426E+01, 6.13426E+01,
6.13426E+01, 6.13426E+01, 1.23211E+02, 1.23211E+02, 6.39394E+02, 6.39394E+02,
8.50341E+02, 3.50847E+02, 3.68026E+02
2100,"POPRSK","ALL","RAD","SUMRISK","Risk", 3.42799E-02, 3.42799E-02,
3.42799E-02, 3.42799E-02, 5.49149E-02, 5.49149E-02, 4.24109E-01, 4.24109E-01,
6.47383E-01, 2.40123E-01, 2.81275E-01
```

This file can have up to nine rows of information for every combination of time, location, and analyte. Therefore, this file can become very large. As an example, a 398 KB file was generated for a case involving 11 locations, 10 analytes, 5 realizations, and 3 times. The file size directly scales with the number of analytes, locations, and times. The file size grows more slowly than a direct scaling by the number of realizations. As another example, a 466 MB file was generated for a case involving 1618 locations, 6 analytes, 11 realizations, and 35 times, using all details output options. The file size can be reduced by selecting fewer statistics solutions types.

14.4 Keyword Descriptions for the HUMAN Code

This section defines keywords needed to control the HUMAN code directly. Most of these keywords can be entered in any order. The only restriction on keyword order is that the END keyword must be the last keyword in the file. General rules for reading the keyword descriptions are explained in Section 1.4. Section 18.0 presents a more detailed description of keyword language syntax.

14.4.1 ANALYTE Keyword for HUMAN

The ANALYTE keyword is used to define the analytes to be used in the simulation. The following is this keyword's syntax:

```
ANALYTE [ID="quote1"] [RADIOACTIVE | {CARCINOGEN} {HAZARDOUS}] {OUTPUT}
   {VERBOSE} {RFDING} {RFDINH} {SFING} {SFINH}
```

The analytes requested must be a subset of the analytes for which environmental data were computed and stored by the inventory, release, and transport modules. Table 14.7 describes the modifiers associated with the ANALYTE keyword.

Table 14.7 Modifiers Associated with the ANALYTE Keyword in the HUMAN Code

Modifier	Description
ID	The quote string associated with the ID modifier is an analyte identification string up to six characters long. The analyte identification string is case sensitive, and spaces or hyphens change the definition. All data in the analyte identification strings must satisfy the following conventions: • Only the first entry in the analyte identification string is capitalized • No embedded spaces or hyphens are used, even for radionuclides • Individual elements are defined using the standard element abbreviation
RADIOACTIVE	The presence of this modifier indicates to treat this analyte as a radioactive analyte.
CARCINOGEN	The presence of this modifier indicates to treat this analyte as a chemical carcinogen.
HAZARDOUS	The presence of this modifier indicates to treat this analyte as a hazardous chemical that is not carcinogenic.
OUTPUT	If the modifier OUTPUT is entered, then outputs requested by the DETAILS and STATISTICS keywords will be written to the output files for this analyte. Otherwise, the calculations will occur, but no data will be output to these two files for this analyte.
VERBOSE	If the modifier VERBOSE is entered, then intermediate calculations for each component of the pathway dose, risk or hazard quotient calculations will be output to the report file for this analyte. This output selection can cause the report file to become excessively large if a large number of times, locations, and realizations are used in the run.
RFDING	The presence of this optional modifier for hazardous analytes is the indication that reference dose calculations for ingestion are desired. The user must also supply the reference dose values using the STOCHASTIC keyword.

Modifier	Description
RFDING	The presence of this optional modifier for hazardous analytes is the indication that reference dose calculations for inhalation are desired. The user must also supply the reference dose values using the STOCHASTIC keyword.
SFING	The presence of this optional modifier for carcinogenic analytes is the indication that risk calculations for ingestion are desired. The user must also supply the slope factor values using the STOCHASTIC keyword.
SFINH	The presence of this optional modifier for carcinogenic analytes is the indication that risk calculations for inhalation are desired. The user must also supply the slope factor values using the STOCHASTIC keyword.

Even though the HUMAN code can treat each analyte in three different fashions: as a radioactive analyte, as a noncarcinogenic hazardous chemical, and as a carcinogenic chemical. Each analyte can only be handled in one fashion in a given run of the code. Treating an analyte in all three fashions would require running the code three times.

The following are example entries for a radioactive analyte:

```
ANALYTE ID="Np237" RADIOACTIVE
ANALYTE ID="Np237" RADIOACTIVE OUTPUT
ANALYTE ID="Np237" RADIOACTIVE OUTPUT VERBOSE
```

The following are example entries for a noncarcinogenic (hazardous) analyte. In the first example the calculations will be performed for ingestion but not inhalation.

```
ANALYTE ID="U" HAZARDOUS OUTPUT RFDING
ANALYTE ID="U" HAZARDOUS OUTPUT RFDING RFDINH
ANALYTE ID="U" HAZARDOUS OUTPUT VERBOSE RFDING RFDINH
```

The following is an example entry for a carcinogenic analyte:

```
ANALYTE ID="Cr" CARCINOGENIC  SFINH
```

The following entry illustrates definition of an analyte that is both a hazardous chemical and a carcinogen.

```
ANALYTE ID="CCl4" HAZARDOUS CARCINOG SFING SFINH RFDING RFDINH
   OUTPUT VERBOSE
```

14.4.2 AVERAGE Keyword for HUMAN

The optional AVERAGE keyword is used to define averaging time for human risk calculations for carcinogenic or hazardous analytes. This keyword is not used for radioactive analytes. The following is this keyword's syntax:

```
AVERAGE {CARCINOG=Value1} {HAZARDOU=Value2}
```

The numerical entry associated with the CARCINOG modifier is the number of years in the averaging time for carcinogenic analytes. The numerical entry associated with the HAZARDOU modifier is the number of years in the averaging time for hazardous analytes. No default averaging time is implemented. The averaging time for carcinogenic analytes is typically set to a lifetime of 50 or 70 years, although a value of 1 may sometimes be used for a 1-year exposure scenario. The averaging time for hazardous analytes should be set to the exposure duration because the hazardous effects model does not consider latent effects from hazardous analytes. The averaging times are converted to days after the inputs are read

using a conversion factor of 365.25 days/year. The following example keyword sets the averaging time to 50 years for carcinogenic analytes and 1 year for hazardous analytes:

```
AVERAGE CARCINOG=50 HAZARDOU=1
```

The same effect can be obtained using the following two AVERAGE keywords:

```
AVERAGE CARCINOG=50
AVERAGE HAZARDOU=1
```

There are no quote strings associated with the AVERAGE keyword.

14.4.3 DEBUG Keyword for HUMAN

The DEBUG keyword is used to activate dumping of intermediate calculations to the report file. It should be used sparingly and with only one or two realizations; otherwise, the volume of output could fill the user's hard drive. The following is this keyword's syntax:

```
DEBUG [modifier 1] {modifier 2}…{modifier 9}
```

Multiple DEBUG records can be entered with combinations of modifiers, or a single record can be entered containing all of the modifiers. The modifiers can be entered in any order. Table 14.8 describes the modifiers associated with the DEBUG keyword.

Table 14.8 Modifiers Associated with the DEBUG Keyword in the HUMAN Code

Modifier	Description
CARCINOG	Intermediate outputs on calculations for carcinogenic analytes.
CONCENTR	Intermediate outputs on reading and processing media concentrations.
FOOD	Intermediate outputs on calculating concentrations in food items.
HAZARDOU	Intermediate outputs on calculations for hazardous analytes.
RADIONUC	Intermediate outputs on calculations for radioactive analytes.
STOCHAST	Write out all generated stochastic values.
DEFINITI	Output the definition of all stochastic variables.
STATISTI	Output summary statistics for all generated stochastic variables.
VERBOSE	Output additional information to the report file.

The following entries are examples of the use of the DEBUG keyword:

```
DEBUG CARCINOGENIC RADIONUCLIDES STOCHASTIC
DEBUG STOCHASTIC
```

There are no quote strings associated with the DEBUG keyword.

14.4.4 DETAILS Keyword for HUMAN

The DETAILS keyword is used to control writing detailed data for all realizations to the output details file for a variety of solution types. The following is this keyword's syntax:

```
DETAILS {modifier 1} {modifier 2} … {modifier13}
```

Multiple DETAILS cards can be entered with combinations of modifiers, or a single card can be entered containing all of the modifiers. The modifiers can be entered in any order. The modifiers associated with the DETAILS keyword are given in Table 14.9. Also shown are possible solution IDs that will be contained in the details output file.

Table 14.9 Modifiers Associated with the DETAILS Keyword in the HUMAN Code

Modifier	Solution ID	Description
CONCEN	CONMEDIA	This modifier activates output of detailed media concentration data for those analytes and locations whose OUTPUT flags have been activated.
FOODS	CONFOODS	This modifier activates output of detailed food concentration data for those analytes and locations whose OUTPUT flags have been activated.
SUMDOSE	SUMDOSE	This modifier activates output of the dose for combined pathways that is summed over all radioactive analytes. This solution does not apply to carcinogenic or hazardous analytes. Detailed information is written out for every time and location combination.
SUMRISK	SUMRISK	This modifier activates output of the risk or hazard quotient that is summed over all analytes of the same type (radioactive, carcinogenic, or hazardous). Detailed information is output for every time and location combination.
ANADOSE	ANADOSE	This modifier activates output of the dose for each analyte. Detailed information is output for every time, location and analyte combination.
ANARISK	ANARISK	This modifier activates output of the risk or hazard quotient for each analyte. Detailed information is output for every time, location, and analyte combination.
PATHDOSE	DOSEDER DOSEEXT DOSEING DOSEINH	This modifier activates output of the pathway dose for each analyte. Pathways include external (for radionuclides), dermal (for hazardous and carcinogenic analytes), ingestion, and inhalation routes. Detailed information is output for every applicable pathway for every location, analyte, and time step combination.
PATHRISK	RISKDER RISKEXT RISKING RISKINH	This modifier activates output of the pathway risk or hazard quotient for each analyte. Pathways include external (for radionuclides), dermal (for hazardous and carcinogenic analytes), ingestion, and inhalation routes. Detailed information is output for every applicable pathway for every location, analyte, and time step combination.
POPDOSE	POPDOSE	This modifier activates output of a population dose summed over all radioactive analytes. Detailed information is output for every time step.
POPRISK	POPRISK	This modifier activates output of a population risk summed over all radioactive analytes. Detailed information is output for every time step.

The following entries provide examples of the use of the DETAILS keyword:

```
DETAILS ANADOSE
DETAILS ANADOSE POPDOSE SUMRISK
```

There are no quote strings associated with the DETAILS keyword.

14.4.5 END Keyword for HUMAN

The END keyword signifies the end of all keyword data. It should be the last keyword in the keyword file. All data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

There are no modifiers or quote strings associated with the END keyword.

14.4.6 EXECUTE Keyword for HUMAN

The EXECUTE keyword signifies that the user wishes to perform problem execution. If this keyword is not entered, then the inputs are checked for consistency, but the problem will not be executed. This is useful if the run being set up is expected to take a significant amount of computation time. The following is this keyword's syntax:

```
EXECUTE
```

There are no modifiers or quote strings associated with the EXECUTE keyword.

14.4.7 FILE Keyword for HUMAN

The FILE keyword is used to enter the names of input and output files except for the report file. The names of the files providing concentration data are contained in the environmental scenario file rather than in the keyword file. The following is this keyword's syntax:

```
FILE [modifier1="quote1"] {modifier2="quote2"} ... {modifier5="quote7"}
```

The file names are entered in quote strings, which must be enclosed in double quotation marks. Path names up to 72 characters long are supported. The file name associated with a modifier must be entered before the next modifier is entered. At least one FILE keyword is required for every run of the code. Table 14.10 describes the modifiers associated with the FILE keyword.

Table 14.10 Modifiers Associated with the FILE Keyword in the HUMAN Code

Modifier	Description
DETAIL	Output file containing the calculated risk for each analyte and segment for every realization of the code. The risks are written in tabular form so they can be imported easily into a spreadsheet or other software. This file is optional. It is required if any modifier is entered on the DETAILS keyword. The file is written in comma separated variables format, so a file name extension of *.csv is recommended.
ESD	Input environmental settings definition file that contains the definition of the environmental runs from which impacts are to be calculated.
HEADER	Output file containing information needed by post-processor programs to allow easy abstraction of the data output of the data code.
STATS	Output file containing summary statistics on the risks for every analyte at every location. This file is optional. It is required if any modifier is entered on the STATISTICS keyword. The file is written in comma separated variables format, so a file name extension of *.csv is recommended.

Modifier	Description
VALUES	Output file containing the generated stochastic values for every stochastic variable used in the run. The values are written in tabular form so they can be imported easily into a spreadsheet or other software. This file is optional. Entry of this modifier and the file name initiates data output.

The following are two example entries:

```
FILE  HEADER "TestCase.hdr"
FILE  DETAIL "TestCase.det"
```

The following set of two entries has the same effect as the single entry above.

```
FILE HEADER="TestCase.hdr"  DETAIL="TestCase.det"
```

14.4.8 FOOD Keyword for HUMAN

The FOOD keyword defines the path to the directory where all of the food files from a given run of ECEM reside. The MAP modifier identifies the record number map file for use with all food concentration (FCDA) data files. The following is this keyword's syntax:

```
FOOD [PATH="Q1"] [MAP="Q2"]
```

The keyword can also be written using the following syntax to match the entry in the ECEM code:

```
FOODS [PATH="Q1"] [MAP="Q2"]
```

The path to the directory is entered in a set of double quotes. The path name must end with a "\" for locations under a Windows operating environment or "/" for locations under a Linux operating environment. The path must be nonblank. An example for this keyword (for the Windows operating system) is the following:

```
FOOD PATH="C:\SAC_1\ECEM\FOODS\"
   MAP="Food_Map.Dat"
```

14.4.9 FOODSOIL Keyword for HUMAN

The optional FOODSOIL keyword is used to define the type of soil at upland locations to be used in the exposure calculations. This keyword is not needed if no upland locations are defined. The following is this keyword's syntax:

```
FOODSOIL  [ SODR | SOGW | SOSW ]
```

The same soil type is used for the entire run; it also determines the soil type used for the food calculations. Table 14.11 describes the modifiers associated with the FOODSOIL keyword.

Table 14.11 Modifiers Associated with the FOODSOIL Keyword in the HUMAN File

Modifier	Description
SODR	The food concentrations for the species were generated using dry land assumptions (no irrigation).
SOGW	The food concentrations for the species were generated using the assumption that the water source for irrigation was local groundwater.

Modifier	Description
SOSW	The food concentrations for the species were generated using the assumption that the water source for irrigation was surface water from the location identified in the ESD keyword file.

The following is an example entry for using food crops grown in soil irrigated with surface water:

```
FOODSOIL SOSW
```

14.4.10 FOODSOUR Keyword for HUMAN

The FOODSOUR(CE) keyword is used to set a single source location for all food consumption for birds, meat, or fish. Use of the FOODSOUR keyword overrides any food source locations provided on individual LOCATION keywords. The following is this keyword's syntax:

```
FOODSOUR  {BIRD= "Location ID"} {MEAT"Location ID"} {FISH "Location ID"}
   {FISH "Location ID"} {FISH "Location ID"}
```

Multiple FOODSOUR keywords can be entered. Table 14.12 describes the modifiers associated with the FOODSOUR keyword.

Table 14.12 Modifiers Associated with the FOODSOUR Keyword in the HUMAN File

Modifier	Description
BIRD	The quote string (location ID) associated with BIRD modifier indicates that food concentrations for the location identified by the location ID will be used at all locations in calculations where a human eats a bird.
FISH	The quote string (location ID) associated with FISH modifier indicates that food concentrations for the location identified by the location ID will be used at all locations in calculations where a human eats a fish.
FISH_2	The quote string (location ID) associated with FISH_2 modifier indicates that food concentrations for the location identified by the location ID will be used at all locations in calculations where a human eats the second variety of fish.
FISH_3	The quote string (location ID) associated with FISH modifier indicates that food concentrations for the location identified by the location ID will be used at all locations in calculations where a human eats the third variety of fish.
MEAT	The quote string (location ID) associated with MEAT modifier indicates that food concentrations for the location identified by the location ID will be used at all locations in calculations where a human eats meat.

The following is an example entry for assigning the food source location for meat and two varieties of fish:

```
FOODSOUR MEAT="UH1876" FISH="QHP013" FISH_3="QHP012"
```

14.4.11 INGESTION Keyword for HUMAN

The INGESTION keyword associates a food item for the HUMAN code with a concentration file prepared by the ECEM code for a food (species). The following is this keyword's syntax:

```
INGESTIO [BIRD= "Species ID 1"] [FISH= "Species ID 2"]
```

```
[LEAFY= “Species ID 3”] [MEAT= “Species ID 4”] [MILK= “Species ID 5”]
[ROOT= “Species ID 6”] [GRAIN= “Species ID 7”] [FRUIT= “Species ID 8”]
[EGGS= “Species ID 9”] {FISH_2= “Species ID 10”}
{FISH_3= “Species ID 11”}
```

Multiple INGESTIO keywords can be entered. Table 14.13 describes the modifiers associated with the INGESTIO keyword.

Table 14.13 Modifiers Associated with the INGESTIO Keyword in the HUMAN File

Modifier	Description
BIRD	The quote string (species ID) associated with BIRD modifier indicates that concentrations for the species identified by the species ID will be used in calculations where a human eats a bird. The quote string “NONE” should be used as the species definition for any food type not eaten.
FISH	The quote string (species ID) associated with FISH modifier indicates that concentrations for the species identified by the species ID will be used in calculations where a human eats fish. The quote string “NONE” should be used as the species definition for any food type not eaten.
FISH_2	The quote string (species ID) associated with optional FISH_2 modifier indicates that concentrations for the species identified by the species ID will be used in calculations where a human eats a second type of fish. The quote string “NONE” should be used as the species definition for any food type not eaten.
FISH_3	The quote string (species ID) associated with optional FISH_3 modifier indicates that concentrations for the species identified by the species ID will be used in calculations where a human eats a third kind of fish. The quote string “NONE” should be used as the species definition for any food type not eaten.
LEAFVEG	The quote string (species ID) associated with LEAFVEG modifier indicates that concentrations for the species identified by the species ID will be used in calculations where a human eats leafy vegetables. The quote string “NONE” should be used as the species definition for any food type not eaten.
MEAT	The quote string (species ID) associated with MEAT modifier indicates that concentrations for the species identified by the species ID will be used in calculations where a human eats meat. The quote string “NONE” should be used as the species definition for any food type not eaten.
MILK	The quote string (species ID) associated with MILK modifier indicates that concentrations for the species identified by the species ID will be used in calculations where a human drinks milk. The quote string “NONE” should be used as the species definition for any food type not eaten.
ROOTVEG	The quote string (species ID) associated with ROOTVEG modifier indicates that concentrations for the species identified by the species ID will be used in calculations where a human eats a root vegetable. The quote string “NONE” should be used as the species definition for any food type not eaten.
GRAIN	The quote string (species ID) associated with GRAIN modifier indicates that concentrations for the species identified by the species ID will be used in calculations where a human eats grain. The quote string “NONE” should be used as the species definition for any food type not eaten.
FRUIT	The quote string (species ID) associated with FRUIT modifier indicates that concentrations for the species identified by the species ID will be used in calculations where a human eats fruits. The quote string “NONE” should be used as the species definition for any food type not eaten.

Modifier	Description
EGGS	The quote string (species ID) associated with EGGS modifier indicates that concentrations for the species identified by the species ID will be used in calculations where a human eats eggs. The quote string "NONE" should be used as the species definition for any food type not eaten.

The NONE entry will override any consumption information entered for that food type. The following example entry assigns the ECEM species for meat, leafy vegetables, and fruit to be used as food sources:

```
INGESTIO MEAT="UH1876" LEAFVEG="QHP013" FRUIT="QHP013"
```

The following example entry assigns the ECEM species for meat and leafy vegetables while fruit is not consumed in the exposure scenario:

```
INGESTIO MEAT="UH1876" LEAFVEG="QHP013" FRUIT="NONE"
```

14.4.12 LOCATION Keyword for HUMAN

The LOCATION keyword identifies the locations for human impact calculations that will be generated. Multiple LOCATION keywords are required if more than one location is requested. The locations must be a subset of the locations at which environmental data were computed and stored by the inventory, release, and transport modules. The list of desired locations builds sequentially with each LOCATION record. Upon program entry, no locations are active. The following is this keyword's syntax:

```
LOCATION [PRIMARY="quote 1"] [SECOND="quote 2"] [THIRD="quote 3"] {POP=N1}
   {BIRD="quote 4"} {FISH="quote 5"} {MEAT="quote 6"} {FISH_2="quote 7"}
   {FISH_3="quote 8"} {OUTPUT}
```

The human impact module is activated at a location by entering the location ID string in association with the PRIMARY modifier. A LOCATION keyword is required at each location to activate calculations. Table 14.14 describes the modifiers associated with the LOCATION keyword.

Table 14.14 Modifiers Associated with the LOCATION Keyword in the HUMAN File

Modifier	Description
PRIMARY	The PRIMARY modifier is used to provide the ID for the assessment location. All results for this location will by associated with this location ID.
SECOND	The SECOND modifier is used to provide the ID for the optional secondary assessment location. Any environmental concentrations that are not available at the primary location are taken from the secondary location if they are available.
THIRD	The THIRD modifier is used to provide the ID for the optional tertiary assessment location. Any environmental concentrations that are not available at the primary or secondary locations are taken from the tertiary location if they are available.
POP	The POP modifier is associated with the population at the primary location. If no POP modifier is present, the population from the ESD location keyword will be used for this location.
BIRD	The quote string (location ID) associated with BIRD modifier indicates that concentrations for the location identified by the location ID will be used in calculations where a human eats a bird.

Modifier	Description
FISH	The quote string (location ID) associated with FISH modifier indicates that concentrations for the location identified by the location ID will be used in calculations where a human eats a fish.
FISH_2	The quote string (location ID) associated with FISH_2 modifier indicates that concentrations for the location identified by the location ID will be used in calculations where a human eats the second type of fish.
FISH_3	The quote string (location ID) associated with FISH_3 modifier indicates that concentrations for the location identified by the location ID will be used in calculations where a human eats the third type of fish.
MEAT	The quote string (location ID) associated with MEAT modifier indicates that concentrations for the location identified by the location ID will be used in calculations where a human eats meat.
OUTPUT	If the modifier OUTPUT is entered, then outputs requested by the DETAILS and STATISTICS keywords will be written to the output files for this location. Otherwise, the calculations will occur, but no data will be output for this location.

The following are example LOCATION keywords:

```
LOCATION PRIMARY="UH0001" SECOND="QHP220" POP=0 BIRD="UH0001"
   MEAT="UH0001" FISH="QHP220" OUTPUT
LOCATION PRIMARY="RHP250" SECOND="RHP250" POP=0 BIRD="RHP250"
   MEAT="RHP250" FISH="QHP220" FISH_2="QHP225" OUTPUT
```

14.4.13 REALIZAT Keyword for HUMAN

The REALIZAT (or REALIZATION) keyword defines the number of realizations to generate. The following is this keyword's syntax:

```
REALIZATION value1
```

The integer value1 has a minimum value of 1 and a maximum of the number of realizations defined in the environmental scenario definition file. If the number of realizations is fewer than the number of realizations in the concentration data files, then only the first realizations will be used. The following keyword record sets the number of realizations to 10:

```
REALIZAT 10
```

14.4.14 REPORT Keyword for HUMAN

The REPORT keyword is used to define the name of the output report (log) file. It must be the first keyword entered in the keyword file. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The name of the report file is entered in a quote string. File names up to 72 characters long are supported, and path names can be included. The following is an example REPORT keyword record:

```
REPORT "/SAC/SystemCodes/Cultural/Test1.rpt"
```

14.4.15 SEED Keyword for HUMAN

The SEED keyword sets the value for the seed for the random number generator. The following is this keyword's syntax:

```
SEED Value1
```

The value for Value1 must be an integer or real number in the range 1 to 999999. The following is an example keyword record:

```
SEED 344443
```

There are no modifiers or quote strings associated with the SEED keyword.

14.4.16 STATISTIC Keyword for HUMAN

The STATISTIC keyword is used to control writing summary statistics to the output summary statistics file for a variety of solution types. The following is this keyword's syntax:

```
STATISTIC [modifier 1] {modifier 2}…{modifier 11}
```

Multiple STATISTIC cards can be entered with combinations of modifiers, or a single card can be entered containing all of the modifiers. The modifiers can be entered in any order. Table 14.15 describes the modifiers associated with the STATISTIC keyword.

Table 14.15 Modifiers Associated with the STATISTIC Keyword in the HUMAN Code

Modifier	Solution ID	Description
CONCEN	CONMEDIA	This modifier activates output of statistics on media concentration for those analytes and locations whose OUTPUT flags have been activated.
FOODS	CONFOODS	This modifier activates output of statistics on food concentration data for those analytes and locations whose OUTPUT flags have been activated.
SUMDOSE	SUMDOSE	This modifier activates output of statistics on the dose for combined pathways that is summed over all radioactive analytes. This solution does not apply to carcinogenic or hazardous analytes. Information is written out for every time and location combination.
SUMRISK	SUMRISK	This modifier activates output of statistics for the risk or hazard quotient that is summed over all analytes of the same type (radioactive, carcinogenic, or hazardous). Information is output for every time and location combination.
ANADOSE	ANADOSE	This modifier activates output of statistics for the dose for each analyte. Information is output for every time, location, and analyte combination.
ANARISK	ANARISK	This modifier activates output of statistics for the risk or hazard quotient for each analyte. Information is output for every time, location, and analyte combination.
PATHDOSE	DOSEDER DOSEEXT DOSEING DOSEINH	This modifier activates output of statistics for the pathway dose for each analyte. Pathways include external (for radionuclides), dermal (for hazardous and carcinogenic analytes), ingestion, and inhalation routes. Information is output for every applicable pathway for every location, analyte, and time step combination.

Modifier	Solution ID	Description
PATHRISK	RISKDER RISKEXT RISKING RISKINH	This modifier activates output of statistics for the pathway risk or hazard quotient for each analyte. Pathways include external (for radionuclides), dermal (for hazardous and carcinogenic analytes), ingestion, and inhalation routes. Information is output for every applicable pathway for every location, analyte, and time step combination.
POPDOSE	POPDOSE	This modifier activates output of statistics for population dose summed over all radioactive analytes. Information is output for every time step.
POPRISK	POPRISK	This modifier activates output of statistics for population risk summed over all radioactive analytes. Information is output for every time step.

The following entries provide examples of the use of the STATISTIC keyword:

```
STATISTIC ANADOSE
STATISTIC ANADOSE PATHDOSE POPDOSE POPRISK
```

There are no quote strings associated with the STATISTIC keyword.

14.4.17 STOCHASTIC Keyword for HUMAN

The STOCHASTIC keyword is used to enter the definition of a statistical distribution for stochastic variables. The following is this keyword's syntax:

```
STOCHASTIC ["Quote1"] [Dist_Index Parameters] {TRUNCATE U1 U2}
   {"Quote2"}
```

The entry for Quote1 must be a unique character string of up to 20 characters that will be used to identify this stochastic variable in subsequent uses. It is case sensitive and embedded spaces are significant. It is sometimes useful to make the character string some combination of a variable name and other data such that it can be recreated easily when stochastic data is needed. The entry for Quote2 is a description for the stochastic variable that can be up to 64 characters long. An entry for Quote2 is not required.

The entry for Dist_Index must be an integer in the range 1 to 13 that identifies the index of a statistical distribution. The statistical distributions are defined in Section 19.0, Table 17.3. The word Parameters in the general syntax statement indicates the numerical values of parameters required for defining the statistical distribution. The additional modifier TRUNCATE can be used for all distribution types except 1, 3, and 10. If TRUNCATE is entered, it must be followed by two values in the interval 0 to 1, inclusive. The lower value must be less than the upper value. These two values specify the tail probabilities at which to impose range truncation for the distribution. Truncation data must be entered after all of the other parameters that define the distribution.

The following is an example stochastic record for the ingestion rate of soil for an adult that is uniformly distributed between 0.01 and 0.15:

```
STOCHASTIC "IRSOILADULT" 2 0.01 0.15 "Soil ingestion rate for an adult"
```

Although this section gives the general form of a STOCHASTIC keyword entry, it does not describe the entire set of STOCHASTIC keywords required to run the HUMAN code. A more complete set of example STOCHASTIC keywords is provided in Section 14.5. The example keywords are grouped by variable types as outlined in Table 14.16.

Table 14.16 Cross Reference to Example STOCHASTIC Keywords for the HUMAN Code

Cross-Reference	Multiple Dependencies	Type of Data Defined Using STOCHASTIC Keywords
Table 14.17	None	Exposure frequencies for different human activities.
Table 14.18	None	Exposure times for different human activities.
Table 14.19	None	Ingestion rates for water and food types.
Table 14.20	None	Miscellaneous variables.
Table 14.21	None	Data describing the body variability in humans.
Table 14.22	Analyte	Volatilization and Permeability Data.
Table 14.23	Analyte	Reference Doses for inhalation and ingestion that are used to compare intake to levels of concern. These data are required only for the analytes modeled as hazardous constituents.
Table 14.24	Analyte	Dose factors for converting external exposure and intake of radionuclides to dose. These data are required only for the radioactive analytes.
Table 14.25	Analyte	Slope factors for inhalation and ingestion that are used to compare intake to risk. These data are required only for the analytes modeled as carcinogenic constituents.

14.4.18 SWEAT Keyword for HUMAN

The SWEAT keyword is used to define the source of water to be used in the sweat lodge calculations. The following is this keyword's syntax:

```
SWEAT [ GROUND | RIVER | SEEP | NONE ]
```

If the SWEAT keyword is not used or the modifier NONE is entered, then the sweat portion of the impact equations will yield a zero impact. The following is the keyword entry to select river water as the water source for sweat lodge calculations:

```
SWEAT RIVER
```

There are no quote strings or numerical values associated with the SWEAT keyword.

14.4.19 TIMES Keyword for HUMAN

The TIMES keyword identifies the times at which the calculations are to be performed. The following is this keyword's syntax:

```
TIMES [ [T1] {T2} … {Tn} | {ALL} ]
```

The numerical entries T1, T2, …, Tn are the times (whole number years) when human impacts calculations are desired. These times must be a subset of the times at which environmental data were computed and stored by the inventory, release, and transport modules. Multiple TIMES keywords can be entered. If the modifier ALL is used, results will be calculated for every time in the ESD keyword file. If the modifier ALL is used, no numerical values should be entered. The following is an example TIMES keyword that requests output for the three years 2020, 2075, and 3014:

```
TIMES 2020 2075 3014
```

The following is an example TIMES keyword where all times from the ESD keyword file are requested:

```
TIMES ALL
```

There are no quote strings associated with the TIMES keyword.

14.4.20 TITLE Keyword for HUMAN

The TITLE keyword is used to define a single-line problem title. The problem title will be written to output files. If the title is not supplied, then the program will error terminate. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 72 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the human impacts code."
```

There are no modifiers associated with the TITLE keyword.

14.4.21 USER Keyword for HUMAN

The USER keyword is used to identify the user of the program. The user name will be written to output files. If the user name is not supplied, then the program will error terminate. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

There are no modifiers associated with the USER keyword.

14.5 Example Stochastic Keywords for the HUMAN Code

The equations in Section 14.1.1 reference exposure frequencies for a number of activities. Table 14.17 provides example statistical distributions for these activities and the resulting keywords that implement the definitions.

Table 14.17 Example HUMAN Keywords for Entering Exposure Frequencies

Variable	Description	Units	Statistical Distribution
EF_{boat}	Exposure frequency for boating	day/yr	Constant of 5
`STOCHASTIC "EFBOAT" 1 5` `"Exposure frequency for boating"`			

Variable	Description	Units	Statistical Distribution
EF_{river}	Exposure frequency to volatile river water	day/yr	Uniform on 270 to 365
`STOCHASTIC "EFRIVER" 2 270 365` `"Exposure frequency to volatile river water"`			
EF_{sed}	Exposure frequency for sediment	day/yr	Uniform on 1 to 20
`STOCHASTIC "EFSED" 2 1 20` `"Exposure frequency to sediment"`			
EF_{seep}	Exposure frequency volatilized seep water	day/yr	Uniform on 270 to 365
`STOCHASTIC "EFSEEP" 2 270 365` `"Exposure frequency volatile seep water"`			
EF_{soil}	Exposure frequency for soil	day/yr	Uniform on 270 to 365
`STOCHASTIC "EFSOIL" 2 270 365` `"Exposure frequency for soil"`			
EF_{swim}	Exposure frequency for swimming	day/yr	Uniform on 1 to 20
`STOCHASTIC "EFSWIM" 2 1 20` `"Exposure frequency for swimming"`			
EF_{sweat}	Exposure frequency for sweat lodge	day/yr	Constant of 0
`STOCHASTIC "EFSWEAT" 1 0` `"Exposure frequency for sweat lodge"`			
EF_{ground}	Exposure frequency for drinking groundwater	day/yr	Uniform on 270 to 365
`STOCHASTIC "EFGROUND" 2 270 365` `"Exposure frequency for drinking groundwater"`			
EF_{leafy}	Exposure frequency for leafy vegetables	day/yr	Uniform on 270 to 365
`STOCHASTIC "EFLEAFY" 2 270 365` `"Exposure frequency for leafy vegetables"`			
EF_{root}	Exposure frequency for eating root vegetables	day/yr	Uniform on 270 to 365
`STOCHASTIC "EFROOT" 2 270 365` `"Exposure frequency for eating root vegetables"`			

Variable	Description	Units	Statistical Distribution
EF_{meat}	Exposure frequency for eating meat	day/yr	Uniform on 270 to 365
`STOCHASTIC "EFMEAT" 2 270 365` `"Exposure frequency for eating meat"`			
EF_{milk}	Exposure frequency for drinking milk	day/yr	Uniform on 270 to 365
`STOCHASTIC "EFMILK" 2 270 365` `"Exposure frequency for drinking milk"`			
EF_{bird}	Exposure frequency for eating birds (poultry)	day/yr	Uniform on 270 to 365
`STOCHASTIC "EFBIRD" 2 270 365` `"Exposure frequency for eating birds (poultry)"`			
EF_{fish}	Exposure frequency for eating fish	day/yr	Uniform on 270 to 365
`STOCHASTIC "EFFISH" 2 270 365` `"Exposure frequency for eating fish"`			
EF_{fish_2}	Exposure frequency for eating fish	day/yr	Uniform on 270 to 365
`STOCHASTIC "EFFISH_2" 2 270 365` `"Exposure frequency for eating optional second variety of fish"`			

The equations in Section 14.1.1 reference exposure times and durations for a number of activities. Table 14.18 provides example statistical distributions for these activities and the resulting keywords that implement the definitions.

Table 14.18 Example HUMAN Keywords for Entering Exposure Times

Variable	Description	Units	Statistical Distribution
ET_{boat}	Exposure time for boating	hr/day	Constant of 0
`STOCHASTIC "ETBOAT" 1 0` `"Exposure time for boating"`			
ET_{river}	Exposure time to volatile river water	hr/day	Uniform on 10 to 20
`STOCHASTIC "ETRIVER" 2 10 20` `"Exposure time to volatile river water"`			
ET_{sed}	Exposure time for sediment	hr/day	Constant of 0
`STOCHASTIC "ETSED" 1 0` `"Exposure time for sediment"`			

Variable	Description	Units	Statistical Distribution
ET_{seep}	Exposure time volatile seep water	hr/day	Uniform on 10 to 24
`STOCHASTIC "ETSEEP" 2 10 24` `"Exposure time volatile seep water"`			
ET_{soil}	Exposure time for soil	hr/day	Uniform on 8 to 24
`STOCHASTIC "ETSOIL" 2 8 24` `"Exposure time for soil"`			
ET_{swim}	Exposure time for swimming	hr/day	Uniform on 0 to 8
`STOCHASTIC "ETSWIM" 2 0 8` `"Exposure time for swimming"`			
ET_{sweat}	Exposure time for sweat lodge	hr/day	Uniform on 10 to 24
`STOCHASTIC "ETSWEAT" 1 0` `"Exposure time for sweat lodge"`			
ED_{child}	Exposure duration for a child	yr	Uniform on 1 to 6
`STOCHASTIC "EDCHILD" 2 1 6` `"Exposure duration for a child"`			
ED_{adult}	Exposure duration for an adult	yr	Uniform on 1 to 64
`STOCHASTIC "EDADULT" 2 1 64` `"Exposure duration for an adult"`			

The equations in Section 14.1.1 reference inhalation and ingestion rates for a number of foods. Table 14.19 provides example statistical distributions for these activities and the resulting keywords that implement the definitions.

Table 14.19 Example HUMAN Keywords for Entering Ingestion Rates

Variable	Description	Units	Statistical Distribution
IRATE	Inhalation rate	m^3/day	Uniform on 15 to 30
`STOCHASTIC "IRATE" 2 15 30` `"Inhalation rate"`			
$IR_{soilchild}$	Ingestion rate, soil child	kg/day	Uniform on 0.00002 to 0.0005
`STOCHASTIC "IRSOILCHILD" 2 0.00002 0.00050` `"Soil ingestion rate for a child"`			
$IR_{soiladult}$	Ingestion rate, soil adult	kg/day	Uniform on 0.00001 to 0.00015

Variable	Description	Units	Statistical Distribution
STOCHASTIC "IRSOILADULT" 2 0.00001 0.00015 "Soil ingestion rate for an adult"			
$IR_{sedchild}$	Ingestion rate, sediment – child	kg/day	Uniform on 0.00002 to 0.0005
STOCHASTIC "IRSEDCHILD" 2 0.00002 0.00050 "Sediment ingestion rate for a child"			
$IR_{sedadult}$	Ingestion rate, sediment – adult	kg/day	Uniform on 0.00001 to 0.00015
STOCHASTIC "IRSEDADULT" 2 0.00001 0.00015 "Sediment ingestion rate for an adult"			
IR_{river}	Ingestion rate, river water	L/day	Uniform on 0 to 3
STOCHASTIC "IRRIVER" 2 0 3 "River water ingestion rate"			
IR_{ground}	Ingestion rate, ground water	L/day	Uniform on 0 to 3
STOCHASTIC "IRGROUND" 2 0 3 "Ground water ingestion rate"			
IR_{seep}	Ingestion rate, seep water	L/day	Constant of 0
STOCHASTIC "IRSEEP" 1 0 "Seep water ingestion rate"			
IR_{fish}	Ingestion rate, fish	kg/day	Uniform on 0 to 0.1
STOCHASTIC "IRFISH" 2 0 0.1 "Ingestion rate for fish"			
IR_{fish_2}	Ingestion rate, fish	kg/day	Uniform on 0 to 0.1
STOCHASTIC "IRFISH_2" 2 0 0.1 "Ingestion rate for optional second variety fish"			
IR_{leafy}	Ingestion rate, leafy vegetables	kg/day	Uniform on 0 to 0.5
STOCHASTIC "IRLEAFY" 2 0 0.5 "Ingestion rate for leafy vegetables"			
IR_{root}	Ingestion rate, root vegetables	kg/day	Constant of 0
STOCHASTIC "IRROOT" 1 0 "Ingestion rate for root vegetables"			
IR_{meat}	Ingestion rate, meat	kg/day	Uniform on 0 to 0.25

Variable	Description	Units	Statistical Distribution
STOCHASTIC "IRMEAT" 2 0 0.25 "Ingestion rate for meat"			
IR_{milk}	Ingestion rate, milk	L/day	Uniform on 0.1 to 1
STOCHASTIC "IRMILK" 2 0.1 1 "Milk ingestion rate"			
IR_{bird}	Ingestion rate, birds	kg/day	Constant of 0
STOCHASTIC "IRBIRD" 1 0 "Ingestion rate for bird meat"			

The equations in Section 14.1.1 reference several soil and air concentration related variables. Table 14.20 provides example statistical distributions for these activities and the resulting keywords that implement the definitions.

Table 14.20 Example HUMAN Keywords for Entering Concentration Variables

Variable	Description	Units	Statistical Distribution
ML	Mass loading of soil in air	kg/m^3	Constant of 0.00000005
STOCHASTIC "ML" 1 0.00000005 "Mass loading of soil in air"			
AF_{soil}	Adherence factor for soil	$mg/cm^2/day$	Uniform on 0.05 to 0.5
STOCHASTIC "AFSOIL" 2 0.05 0.50 "Adherence factor for soil"			
AF_{sed}	Adherence factor for sediment	$mg/cm^2/day$	Uniform on 0.05 to 0.5
STOCHASTIC "AFSED" 2 0.05 0.50 "Adherence factor for sediment"			
IRGRATE	Irrigation rate	L/m^2 per yr	Uniform on 500 to 1000
STOCHASTIC "IRGRATE" 2 500 1000 "Irrigation rate"			
SHIELDSOIL	Soil shielding factor	unitless	Constant of 0.8
STOCHASTIC "SHIELDSOIL" 1 0.8 "Soil shielding factor"			
SHIELDSED	Sediment shielding factor	unitless	Constant of 0.2
STOCHASTIC "SHIELDSED" 1 0.2 "Sediment shielding factor"			

Variable	Description	Units	Statistical Distribution
CF_{sweat}	Air concentration factor for sweat lodge	L/m^3	Uniform on 0.1 to 0.3
`STOCHASTIC "CFSWEAT" 2 0.1 0.3` `"Air concentration factor for sweat lodge"`			

The equations in Section 14.1.1 reference several body size variables. Table 14.21 provides example statistical distributions for these activities and the resulting keywords that implement the definitions.

Table 14.21 Example Keywords for Entering Body Data in the HUMAN Code

Variable	Description	Units	Statistical Distribution
BW_{child}	Body weight for a child	kg	Constant of 16
`STOCHASTIC "BWCHILD" 1 16` `"Body weight for a child"`			
BW_{adult}	Body weight for an adult	kg	Constant of 70
`STOCHASTIC "BWADULT" 1 70` `"Body weight for an adult"`			
SA_{soil}	Body surface area – soils	cm^2	Constant of 5000
`STOCHASTIC "SASOIL" 1 5000` `"Body surface area for soil exposure"`			
SA_{sed}	Body surface area – sediments	cm^2	Constant of 5000
`STOCHASTIC "SASED" 1 5000` `"Body surface area for sediment exposure"`			
SA_{seep}	Body surface area - seep water	cm^2	Constant of 20000
`STOCHASTIC "SASEEP" 1 20000` `"Body surface area for seep water exposure"`			
SA_{river}	Body surface area - river water	cm^2	Constant of 20000
`STOCHASTIC "SARIVER" 1 20000` `"Body surface area for river water exposure"`			
SA_{other}	Body surface area - river water	cm^2	Constant of 0
`STOCHASTIC "SAOTHER" 1 0` `"Body surface area for other (Native American) activities"`			
SA_{sweat}	Body surface area - sweat lodge	cm^2	Constant of 20000

Variable	Description	Units	Statistical Distribution
STOCHASTIC "SASWEAT" 1 20000 "Body surface area sweat lodge calculations"			

The equations in Section 14.1.1 reference volatilization, permeability, and skin absorption variables. Values for these variables must be entered for every analyte. Table 14.22 provides example statistical distributions for these activities and the resulting keywords that implement the definitions.

Table 14.22 Example HUMAN Keywords for Volatilization and Permeability Data

Analyte	Variable	Description	Units	Statistical Distribution
CCl4	VF	CCL4 Volatilization Factor	L/m^3	Loguniform on Lower Limit 0.001, Upper Limit 0.1
STOCHASTIC "CCl4 VF" 4 0.001 0.1 "CCL4 Volatilization Factor"				
CrVI	KP	Cr Skin Permeability Coefficient	cm/hr	Loguniform on Lower Limit 0.0003 Upper Limit 0.003
STOCHASTIC "CrVI KP" 4 0.0003 0.0030 "Cr Skin Permeability Coefficient"				
U	ABS	U Skin Absorption Factor	unitless	Loguniform on Lower Limit 0.0001, Upper Limit 0.01
STOCHASTIC "U ABS" 4 0.0001 0.0100 "U Skin Absorption Factor"				

The equations in Section 14.1.1 refer to oral and inhalation reference doses for hazardous analytes. These values must be entered for every analyte. Table 14.23 provides example statistical distributions for these activities and the resulting keywords that implement the definitions.

Table 14.23 Example HUMAN Keywords for Entering Reference Doses

Analyte	Variable	Description	Units	Statistical Distribution
CrVI	RFD_{inh}	Cr(VI) reference dose for inhalation	mg(intake)/(kg(bodyweight)/day)	Triangular on Lower Limit 1.00E-03, Mode 0.005, Upper Limit 0.015
STOCHASTIC "CrVI RFDINH" 6 0.001 0.005 0.015 "Cr(VI) reference dose for inhalation"				
CrVI	RFD_{ing}	Cr(VI) reference dose for ingestion	mg(intake)/(kg(bodyweight)/day)	Triangular on Lower Limit 0.001, Mode 0.005, Upper Limit 0.015
STOCHASTIC "CrVI RFDING" 6 0.001 0.005 0.015 "Cr(VI) reference dose for ingestion"				

Analyte	Variable	Description	Units	Statistical Distribution
CCl4	RFD_{inh}	CCl4 reference dose for inhalation	mg(intake)/(kg(bodyweight) /day)	Loguniform on Lower Limit 7.00E-06, Upper limit 7.00E-04
`STOCHASTIC "CCL4 RFDINH" 5 7.0E-06 7.0E-04 "CCl4 reference dose for inhalation"`				
CC4	RFD_{ing}	CCl4 reference dose for ingestion	mg(intake)/(kg(bodyweight) /day)	Loguniform on Lower Limit 7.00E-06, Upper Limit 7.00E-04
`STOCHASTIC "CCL4 RFDING" 5 7.0E-06 7.0E-04 "CCl4 reference dose for ingestion"`				
U	RFD_{inh}	U reference dose for inhalation	mg(intake)/(kg(bodyweight) /day)	Loguniform on Lower Limit 1.40E-06, Upper Limit 1.40E-03
`STOCHASTIC "U RFDINH" 5 1.4E-06 1.4E-03 "U reference dose for inhalation"`				
U	RFD_{ing}	reference dose for ingestion	mg(intake)/(kg(bodyweight) /day)	Loguniform on Lower Limit 3.00E-06, Upper Limit 3.00E-03
`STOCHASTIC "U RFDING" 5 3.0E-06 3.0E-03 "U reference dose for ingestion"`				

The equations in Section 14.1.1 reference dose factors for radioactive analytes. The dose factors must be entered for every radioactive analyte. Table 14.24 provides example statistical distributions for these activities and the resulting keywords that implement the definitions.

Table 14.24 Example HUMAN Keywords for Entering Radiation Dose Factors

Analyte	Variable	Description	Units	Statistical Distribution
Cs137	DF_{soil}	Cs/Ba137 dose factor for soil	rem/hr per pCi/g	Triangular on Lower Limit 2.50E-08, Mode 5.00E-08, Upper Limit 1.00E-07
`STOCHASTIC "U HQING" 5 3.0E-06 3.0E-03 "U dose factor for soil exposure"`				
Cs137	DF_{swim}	Cs/Ba137 dose factor for swimming	rem/hr per pCi/L	Triangular on Lower Limit 4.20E-10, Mode 8.30E-10, Upper Limit 1.70E-09
`STOCHASTIC "Cs137 DFSWIM" 6 4.20E-10 8.30E-10 1.70E-09 "Cs/Ba137 dose factor for swimming"`				
Cs137	DF_{boat}	Cs/Ba137 dose factor for boating	rem/hr per pCi/L	Triangular on Lower limit 2.10E-10, mode 4.20E-10, Upper Limit 8.30E-10

Analyte	Variable	Description	Units	Statistical Distribution
STOCHASTIC "Cs137 DFBOAT" 6 2.10E-10 4.20E-10 8.30E-10 "Cs/Ba137 dose factor for boating"				
Cs137	DF_{ing}	Cs137 dose factor for ingestion	rem/pCi	Lognormal on Mean -7.30103, Standard Deviation of Logarithms 3.01E-01
STOCHASTIC "Cs137 DFING" 8 -7.30103E+00 3.01E-01 "Cs137 dose factor for ingestion"				
Cs137	DF_{inh}	Cs137 dose factor for inhalation	rem/pCi	Lognormal on Mean -7.49485, Standard Deviation of Logarithms 3.01E-01
STOCHASTIC "Cs137 DFINH" 8 -7.49485E+00 3.01E-01 "Cs137 dose factor for inhalation"				
H3	DF_{soil}	H3 dose factor for soil	rem/hr per pCi/g	Constant of 0
STOCHASTIC "H3 DFSOIL" 1 0 "H3 dose factor for soil"				
H3	DF_{swim}	H3 dose factor for swimming	rem/hr per pCi/L	Constant of 0
STOCHASTIC "H3 DFSWIM" 1 0 "H3 dose factor for swimming"				
H3	DF_{boat}	H3 dose factor for boating	rem/hr per pCi/L	Constant of 0
STOCHASTIC "H3 DFBOAT" 1 0 "H3 dose factor for boating"				
H3	DF_{ing}	H3 dose factor for ingestion	rem/pCi	Lognormal on Mean -10.1938, Standard Deviation of Logarithms 3.01E-01
STOCHASTIC "H3 DFING" 8 -1.01938E+01 3.01E-01 "H3 dose factor for ingestion"				
H3	DF_{inh}	H3 dose factor for inhalation	rem/pCi	Lognormal on Mean -10.0177, Standard Deviation of Logarithms 3.01E-01
STOCHASTIC "H3 DFINH" 8 -1.00177E+01 3.01E-01 "H3 dose factor for inhalation"				

The equations in Section 14.1.1 reference slope factors for carcinogenic analytes. The slope factors must be defined for every carcinogenic analyte. Table 14.25 provides example statistical distributions for these activities and the resulting keywords that implement the definitions.

Table 14.25 Example HUMAN Keywords for Entering Slope Factors

Analyte	Variable	Description	Units	Statistical
CCl4	SF_{inh}	CCl4 slope factor for inhalation	risk per mg(intake)/(kg(bodyweight)/day)	Lognormal on Mean -1.27572, Standard Deviation of Logarithms 0.47712
`STOCHASTIC "CCl4 SFINH" 8 -1.27572 0.47712` `"CCl4 slope factor for inhalation"`				
CCl4	SF_{ing}	CCl4 slope factor for ingestion	risk per mg(intake)/(kg(bodyweight)/day)	Lognormal Mean -0.88606, Standard Deviation of Logarithms 0.47712
`STOCHASTIC "CCl4 SFING" 8 -0.88606 0.47712` `"CCl4 slope factor for ingestion"`				
CrVI	SF_{inh}	Cr slope factor for inhalation	risk per mg(intake)/(kg(bodyweight)/day)	Triangular on Lower Limit 21, Mode 42, Upper Limit 290
`STOCHASTIC "CrVI SFINH" 6 21 42 290` `"Cr slope factor for inhalation"`				
CrVI	SF_{ing}	Cr slope factor for ingestion	risk per mg(intake)/(kg(bodyweight)/day)	User-defined cumulative distribution function

`STOCHASTIC "CrVI SFING" 10`
`"Cr slope factor for ingestion" 8 (0,0) (0.7999,0) (0.8,21)`
`(0.8499,21) (0.85,42) (0.8999,42) (0.9,290) (1,290)`				

15.0 RIPSAC – Riparian Zone Module

15.1 Code Purpose

The riparian zone module (RIPSAC) calculates the concentrations of analytes in seep water and soil. The riparian zone model algorithms apply only in the region along the edge of the river where there is significant interaction between groundwater and river water. RIPSAC reads analyte concentrations in groundwater and surface water from ECDA files (see Section 2.2), calculates the concentrations for seep water and soil, and writes the calculated concentrations back into the same files.

15.2 Algorithms and Assumptions

Concentrations of analytes in seep water (groundwater seepage face boundaries flowing to the river) are calculated from the concentration in groundwater using the following equation:

$$C_{seep} = \left(Df_{seep} C_{gw}\right) + \left(1 - Df_{seep}\right) C_{river}$$

where

C_{seep} = Concentration of an analyte in seep water (Ci/m^3 or kg/m^3)
C_{gw} = Concentration of an analyte in ground water (Ci/m^3 or kg/m^3)
C_{river} = Concentration of an analyte in river (surface) water (Ci/m^3 or kg/m^3)
Df_{seep} = Dilution factor controlling the mixing of groundwater and river water (unitless).

Concentrations of analytes in the upper layer of riparian zone soil are calculated from the concentration in seep water using the following equation:

$$C_{soil} = C_{seep}\ Kd_{soil}$$

where

C_{soil} = Concentration of an analyte in soil (Ci/kg soil or kg/kg soil)
C_{seep} = Concentration of an analyte in seep water (Ci/m^3 or kg/m^3)
Kd_{soil} = Partition coefficient for the analyte between water and soil (m^3/kg).

15.3 Code Execution Environment

The RIPSAC code is invoked in a standalone mode.

15.3.1 Location in the Processing Sequence

The general processing sequence for TIIA environmental runs is outlined in Figure 1.1. RIPSAC is an optional step in the environmental transport sequence and operates using internal realization looping. Thus, only one run of RIPSAC is required to process all realizations for all analytes. RIPSAC may also be run on a subset of data for any combination of realizations and analytes.

15.3.2 How the Code Is Invoked

RIPSAC may be used in either Microsoft Windows or Linux environments, provided that the code has been compiled by a Fortran 95 compiler appropriate for the environment. In the Microsoft Windows (Release XP) environment, RIPSAC is executed either of the following DOS commands:

```
RIPSAC "Keyword File"
RIPSAC
```

In the Linux environment, RIPSAC is executed through either of the following Bourne Shell or C Shell commands:

```
ripsac-1.exe "keyword file"
ripsac-1.exe
```

In the first example for both operating systems, RIPSAC is invoked and assumes the file identified by "keyword file" (file names are case sensitive under Linux), which contains the controlling keywords for RIPSAC. In the second example, the keyword file name is missing from the command line, thus RIPSAC queries the user for the name of the file. In either example, if the keyword file is not found, RIPSAC writes an error message and terminates execution.

15.4 Keyword Descriptions for the RIPSAC Code

In general, the keywords for RIPSAC (Table 15.1) can be entered in any order. The only restriction on keyword order is that the END keyword must be the last keyword in the file.

Table 15.1 Summary of Keywords Used by RIPSAC

Keyword	Description
ANALYTE	The ANALYTE keyword defines the analytes to be used in a run of RIPSAC.
DEBUG	The DEBUG keyword is used to activate dumping of intermediate calculations to the report file.
END	The END keyword signifies the end of all keyword data.
EXECUTE	The EXECUTE keyword indicates the problem will be executed in addition to performing input consistency checks.
FILE	The FILE keyword is used to enter the name of the ESD keyword file.
KDSOIL	The KDSOIL keyword is used to assign soil-water partition coefficients to locations for use in the soil concentration calculations.
LOCATION	The LOCATION keyword is used to associate groundwater and surface water concentrations with dilution factors in order to complete soil and seep water concentration calculations.
REALIZATION	The REALIZATION keyword is used to define the realizations to be processed in a run of RIPSAC.
REPORT	The REPORT keyword is used to define the name of the output report (log) file.
TITLE	The TITLE keyword is used to define a single-line problem title.
USER	The USER keyword is used to identify the user of the program.

15.4.1 ANALYTE Keyword for RIPSAC

The ANALYTE keyword is used to define the analytes to be used in the simulation. The following is this keyword's syntax:

```
ANALYTE ["quote1"] {"quote2"} … {"quoteN"}
```

One or more analyte IDs are entered in quote strings. The analyte IDs entered must be a subset of the analytes defined in the ESD keyword file. Multiple ANALYTE keywords may be entered, and multiple analytes can be processed in a single run of the code. Two example keywords are the following:

```
ANALYTE "H3"
ANALYTE "C14" Cl36" Se79" Sr90"
```

15.4.2 DEBUG Keyword for RIPSAC

The DEBUG keyword is used to activate dumping of intermediate calculations to the report file. It should be used only on small problem definitions with only one or two realizations; otherwise the volume of output can easily exceed 2 gigabytes. The following is this keyword's syntax:

```
DEBUG
```

15.4.3 END Keyword for RIPSAC

The END keyword signifies the end of all keyword data. It should be the last keyword in the keyword file. All data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

15.4.4 FILE Keyword for RIPSAC

The FILE keyword is used to enter the name of the ESD keyword file for the assessment. The names of the files providing concentration data are contained in the ESD keyword file rather than in the RIPSAC keyword file. The following is this keyword's syntax:

```
FILE [ESD="quote1"]
```

The file name must be entered in a quote string,. Path names up to 200 characters long are supported. An example entry is the following:

```
FILE ESD "G:\RIPSAC\Tests\Test_Case_12.Key"
```

15.4.5 KDSOIL Keyword for RIPSAC

The KDSOIL keyword is used to assign soil-water partition coefficients to locations for use in the soil concentration calculations. The coefficients are extracted from a library of values that are defined in the ESD keyword file (see Section 2.4.2). The KDSOIL keywords in RIPSAC are assigned as a function of location and analyte. The following is this keyword's syntax:

```
KDSOIL [ANALYTE="quote1"] [KDSOIL="quote2"] [LOCATION="quote2"
   {"quote4"} … {"quoteN"}|TERSE]
```

Multiple KDSOIL keyword entries may be required if there is more than one analyte and more than one riparian zone location. The KDSOIL keywords must cover every combination of analyte and riparian zone locations where soil concentrations are to be computed.

The quote string associated with the ANALYTE modifier must contain the ID of an analyte identified in the ESD keyword file (see Section 5.3.1). The quote string associated with the KDSOIL modifier must contain the ID string of KDSOIL variable identified in the ESD keyword file (see Section 5.3.8).

Only one of the TERSE and LOCATION modifiers can be used. If the TERSE modifier is entered then the same KDSOIL definition will be used for all locations. If the LOCATION modifier is used it must be associated with one or more quote strings containing location ID's for riparian zone locations that were defined in the ESD keyword file.

Example keyword entries include the following:

```
KDSOIL TERSE ANALYTE="H3"    KDSOIL="KDH"
KDSOIL TERSE ANALYTE="C14"   KDSOIL="KDC"
KDSOIL ANALYTE="Sr90" KDSOIL="KDSr" LOCATION= "RFP001" "RFP002" "RFP003"
```

15.4.6 LOCATION Keyword for RIPSAC

The LOCATION keyword is used to associate groundwater and surface water concentrations with dilution factors in order to complete soil and seep water concentration calculations. The dilution factor coefficients are extracted from a library of values that are defined in the ESD keyword file. The following is this keyword's syntax:

```
LOCATION [PRIMARY="quote1"] [SECOND="quote2"] [DF="quote3"]
```

There must be a LOCATION keyword entry for every location where seep water or soil concentrations are to be computed. The quote string associated with the PRIMARY modifier must contain the ID string of a riparian location defined in the ESD keyword (see Section 5.3.10). This location must have the groundwater concentration solution activated. The quote string associated with the SECOND modifier must contain the ID string of a location where a surface water concentration solution has been identified in the ESD keyword file. The quote string associated with the DF modifier must contain the ID string of a dilution variable (see Section 5.3.3) identified in the ESD keyword file.

Example keyword entries include the following:

```
LOCATION PRIMARY="RHP001" SECOND="QHP001" DF="DF5m"
LOCATION PRIMARY="RHP002" SECOND="QHP002" DF="DF5m"
LOCATION PRIMARY="RHP003" SECOND="QHP003" DF="DF5m"
LOCATION PRIMARY="RHP004" SECOND="QHP004" DF="DF5m"
LOCATION PRIMARY="RHP005" SECOND="QHP005" DF="DF5m"
```

15.4.7 REALIZATION Keyword for RIPSAC

The REALIZATION keyword is used to define the realizations to be processed in the RIPSAC code. The following is this keyword's syntax:

```
REALIZATION [ALL | LIST N1 {N2 ... Nn} | RANGE N1 N2 ]
```

The ESD keyword file defines the total number of realizations that will be processed in the suite of environmental and impacts codes. The RIPSAC code can process all realizations at one time, or it can process a subset of the realizations. Table 15.2 describes the modifiers used on the REALIZATION keyword. Only one of the ALL, LIST or RANGE modifiers is allowed on a single entry of the REALIZATION keyword. Upon entry to the code, none of the realizations are selected for processing.

Multiple REALIZATION keyword entries may be used with the definition of active realizations building with each additional keyword entry.

Table 15.2 Modifiers for the REALIZATION Keyword in RIPSAC

Modifier	Description
ALL	The presence of this modifier will activate processing of all realizations defined in the ESD keyword file.
LIST	The LIST modifier must be accompanied by one or more realization indices. All realization indices in the list will be processed. The realization indices do not have to be entered in any particular order.
RANGE	The RANGE modifier must be accompanied by two realization indices. All realizations from the first to the second indices, inclusive of the end points, will be processed. The second index must be equal to, or greater than, the first index.

The following REALIZATION keyword in the RIPSAC keyword file would invoke processing for all realizations defined in the ESD keyword file.

```
REALIZATION ALL
```

The following set of REALIZATION keywords assume that 100 realizations are defined in the ESD keyword file. These keywords define processing in RIPSAC for realization numbers 2, 4, 6, 12, 13, 14, 15, 99, and 100.

```
REALIZATION LIST 2 4 6 100 99
REALIZATION RANGE 12 15
```

15.4.8 REPORT Keyword for RIPSAC

The REPORT keyword is used to define the name of the output report (log) file. It must be the first keyword entered in the keyword file. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The name of the report file is entered in a quote string, which must be enclosed in double quotation marks. File names up to 200 characters long are supported, and path names can be included. An example REPORT keyword is the following:

```
REPORT "/SAC/SystemCodes/Test.rpt"
```

15.4.9 TITLE Keyword for RIPSAC

The TITLE keyword is used to define a single-line problem title. The problem title will be written to output files. If the title is not supplied the program will error terminate. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 72 characters long are supported. The following example defines a title for a run of the code.

```
TITLE "Example title line for the RIPSAC code."
```

15.4.10 USER Keyword for RIPSAC

The USER keyword is used to identify the user of the program. The user name will be written to output files. If the user name is not supplied, the program will error terminate. The following is this keyword's syntax:

```
USER "John Q. Public"
```

15.5 Data Files

The RIPSAC code reads four or more input files and writes a number of output files. The number of input and output files depends on the number of contaminants being analyzed. The following sections describe these files.

15.5.1 Input Files

The input files for RIPSAC are two keyword files, a KDSOIL data file, a DILUTE data file, and a suite of concentration data files. The RIPSAC keyword file controls the case RIPSAC will execute, and it points to the ESD keyword file. The suite of concentration data files are all identified in the ESD keyword file—the user of the RIPSAC only needs to identify the ESD keyword file.

15.5.1.1 ESD Keyword File

RIPSAC reads keywords from the ESD keyword file. These keywords are read from a different file and can have a different definition than for keywords defined for internal use in RIPSAC. Section 2.1 defines the ESD keywords. The following keywords are required:

- ANALYTE – defines analytes in the assessment
- END – end of the ESD keyword data
- FILE – file names for ECDA-related files
- LOCATION – locations defined in the assessment
- REALIZAT – number of realizations to be simulated
- TIMES – times at which ECDA data are saved for the the impacts codes
- TITLE – title line from the ESD keyword file.

15.5.1.2 RIPSAC Keyword File

Section 15.4 describes the individual keywords for RIPSAC. Table 15.3 provides an example RIPSAC keyword file for two analytes and four riparian locations using the TERSE option on the KDSOIL keyword.

Table 15.3 Example RIPSAC Keyword File

```
REPORT "RipSac_CA1_median.Rpt"
FILE ESD "/home/ANALYSIS4/CA1_median/ESD_CA1_median.key"
TITLE "2004 CA - RIPSAC keyword file"
USER "Paul W. Eslinger"
REALIZATION ALL
ANALYTE ID="H3"
```

```
ANALYTE ID="C14"
EXECUTE
KDSOIL TERSE ANALYTE="H3"    KDSOIL="KDH"
KDSOIL TERSE ANALYTE="C14"   KDSOIL="KDC"
! PRIMARY location is for groundwater on the shore - Hanford
! SECOND location is for the associated surface water - Hanford
! Riparian and Aquatic - Hanford Shore
LOCATION PRIMARY="RHP001" SECOND="QHP001" DF="DF5m"
LOCATION PRIMARY="RHP002" SECOND="QHP002" DF="DF5m"
LOCATION PRIMARY="RHP003" SECOND="QHP003" DF="DF5m"
LOCATION PRIMARY="RHP004" SECOND="QHP004" DF="DF5m"
END
```

15.5.1.3 DILUTE Stochastic Data

The file containing dilution factors for groundwater and river water interaction coefficients is used for every run of the code. This file is generated by the ECDA program from DILUTE keywords contained in the ESD keyword file. Section 2.4.1 defines the file format and provides an example file. The file name is supplied in the ESD keyword file by using the FILE keyword and the DILUTE modifier. Typically, the user of the RIPSAC code will not modify this file.

15.5.1.4 KDSOIL Stochastic Data

The file containing stochastic values for the soil-water partition coefficients is used for every run of the code. This file is generated by the ECDA program from KDSOIL keywords contained in the ESD keyword file. Section 2.4.2 defines the file format and provides an example file. The file name is supplied in the ESD keyword file by using the FILE keyword and the KDSOIL modifier. Typically, the user of the RIPSAC code will not modify this file.

15.5.1.5 Concentration Data Files

Concentration data for different analytes are contained in separate ECDA files. RIPSAC reads from, and writes to, a concentration data file for every analyte being simulated. If there are ten analytes, then ten concentration data files will be required, along with one record map file. Section 2.2 describes the format for each of these files. The ECDA data and map file names are defined in the ESD keyword file.

15.5.2 Output Files

RIPSAC writes a report file, a run-time signal file named “RIPSAC.Run”, and a run completion signal file named “RIPSAC.Done” as well as modifies ECDA concentration data files. The number of modified concentration data files depends on the options selected in the scenario being analyzed. The following sections describe the output files.

15.5.2.1 RIPSAC Report File

The RIPSAC report file contains run information and error messages, if any. The file contains program identification and an echo of the basic options selected for the code run. Table 15.4 provides excerpted records from an example RIPSAC report file.

Table 15.4 Excerpted Records from a RIPSAC Report File

```
              RRRRR    IIIIIII  PPPPP      SSS     AAAAA     CCC
              R    RR     I     P    PP  S    SS  A     A   C   CC
              R    RR     I     P    PP   S     S  A     A  C
              RRRRR       I     PPPPP      SS     AAAAAAA  C
              R    R      I     P        S   S    A     A  C
              R     R     I     P        SS   S   A     A   C   CC
              R     R  IIIIIII  P          SSS    A     A    CCC


                                 RipSac   2.00.A.1
                            Last Modified on 17 Jun 2003


                          Stochastic River-Shore Analysis
                     Systems Assessment Capability (SAC), Revision 0
                     ------------------------------------------------
                                 Developed By Battelle
                           Pacific Northwest National Laboratory
                                 Richland, Washington
                     ------------------------------------------------

          Current Run ID = 200407121935   User Name = Paul W. Eslinger
               System Date = 07-12-2004   System Time = 19:35:06


           The software used to generate this output is experimental
              and has not been formally tested or peer reviewed.


                                  Review Signatures

Input Prepared By: _____________________________       Date: _______________

Input Reviewed By: _____________________________       Date: _______________

======================== Echo of the Problem Definition ========================

Title: 2004 CA - RIPSAC keyword file
User:  Paul W. Eslinger
1 Realizations identified in the ESD keyword file
1 Realizations utilized in this run

A map of realization activations (true/false) is:
   1-  1  T

File Name for RIPSAC Input Keyword Data
File: RipSac_CA1_median.key

File Name for ESD Input Keyword Data
File: /home/ANALYSIS4/CA1_median/ESD_CA1_median.key

File Name for Dilution Data
File: /home/ANALYSIS4/CA1_median/ecda/DILUTE_CA1_median.Dat

File Name for KDSOIL Data
File: /home/ANALYSIS4/CA1_median/ecda/KDSOIL_CA1_median.dat

File Name for Concentration Index Map File
File: /home/ANALYSIS4/CA1_median/ecda/ECDA_CA1_median.map

File Name for Media Concentrations: Analyte ID="C14"
```

```
File: /home/ANALYSIS4/CA1_median/ecda/C14_CA1_median.dat

<data rows deleted>

Analye Information for 15 analytes.
    1 : C14    : Carbon-14
<data rows deleted>
   15 : U238   : Uranium-238
A total of 12 analytes have been requested.

Number of times is 272
Index    Year
     1 1945
     2 1950
<data rows deleted>
   271 12000
   272 12050

Number of locations is 4351
Index   Location ID
     1 UH0001
     2 UH0002
<data rows deleted>
  4350 QTV010
  4351 QHRWI1

Soil-Water KD and Dilution Factor Mapping
  Location      Analyte      KDSOIL ID String      DILUTE ID String
  ------------  -----------  --------------------  --------------------
  2864: RFP001    1: C14     KDC                   DF5m
  2864: RFP001    2: Cs137   KDCs                  DF5m
<data rows deleted>
  4057: R21I08   14: U235    KDU                   DF5m
  4057: R21I08   15: U238    KDU                   DF5m

======================== End of the Problem Definition ========================

Message originating in routine PROCESS_IMPACTS
Message: Entering subroutine for analyte "C14"
         On 07/12/2004 at 19:35:16.973

<data rows deleted>

Message originating in routine PROCESS_IMPACTS
Message: Entering subroutine for analyte "U238"
         On 07/12/2004 at 19:55:06.954

Message originating in routine RipSac
Message: Normal Termination
         Run Completed on 07/12/2004 at 19:56:56.033
```

15.5.2.2 "RIPSAC.Run" File

A file named "RipSac.Run" is always written just as RIPSAC starts execution. Presence of the file signals the ESP that a RIPSAC run is in progress. This file does not contain any data. The file is closed and deleted when the RIPSAC run terminates.

15.5.2.3 "RIPSAC.Done" File

A file named "RipSac.Done" is always written just as RIPSAC finishes a run. This file contains a single line of text data. If the run was successful, the line reads as follows:

```
"0 Normal termination"
```

If the run was not successful, the line will have the following form:

```
"1 Error termination"
```

The first entry on the line for runs that terminate with errors will be a nonzero error code that can be used to help trace the source of the error. Typically, the ending lines in the report file (see Table 15.4) will contain more detailed information about the type of error encountered.

15.5.2.4 Concentration Data Files

Concentration data for different analytes are contained in separate ECDA files. RIPSAC reads from, and writes to, a concentration data file for every analyte being simulated. If there are ten analytes, then ten concentration data files will be required, along with one record map file. Sections 0 describes the format for each of these files. The ECDA data and map file names are defined in the ESD keyword file using the FILE keyword.

16.0 SOIL – Soil Accumulation Module

16.1 Code Purpose

The soil accumulation module (SOIL) calculates the concentrations of analytes in near-surface soil. The soil model algorithms apply to dry land locations as well as locations that use irrigation. SOIL reads air deposition rates and analyte concentrations in groundwater and surface water from ECDA files (see Section 2.2), calculates the concentrations in soil, and writes the calculated concentrations back into the same data files.

16.2 Algorithms and Assumptions

The soil concentration model includes the effects of air deposition, precipitation and evaporation, irrigation with contaminated water, leaching from soil due to precipitation and irrigation, and radioactive decay. These processes are modeled in the upper soil layer, which is nominally assumed to be 15 cm in depth. The general equation for the rate of analyte accrual in the upper soil layer while irrigation is occurring is the following:

$$M'(t) = \frac{I(t) \times 0.01}{F_{yi}} \times C_{water}(t) + A_{dep}(t) - M(t) \times \left(\lambda_L(t) + \lambda_{Rad}\right)$$

where

M'(t)	=	rate of change in the amount of analyte in the upper soil layer [Ci/(m^2-yr) or kg/(m^2-yr)]
M(t)	=	amount of analyte in the upper soil layer (Ci/m^2 or kg/m^2)
I(t)	=	applied irrigation (cm), set to zero outside the growing season
F_{yi}	=	fraction of the year that irrigation is applied (yr)
0.01	=	conversion factor (m/cm)
$C_{water}(t)$	=	concentration of analyte in the irrigation water (Ci/m^3 or kg/m^3)
$A_{dep}(t)$	=	air deposition of the analyte [Ci/(m^2-yr)or kg/(m^2-yr)]
M(t)	=	amount of analyte in the upper soil layer (Ci/m^2 or kg/m^2)
$\lambda_L(t)$	=	leach rate constant due to water moving through the upper soil layer (yr^{-1})
λ_{Rad}	=	radioactive decay constant (yr^{-1}) (set to zero for nonradioactive analytes)

The general equation for the rate of analyte accrual in the upper soil layer while irrigation is not occurring is the following:

$$M'(t) = A_{dep}(t) - M(t) \times \left(\lambda_L(t) + \lambda_{Rad}\right)$$

Baes and Sharp (1981) provide a method for estimating the annual leach rate of contaminants out of the upper layer of irrigated soils. The leach rate is represented by:

$$\lambda_L(t) = \frac{P - E + I(t)\frac{F_{yi}}{F_{il}}}{d_s \theta (1 + \frac{\rho}{\theta} K_d)}$$

where

$\lambda_L(t)$ = leach rate (yr^{-1})
P - E = annual net infiltration from natural sources, precipitation less evapotranspiration (cm/yr)
I(t) = applied irrigation (cm), set to zero outside the growing season
F_{yi} = fraction of the year that irrigation is applied (yr)
F_{il} = fraction of the irrigation that is available for leaching below the root zone, nominally 0.2
d_s = depth of surface soil (cm), nominally 15 cm
θ = surface soil volumetric water content (mL/cm^3), nominally 0.5 mL/cm^3
ρ = surface soil density (g/cm^3), nominally 1.5 g/cm^3
K_d = soil distribution coefficient (mL/g)

The mass solution in terms of the original soil formulation while irrigation is being applied is given by:

$$M(t) = \frac{\frac{I(t)\times 0.01}{F_{yi}}\times C_{water}(t) + A_{dep}(t)}{(\lambda_L(t)+\lambda_{Rad})} + e^{-(\lambda_L(t)+\lambda_{Rad})(t-t_i)}\left[M(t_{(i-1)}) - \frac{\frac{I(t)\times 0.01}{F_{yi}}\times C_{water}(t) + A_{dep}(t)}{(\lambda_L(t)+\lambda_{Rad})}\right]$$

The mass solution in terms of the original soil formulation outside the irrigation period is given by:

$$M(t) = \frac{A_{dep}(t)}{(\lambda_L(t)+\lambda_{Rad})} + e^{-(\lambda_L(t)+\lambda_{Rad})(t-t_i)}\left[M(t_{(i-1)}) - \frac{A_{dep}(t)}{(\lambda_L(t)+\lambda_{Rad})}\right]$$

The soil concentration is then computed from:

$$C_{soil}(t) = M(t) / S_{mass}$$

where

$C_{soil}(t)$ = soil concentration (Ci/kg or kg-analyte/kg-soil)
M(t) = amount of analyte in the upper soil layer (Ci/m^2 or kg/m^2)
S_{mass} = mass of soil (kg/m^2) in the upper soil layer, a nominal value is 225 kg/m^2

The soil concentration varies as a function of time due to soil buildup and the seasonal effects of irrigation. However, the solution desired is an annual soil concentration. This concentration is computed and reported as the value at the end of the irrigation season (nominally 120 to 150 days in length) for locations that are irrigated and irrigation has been initiated. This concentration is computed and reported as the value at the end of the calendar year for locations that are not irrigated and locations where irrigation will be initiated at a future date.

16.3 Code Execution Environment

The SOIL is invoked in a standalone mode.

16.3.1 Location in the Processing Sequence

The general processing sequence for TIIA codes is outlined in Figure 1.1. As noted in the figure, the optional SOIL model is executed before the ECEM code. Only one run of SOIL is required to process all realizations for all analytes. SOIL also has the capability to run on a subset of data for any combination of realizations and analytes.

16.3.2 How the Code Is Invoked

SOIL may be used in either Microsoft Windows or Linux environments, provided that the code has been compiled by a Fortran 95 compiler appropriate for the environment. In the Microsoft Windows (Release XP) environment, SOIL is executed by either of the following DOS commands:

```
SOIL-1 "Keyword File"
SOIL-1
```

In the Linux environment, SOIL is executed through either of the following Bourne Shell or C Shell commands:

```
soil-1.exe "keyword file"
soil-1.exe
```

In the first example for both operating systems, SOIL is invoked and assumes the file identified by "keyword file" (file names are case sensitive under Linux) contains the controlling keywords for SOIL. In the second example, the keyword file name is missing from the command line; thus SOIL queries the user for the name of the file. In either case, if the input keyword file is not found, SOIL writes an error message and terminates execution.

16.4 Data Files

The SOIL code reads four or more input files and writes a number of output files. The number of input and output files depends on the number of contaminants being analyzed. The following sections describe these files.

16.4.1 Input Files

The input files for SOIL are two keyword files, a KDSOIL data file, an INFILT data file, and a suite of ECDA files. The SOIL keyword file controls the case SOIL will execute, and it points to the ESD keyword file. The suite of concentration data files are all identified in the ESD keyword file—the user of the SOIL only needs to identify the ESD keyword file.

16.4.1.1 ESD Keyword File

The SOIL code reads a number of keywords from the ESD keyword file. A summary of these keywords is provided in Table 16.1. Typically, the user of the SOIL code will not modify the ESD keyword file. These keywords are described in detail in Section 2.1.

Table 16.1 ESD Keywords Used by SOIL

Keyword	Description
ANALYTE	The ANALYTE keyword defines the analytes to be used in a run of SOIL.
END	The END keyword signifies the end of all keyword data in the ESD keyword file.
FILE	The FILE keyword is used to define the names of the ECDA-related files.
IRRIGATE	The IRRIGATE keyword defines the year to start irrigating and the irrigation rate.
LOCATION	The LOCATION keyword defines the impact locations.
PERIOD	The period keyword defines the time period for the entire analysis.
REALIZATION	The REALIZATION keyword defines the number of realizations in the entire analysis.
TIMES	The TIMES keyword defines the times (set of years) for which impact analyses can be calculated.
TITLE	The TITLE keyword defines a single-line problem title.

16.4.1.2 SOIL Keyword File

Section 16.5 describes the individual keywords for SOIL. Table 16.2 provides an example SOIL keyword file for five analytes. This example file uses four locations for impacts calculations. A SOIL keyword file for a production run incorporating hundreds of locations for several analytes would be several thousand lines long.

Table 16.2 Example SOIL Keyword File

```
REPORT "Soil_CA1_median.rpt"
FILE ESD "/home/ANALYSIS4/CA1_median/ESD_CA1_median.key"
USER "Paul W. Eslinger"
TITLE "2004 CA - SOIL keyword file"
REALIZAT ALL
EXECUTE
!
ANALYTE ID="H3"
ANALYTE ID="C14"
ANALYTE ID="Cl36"
ANALYTE ID="Sr90"
ANALYTE ID="Tc99"
!
KDSOIL TERSE ANALYTE="H3"    KDSOIL="KDH"
KDSOIL TERSE ANALYTE="C14"   KDSOIL="KDC"
KDSOIL TERSE ANALYTE="Cl36"  KDSOIL="KDCl"
KDSOIL TERSE ANALYTE="Sr90"  KDSOIL="KDSr"
KDSOIL TERSE ANALYTE="Tc99"  KDSOIL="KDTc"
!
LOCATION ID="UH0001" INFILT="Wa-s"
LOCATION ID="UH0002" INFILT="Ba-s"
LOCATION ID="UH0003" INFILT="Ba-s"
LOCATION ID="UH0004" INFILT="Ba-s"
!
END
```

16.4.1.3 KDSOIL Stochastic Data

The file containing stochastic values for the soil-water partition coefficients is used for every run of the code. This file is generated by the ECDA program from KDSOIL keywords contained in the ESD keyword file. Section 2.4.2 defines the file format and provides an example file. The file name is supplied in the ESD keyword file by using the FILE keyword and the KDSOIL modifier. Typically, the user of the SOIL code will not modify this file.

16.4.1.4 INFILT Stochastic Data

The file containing stochastic values for the water infiltration data must be supplied for every run of the code. This file is generated by the ESP program from INFILTRATION keywords contained in the ESD keyword file. Section 2.4.3 defines the file format and provides an example file. The file name is supplied in the ESD keyword file by using the FILE keyword and the INFILT modifier. Typically, the user of the SOIL code will not modify this file.

16.4.1.5 ECDA Files

Concentration data for different analytes are contained in separate ECDA files. SOIL reads from, and writes to, a concentration data file for every analyte being simulated. If there are ten analytes, then ten concentration data files will be required, along with one record map file. Section 0 describes the format for each of these files. The ECDA data and map file names are defined in the ESD keyword file.

16.4.2 Output Files

SOIL writes a report file, a run-time signal file named “soil.run”, and a run completion signal file named “soil.done” as well as modifying ECDA files. The number of modified concentration data files depends on the options selected in the scenario being analyzed. The following sections describe the output files.

16.4.2.1 SOIL Report File

The SOIL report file contains run information and error messages, if any. The file contains program identification and an echo of the basic options selected for the code run. Table 16.3 provides excerpts from a SOIL report file. The original file was 6100 lines long.

Table 16.3 Excerpts from a SOIL Report File

```
   SSS     OOOOO   IIIIIII  L
  S    SS  O     O     I     L
   S    S  O     O     I     L
    SS     O     O     I     L
  S   S    O     O     I     L
  SS   S   O     O     I     L
    SSS     OOOOO   IIIIIII  LLLLLLL

            Soil 1.00.D.1
     Last Modified on 29 Dec 2003


Stochastic Soil Concentration Analysis
```

```
               Systems Assessment Capability (SAC), Revision 1
               -----------------------------------------------
                           Developed By Battelle
                     Pacific Northwest National Laboratory
                           Richland, Washington
               -----------------------------------------------

          Current Run ID = 20040824101440   User Name = Paul W. Eslinger
               System Date = 08-24-2004   System Time = 10:14:40.653

           The software used to generate this output is experimental
              and has not been formally tested or peer reviewed.

                              Review Signatures

Input Prepared By: _____________________________       Date: _________________

Input Reviewed By: _____________________________       Date: _________________


======================== Echo of the Problem Definition ========================

Title: 2004 CA - SOIL keyword file - 10,000-year median inputs case
User:  Paul W. Eslinger
   1 Realizations identified in the ESD keyword file
   1 Realizations utilized in this run

A map of realization activations (true/false) is:
   1-  1  T

Year definitionsd
     1944 : Start year for the simulation
     12050 : Stop  year for the simulation
     2070 : Site closure year for the simulation
     2004 : Start year for irrigation

File Name for SOIL Input Keyword Data
File: Soil_CA1_median.key

File Name for ESD Input Keyword Data
File: /home/ANALYSIS4/CA1_median/ESD_CA1_median.key

File Name for Infiltration Data
File: /home/ANALYSIS4/CA1_median/ecda/infilt.dat

File Name for KDSOIL Data
File: /home/ANALYSIS4/CA1_median/ecda/KDSOIL_CA1_median.dat

File Name for Concentration Map File
File: /home/ANALYSIS4/CA1_median/ecda/ECDA_CA1_median.map

File Name for Media Concentrations: Analyte ID="H3"
File: /home/ANALYSIS4/CA1_median/ecda/H3_CA1_median.dat

Analye Information for 15 analytes.
     1 : C14    : ===> Not used
     2 : Cs137  : ===> Not used
     3 : Cl36   : ===> Not used
     4 : I129   : ===> Not used
     5 : Np237  : ===> Not used
     6 : Pa231  : ===> Not used
     7 : Ra226  : ===> Not used
     8 : Se79   : ===> Not used
```

```
     9 : Sr90   : ===> Not used
    10 : Tc99   : ===> Not used
    11 : H3     : Tritium
    12 : Eu152  : ===> Not used
    13 : U233   : ===> Not used
    14 : U235   : ===> Not used
    15 : U238   : ===> Not used
A total of 1 analytes have been requested.

Number of times is 274
  Index   Year
      1   1945
      2   1950
      3   1955
      4   1960
      5   1965
                                <deleted lines>
Total number of locations is 4351
Activated locations are shown below
  Index      ID      SW Irrig   Name
  -----   --------   --------   --------------------------------------------------
      1 : "UH0001" : "QHP025" : "UnsuitableForAgricul"
      2 : "UH0002" : "QHP025" : "UnsuitableForAgricul"
      3 : "UH0003" : "QHP025" : "UnsuitableForAgricul"
      4 : "UH0004" : "QHP025" : "AgExclusionBuffer"
      5 : "UH0005" : "QHP025" : "AgExclusionBuffer"
      6 : "UH0006" : "QHP025" : "AgExclusionBuffer"
      7 : "UH0007" : "QHP025" : "AgExclusionBuffer"
      8 : "UH0008" : "QHP025" : "Upland"
      9 : "UH0009" : "QHP025" : "AgExclusionBuffer"
                                <deleted lines>
Soil-Water KD and Dilution Factor Mapping
  Location         Analyte       KDSOIL ID String        INFILT ID String
  --------------  ------------  ----------------------  ----------------------
      1: "UH0001"  11: "H3    "  "KDH                 "  "Wa-s                "
      2: "UH0002"  11: "H3    "  "KDH                 "  "Ba-s                "
      3: "UH0003"  11: "H3    "  "KDH                 "  "Ba-s                "
                                <deleted lines>
======================== End of the Problem Definition ========================

Header information from the map file
   ECDA_PTITLE = 2004 Composite Analysis 10,000-year (Median Inputs) Assessment
   ECDA_PRGNAM = ECDA
   ECDA_PRGVER = 2.00.A.4
   ECDA_PRGDAT = 16 Oct 2003
   ECDA_USRNAM = Eslinger-DWE-WEN
   ECDA_CRUNID = 20040802132252
   ECDA_BLOCK  = 23155
   ECDA_RECLEN = 18
   ECDA_NREAL  = 1
 Date: 08-24-2004  Time: 10:14:55  Processing impacts for H3

Message originating in routine PROCESS_SOIL
Message: Entering subroutine for analyte "H3"
         On 08/24/2004 at 10:14:55.115

 FN_DONE = "Soil.Done"

Message originating in routine Soil
Message: Normal Termination
    Run Completed on 08/24/2004 at 10:24:38.150
```

16.4.2.2 "soil.run" File

A file named "soil.run" is written just as SOIL starts execution. Presence of the file signals the ESP that a SOIL run is in progress. This file does not contain any data. The file is closed and deleted when the SOIL run terminates.

16.4.2.3 "soil.done" File

A file named "soil.done" is always written just as SOIL finishes a run. This file contains a single line of text data. If the run was successful, the line reads as follows:

```
"0 Normal termination"
```

If the run was not successful, the line will have the following form:

```
"1 Error termination"
```

The first entry on the line for runs that terminate with errors will be a nonzero error code that can be used to help trace the source of the error. Typically, the ending lines in the report file (see Table 16.3) will contain more detailed information about the type of error encountered.

16.4.2.4 Concentration Data Files

Concentration data for different analytes are contained in separate ECDA files. SOIL reads from, and writes to, a concentration data file for every analyte being simulated. If there are 10 analytes, then 10 concentration data files will be required, along with one record map file. Section 0 describes the format for each of these files. The ECDA data and map file names are defined in the ESD keyword file.

16.5 Keyword Descriptions for the SOIL Code

In general, the control keywords specific to the SOIL code can be entered in any order. A summary of the keywords is provided in Table 16.4. The only restriction on keyword order is that the END keyword must be the last keyword in the file.

Table 16.4 Summary of Keywords Used by SOIL

Keyword	Description
ANALYTE	The ANALYTE keyword defines the analytes to be used in a run of SOIL.
DEBUG	The DEBUG keyword is used to activate dumping of intermediate calculations to the report file.
END	The END keyword signifies the end of all keyword data.
EXECUTE	The EXECUTE keyword controls optional execution after the control inputs are checked for consistency.
FILE	The FILE keyword is used to enter the name of the ESD keyword file.
KDSOIL	The KDSOIL keyword is used to assign soil-water partition coefficients to locations for use in the soil concentration calculations.
LOCATION	The LOCATION keyword is used to assign data to locations for use in the soil concentration calculations.
REALIZATION	The REALIZATION keyword is used to define the realizations to be processed in the SOIL code.

Keyword	Description
REPORT	The REPORT keyword is used to define the name of the output report (log) file.
SOIL	The SOIL keyword is an optional keyword used to define the depth of the surface soil layer and the density of the soil.
TITLE	The TITLE keyword is used to define a single-line problem title.
USER	The USER keyword is used to identify the user of the program.

16.5.1 ANALYTE Keyword for SOIL

The ANALYTE keyword is used to define the analytes to be used in the simulation. The following is this keyword's syntax:

```
ANALYTE ["quote 1"] {"quote 2"} ... {"quote n"}
```

Analytes are requested by entering their ID as a quote string, which must be enclosed in double quotation marks. The analytes requested must be defined in the ESD keyword file. A separate ANALYTE keyword may be entered for every analyte, or multiple analytes can be defined on the same keyword. The same analyte ID string must not be entered more than once. Example entries defining for analytes are the following:

```
ANALYTE "Cs137"
ANALYTE "Np237"
```

The same definition can be obtained by entering the following single keyword entry:

```
ANALYTE "Cs137" "Np237"
```

16.5.2 COMPUTE keyword for SOIL

The COMPUTE keyword defines the solutions to be computed in a run of the code. The following is this keyword's syntax:

```
COMPUTE {SODR} {SOGW} {SOSW}
```

The modifiers associated with the COMPUTE keyword are defined in Table 16.5.

Table 16.5 Modifiers for the COMPUTE Keyword in SOIL

Modifier	Description
SODR	The SODR modifier indicates that dry land soil (no irrigation) concentrations will be computed for all locations identified on the LOCATION keyword that had the SODR media activated.
SOGW	The SOGW modifier indicates that groundwater irrigated soil concentrations will be computed for all locations identified on the LOCATION keyword that had the SOGW media activated.
SOSW	The SOSW modifier indicates that surface water irrigated soil concentrations will be computed for all locations identified on the LOCATION keyword that had the SOSW media activated.

The following COMPUTE keyword will cause all three soil concentrations to be computed at every location where they are requested.

```
COMPUTE SODR SOGW SOSW
```

The following COMPUTE keyword will process only dry land soil at every location where it is requested.

```
COMPUTE SODR
```

16.5.3 DEBUG Keyword for SOIL

The DEBUG keyword is used to activate dumping of intermediate calculations to the report file. It should be used only on small problem definitions with only one or two realizations, otherwise the volume of output can easily exceed 2 gigabytes. The following is this keyword's syntax:

```
DEBUG {LOOP} {CONCENTR {BQ}} {COMPUTE}
```

The modifiers associated with the DEBUG keyword are defined in Table 16.6.

Table 16.6 Modifiers for the DEBUG Keyword in SOIL

Modifier	Description
LOOP	The LOOP modifier initiates reporting to the screen that shows program looping and control progress.
CONCENTR	The CONCENTR modifier initiates reporting all media concentrations to the report file. If the additional modifier BQ is entered, the computed soil concentrations written to the report file have activity units of Bq rather than Ci.
COMPUTE	The COMPUTE modifier initiates writing detailed values from the leaching and concentration calculations to the report file.

16.5.4 END Keyword for SOIL

The END keyword signifies the end of all keyword data. It should be the last keyword in the keyword file. All data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

16.5.5 EXECUTE Keyword for SOIL

The EXECUTE keyword (if present) causes a full analysis to be attempted. If the keyword is not present, then the analysis will terminate after reading the input data and performing consistency checks on the data. Running the code without the EXECUTE record is normally performed only to test the input data set. Once the data have been checked, the EXECUTE record should be present. The EXECUTE keyword must be present when SOIL is executed under the control of the ESP or the analysis will not proceed correctly. The following is this keyword's syntax:

```
EXECUTE
```

16.5.6 FILE Keyword for SOIL

The FILE keyword is used to enter the name of the ESD keyword file that defines the assessment. The names of the files providing concentration data are contained in the ESD keyword file rather than in the SOIL keyword file. The following is this keyword's syntax:

```
FILE [ESD="quote1"]
```

The file name must be entered in a quote string, which must be enclosed in double quotation marks. Path names up to 200 characters long are supported. An example entry is the following:

```
FILE ESD "G:\SOIL\Tests\Test_12.Key"
```

16.5.7 KDSOIL Keyword for SOIL

The KDSOIL keyword is used to assign analyte-specific soil-water partition coefficients to locations for use in the soil concentration calculations. The actual numerical values are extracted from a library of values defined in the ESD keyword file (see Section 5.3.8). The KDSOIL keywords in SOIL are assigned as a function of location and analyte. The following is this keyword's syntax:

```
KDSOIL [ANALYTE="quote1"] [KDSOIL="quote2"]
   [LOCATION="quote3" {"quote4"} ... {"quote5"} | TERSE]
```

Multiple KDSOIL keyword entries may be required if there is more than one analyte and more than one soil concentration location. Subsequent KDSOIL entries build upon the definition of previous entries. A KDSOIL keyword entry may be used for every combination of analyte and location where soil concentrations are to be computed. Alternatively, multiple locations can be defined on a single keyword. The modifiers for the KDSOIL keyword can be entered in any order. The modifiers used with the KDSOIL keyword are defined in Table 16.7.

Table 16.7 Modifiers for the KDSOIL Keyword in SOIL

Modifier	Description
ANALYTE	The quote string associated with the ANALYTE modifier must contain the ID of an analyte identified in the ESD keyword file.
KDSOIL	The quote string associated with the KDSOIL modifier must contain the ID string of a KDSOIL variable identified in the ESD keyword file.
LOCATION	One or more quote strings are associated with the LOCATION modifier. Each quote string must contain the ID of a location identified in the ESD keyword file. The LOCATION modifier is not used if the TERSE modifier is used.
TERSE	This modifier can be used instead of the LOCATION modifier. The effect is to assign the same KDSOIL definition for this analyte to every location where a soil concentration solution is to be computed.

Example keyword entries include the following:

```
KDSOIL ANALYTE="U234" LOCATION="HL0012" KDSOIL="KD#042"
KDSOIL ANALYTE="Cr" LOCATION="HL0012" KDSOIL="KD#023"
KDSOIL ANALYTE="Cr" LOCATION="HL0014" KDSOIL="KD#023"
KDSOIL ANALYTE="Cr" LOCATION="HL0015" KDSOIL="KD#023"
KDSOIL ANALYTE="Cr" LOCATION="HL0021" KDSOIL="KD#023"
```

The information in the last four keywords above could be entered by using the single following keyword:

```
KDSOIL ANALYTE="Cr" LOCATION="HL0021" "HL0015" "HL0014" "HL0012"
   KDSOIL="KD#023"
```

The following examples assign the same K_d to every location for each the analyte:

```
KDSOIL TERSE ANALYTE="H3"    KDSOIL="KDH"
KDSOIL TERSE ANALYTE="C14"   KDSOIL="KDC"
KDSOIL TERSE ANALYTE="Cl36"  KDSOIL="KDCl"
KDSOIL TERSE ANALYTE="Se79"  KDSOIL="KDSe"
KDSOIL TERSE ANALYTE="Sr90"  KDSOIL="KDSr"
```

16.5.8 LOCATION Keyword for SOIL

The LOCATION keyword is used to identify groundwater and surface water concentrations and infiltration values in order to complete soil concentration calculations. The infiltration rates are extracted from a library of values that are defined in the ESD keyword file file (see Section 5.3.8). The following is this keyword's syntax:

```
LOCATION [ID="quote 1"] [INFILT="quote 2"]
```

Multiple LOCATION keyword entries may be required. There must be a separate LOCATION keyword entry for every location where soil concentrations are to be computed. If the location is not identified with a LOCATION keyword entry, then no calculations will be carried out at that location. The modifiers for this keyword can be entered in any order. The modifiers for the LOCATION keyword are described in Table 16.8.

Table 16.8 Modifiers for the LOCATION Keyword in SOIL

Modifier	Description
ID	The quote string associated with the ID modifier must contain the ID string of a location identified in the ESD keyword file. The presence of the LOCATION keyword with this ID signifies that one or more soil concentration calculations will occur at this location.
INFILT	The quote string associated with the INFILT modifier must contain the ID string of an infiltration variable identified in the infiltration data library (see Section 2.4.3). This variable defines the infiltration.

The following example illustrates the use of the LOCATION keyword:

```
LOCATION ID="UH0001" INFILT="Wa-s"
```

16.5.9 REALIZATION Keyword for SOIL

The REALIZATION keyword is used to define the realizations to be processed in the SOIL code. The following is this keyword's syntax:

```
REALIZATION [ALL | LIST N1 {N2 ... Nn} | RANGE N1 N2 ]
```

The ESD keyword file defines the total number of realizations that will be processed in the assessment. The SOIL code can process all realizations at one time, or it can process a subset of the realizations. Table 16.9 describes the modifiers used on the REALIZATION keyword. Only one of the modifiers is allowed on a single entry of the REALIZATION keyword. Upon entry to the code, none of the

realizations are selected for processing. Multiple REALIZATION keyword entries may be used with the definition of active realizations building with each additional keyword entry.

Table 16.9 Modifiers for the REALIZATION Keyword in SOIL

Modifier	Description
ALL	The presence of this modifier will activate processing of all realizations defined in the ESD keyword file.
LIST	The LIST modifier must be accompanied by one or more realization indices. All realization indices in the list will be processed. The realization indices do not have to be entered in any particular order.
RANGE	The RANGE modifier must be accompanied by two realization indices. All realizations from the first to the second indices, inclusive of the end points, will be processed. The second index must be equal to, or greater than, the first index.

The following REALIZATION keyword will invoke processing for all realizations defined in the ESD keyword file.

```
REALIZATION ALL
```

The following set of two REALIZATION keywords assume that at least 100 realizations are defined in the ESD keyword file. These keywords define processing in SOIL for realization numbers 2, 4, 6, 12, 13, 14, 15, 99, and 100.

```
REALIZATION LIST 2 4 6 100 99
REALIZATION RANGE 12 15
```

16.5.10 REPORT Keyword for SOIL

The REPORT keyword is used to define the name of the output report (log) file. It must be the first keyword entered in the keyword file. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The name of the report file is entered in a quote string, which must be enclosed in double quotation marks. File names up to 200 characters long are supported, and path names can be included. An example REPORT keyword record is the following:

```
REPORT "/SAC/SystemCodes/Cultural/Test1.rpt"
```

16.5.11 SOIL Keyword for SOIL

The SOIL keyword is an optional keyword used to define the depth of the surface soil layer and the density of the soil. If this keyword is not entered, the soil depth will be 15 cm and the soil density will be 1.5 g/cm^3. The following is this keyword's syntax:

```
SOIL [DEPTH=N1] [DENSITY=N2]
```

The numerical value associated with the DEPTH modifier gives the soil depth (centimeters) for the upper soil layer. If the DEPTH modifier is missing, a value of 15 cm is used. The numerical value associated with the DENSITY modifier gives the soil density (g/cm^3) for the upper soil layer. If the DENSITY modifier is missing, a value of 1.5 g/cm^3 is used. The values for DEPTH and DENSITY are the same for all locations.

16.5.12 TITLE Keyword for SOIL

The TITLE keyword is used to define a single-line problem title. The problem title will be written to output files. If the title is not supplied, the program will error terminate. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 200 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the cultural impacts code."
```

16.5.13 USER Keyword for SOIL

The USER keyword is used to identify the user of the program. The user name will be written to output files. If the user name is not supplied, the program will error terminate. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

17.0 STOCHASTIC – Stochastic Values Generation

17.1 Overview

This utility is a standalone code that generates values defined by statistical distributions. Output options include individual generated values and summary statistics. It can be used to check the effects of stochastic variables before they are included in a simulation.

17.1.1 Location in the Processing Sequence

The STOCHASTIC code is executed independent of other codes in the TIIA processing sequence.

17.1.2 How the Code Is Invoked

STOCHASTIC can run under either the Windows or the Linux operating systems. Under the Windows operating system (Releases XP or 7), STOCHASTIC executes in a DOS box. A run of STOCHASTIC is initiated by entering the following command line:

```
STOCHASTIC "Keyfilename"
```

Under the Linux operating system STOCHASTIC is executed through any of the following Bourne Shell or C Shell commands:

```
stochastic.exe "Keyfilename"
```

For these commands, “STOCHASTIC.EXE” or “stochastic.exe” is the name of the executable program, and “Keyfilename” is the name of an existing control keyword file. Both the name of the executable program and the keyword file may contain path information. If STOCHASTIC is invoked without entering the name of the keyword file, then the code will prompt the user for the file name. If STOCHASTIC cannot find or open the keyword file, then the code will terminate execution after writing an error message to the standard output device.

17.1.3 Memory Requirements

The STOCHASTIC code uses dynamic memory allocation, so the memory requirements depend on the problem being analyzed. A reasonably large example run—where the STOCHASTIC code used six stochastic variables and one million realizations—required 16 MB of memory (on a Windows XP machine).

17.2 File Definitions

The STOCHASTIC code reads a single input file and writes up to three output files.

17.2.1 Input Files

The single input file for the STOCHASTIC code is a control keyword file. An example keyword file is provided in Table 17.1. Detailed descriptions for the individual keywords are provided in Section 17.3.

Table 17.1 Example Keyword File for STOCHASTIC

```
REPORT "Step1.Rpt"
USER "John Q. Doe"
TITLE "Generate Median Values for Vadose Zone Stochastic Data"
SEED 12456564.0
REALIZAT 1000001
SINGLEKEY PERCENT=0.50 FILE="Step1.Val"
!
STOCHASTIC "30" "X" 1   1.000
STOCHASTIC "31" "X" 10  20
     0.00000E+00  1.000000E+00
     5.00000E-01  1.000000E+00
     5.54012E-01  1.044167E+00
     6.04938E-01  1.088333E+00
     6.52778E-01  1.132500E+00
     6.97531E-01  1.176667E+00
     7.39198E-01  1.220833E+00
     7.77778E-01  1.265000E+00
     8.13272E-01  1.309167E+00
     8.45679E-01  1.353333E+00
     8.75000E-01  1.397500E+00
     9.01235E-01  1.441667E+00
     9.24383E-01  1.485833E+00
     9.44444E-01  1.530000E+00
     9.61420E-01  1.574167E+00
     9.75309E-01  1.618333E+00
     9.86111E-01  1.662500E+00
     9.93827E-01  1.706667E+00
     9.98457E-01  1.750833E+00
     1.00000E+00  1.795000E+00
STOCHASTIC "52" "X" 6   1.000  2.590  16.900
!
END
```

17.2.2 Output Files

The STOCHASTIC code writes from one to three output files:

- **Report File.** The report file is an ASCII file containing information about the run of the STOCHASTIC program. It is written for every run of the code. All error messages (except for those indicating the report file could not be opened) are written to this file.
- **SINGLEKEY File.** A revised STOCHASTIC keyword can optionally be written to an output file for every input STOCHASTIC keyword. Output to this file is controlled by the SINGLEKEY keyword. The file contains the new keywords in text format. A typical use of this keyword is to convert the input STOCHASTIC keywords, each defined for a statistical distribution, into new keywords defining a constant set to the median or the mean of the input distribution.
- **Values File.** The generated stochastic values can optionally be written to an output file. Output to this file is controlled by the DEBUG keyword. The file contains the generated values in text format.

17.3 Keyword Definitions for the STOCHASTIC Code

In general, the keywords for the STOCHASTIC code can be entered in any order. The only restriction is that the END keyword must be the last keyword in the file.

17.3.1 DEBUG Keyword for STOCHASTIC

The DEBUG keyword is used to activate dumping of intermediate calculations to the report file, to write generated values to a file, and to write plot data to a file. It should be used sparingly because large output files can result. The following is this keyword's syntax:

```
DEBUG {DEFINITION}{STATISTICS}{STOCHASTIC="Quote 1" {COLUMN}}
   {PLOT="Quote 2" }
```

Multiple DEBUG keywords can be entered with combinations of modifiers, or a single card can be entered containing all of the modifiers. The modifiers can be entered in any order. Table 17.2 describes the modifiers associated with the DEBUG keyword.

Table 17.2 Modifiers Associated with the DEBUG Keyword in STOCHASTIC

Modifier	Description
DEFINITION	The presence of the DEFINITION modifier on the DEBUG keyword will cause the definition of all stochastic variables to be written to the report file.
STATISTICS	The presence of the STATISTICS modifier on the DEBUG keyword will cause summary statistics for all generated variables to be computed and written to the report file.
STOCHASTIC	The presence of the STOCHASTIC modifier on the DEBUG keyword will cause all generated values to be written to the file identified in the associated quote string. If the modifier COLUMN is also present, the values will be written in a single column, otherwise, the values are written in comma-separated format with all values for a single variable on one line.
PLOT	The presence of the PLOT modifier on the DEBUG keyword will cause the empirical cumulative distribution function to be written to the file identified in the associated quote string.

The following sequence of keyword records illustrate the use of the DEBUG keyword:

```
DEBUG STOCHAST "Test_Median.Csv" COLUMN
DEBUG PLOT "Test_Plot_Median.csv"
DEBUG DEFINITI
DEBUG STATISTI
```

17.3.2 END Keyword for STOCHASTIC

The END keyword signifies the end of all keyword data. All data in the keyword file after the END keyword will be ignored. The following is this keyword's syntax:

```
END
```

17.3.3 REALIZAT Keyword for STOCHASTIC

The REALIZAT (or REALIZATION) keyword defines the number of realizations to generate. The following is this keyword's syntax:

```
REALIZATION value1
```

The integer value1 has a minimum value of 1. No specific maximum number of realizations is enforced, but large values may result in large output files. Values up to 5,000,000 have been verified using a small number of variables.

The following keyword record sets the number of realizations to 1000:

```
REALIZAT 1000
```

17.3.4 REPORT Keyword for STOCHASTIC

The REPORT keyword is used to define the name of the output report (log) file. It must be the first keyword entered in the keyword file. The following is this keyword's syntax:

```
REPORT ["quote"]
```

The name of the report file is entered in a quote string, which must be enclosed in double quotation marks. File names up to 200 characters long are supported, and optional path names can be included. The following is an example REPORT keyword record:

```
REPORT "G:\SAC\Sys\EC\Test.rpt"
```

17.3.5 SEED Keyword for STOCHASTIC

The SEED keyword sets the value for the seed for the random number generator. The following is this keyword's syntax:

```
SEED Value1
```

The value for Value1 must be an integer or real number in the range 1 to 999999. The following is an example keyword record:

```
SEED 344443
```

17.3.6 SINGLEKEY Keyword for STOCHASTIC

The SINGLEKEY keyword is used to output an optional file of data for a user-defined sample percentile for all stochastic variables. This option supports generation of median-value data sets for the inventory, vadose zone, and impact codes. The following is this keyword's syntax:

```
SINGLEKEY [PERCENT=Value1|MEAN] [FILE="quote1"]
```

Either the PERCENT modifier or the MEAN modifier is required. The numerical value associated with the modifier PERCENT is used to select the sample percentile for output. A value in the range 0 to 1 is allowed. A value of 0.5 will select the median generated value. The arithmetic mean of the generated values will be used for output if the MEAN modifier is used.

The quote string associated with the FILE modifier identifies the output file where the data will be written. The quote string must be enclosed in double quotation marks, and file names up to 200

characters long are supported. The following example indicates that keywords using median values for two stochastic variables are to be written to the file named "Tmp_Key.Key":

```
SINGLEKEY PERCENT=0.5 File="Tmp_Key.key"
STOCHASTIC KDSOIL "KdI129"  6 0.0 4.0 15.0 "Soil-water Kd for I129"
STOCHASTIC KDSOIL "KdCs137" 9 6.908 0.692 TRUNCATE 0.01 0.99 "Kd Cs137"
```

This example results in the following two output keywords:

```
STOCHASTIC "KdI129"  1  5.9170E+00 "Soil-water Kd for I129"
STOCHASTIC "KdCs137" 1  1.0002E+03 "Kd Cs137"
```

The following example indicates that keywords using the mean values for two stochastic variables are to be written to the file named "Tmp_Key.Key":

```
SINGLEKEY MEAN File="Tmp_Key.key"
STOCHASTIC KDSOIL "KdI129"  6 0.0 4.0 15.0 "Soil-water Kd for I129"
STOCHASTIC KDSOIL "KdCs137" 9 6.908 0.692 TRUNCATE 0.01 0.99 "Kd Cs137"
```

This example results in the following two output keywords:

```
STOCHASTIC "KdI129" 1  6.3333E+00 "Soil-water Kd for I129"
STOCHASTIC "KdCs137" 1  1.2289E+03 "Kd Cs137"
```

17.3.7 STOCHASTIC Keyword for STOCHASTIC

The STOCHASTIC keyword is used to enter the definition of a statistical distribution for stochastic variables. The following is this keyword's syntax:

```
STOCHASTIC ["Quote1"] [Dist_Index Parameters] {TRUNCATE U1 U2} {"Quote2"}
```

- The entry for Quote1 must be a unique character string of up to 20 characters that will be used to identify this stochastic variable in subsequent uses. It is case sensitive, and embedded spaces are significant.
- The entry for Quote1 must be a unique character string of up to 20 characters that will be used to identify this stochastic variable in subsequent uses. It is case sensitive, and embedded spaces are significant.
- The optional entry for Quote2 is a description for the stochastic variable; the description can be up to 64 characters long.
- The entry for Dist_Index must be an integer in the range 1 to 13 that identifies the index of a statistical distribution. The available statistical distributions are defined in Table 17.3.
- The word Parameters in the general syntax statement indicates the numerical values of parameters required for defining the statistical distribution.
- The additional modifier TRUNCATE can be used for all distribution types except 1, 3, and 10 (constant, discrete uniform, and user-defined). If TRUNCATE is entered, it must be followed by two values in the interval 0 to 1, inclusive. The lower value must be less than the upper value. These two values specify the tail probabilities at which to impose range truncation for the distribution. Truncation data must be entered after all of the other parameters that define the distribution. Further information on generation of stochastic variables is provided in Section 19.0.

Table 17.3 Statistical Distributions Available in STOCHASTIC

Index	Distribution	Truncate	Parameters Required
1	Constant	No	Single value.
2	Uniform	Yes	Lower limit, upper limit.
3	Discrete Uniform	No	Smallest integer, largest integer.
4	Loguniform (base 10)	Yes	Lower limit, upper limit.
5	Loguniform (base e)	Yes	Lower limit, upper limit.
6	Triangular	Yes	Lower limit, mode, upper limit.
7	Normal	Yes	Mean, standard deviation.
8	Lognormal (base 10)	Yes	Mean, standard deviation of logarithms.
9	Lognormal (base e)	Yes	Mean, standard deviation of logarithms.
10	User Defined	Yes	Number of pairs, data for pairs of values ($Prob(X_i),X_i$).
11	Beta	Yes	Alpha, beta, lower limit, upper limit. The mean of the distribution would be alpha/(alpha+beta) if the limits were 0 and 1.
12	Log ratio	Yes	Mean, standard deviation (of derived normal), lower limit, upper limit.
13	Hyperbolic arcsine	Yes	Mean, standard deviation (of derived normal).

The following is an example STOCHASTIC keyword for a variable assigned a constant of 234.432:

```
STOCHASTIC "Unique1" 1 234.432 "Define a constant distribution"
```

The following is an example STOCHASTIC keyword for a bioconcentration factor that is normally distributed with a mean of 125 and a standard deviation of 5 for a frog exposed to ^{14}C:

```
STOCHASTIC "BCFC14Frog" 7  125.0  5.0  "Example Distribution"
```

17.3.8 TITLE Keyword for STOCHASTIC

The TITLE keyword is used to define a single-line problem title. The problem title will be written to output files. The program will error terminate if the title is not supplied. The following is this keyword's syntax:

```
TITLE ["quote"]
```

The title is entered in a quote string, which must be enclosed in double quotation marks. Titles up to 200 characters long are supported. The following example defines a title for a run of the code:

```
TITLE "Example title line for the STOCHASTIC code."
```

17.3.9 USER Keyword for STOCHASTIC

The USER keyword is used to identify the user of the program. The user name will be written to output files. The program will error terminate if the user name is not supplied. The following is this keyword's syntax:

```
USER ["quote"]
```

The user name is entered in a quote string, which must be enclosed in double quotation marks. User names up to 16 characters long are supported. The following example defines John Q. Public as the user running the code:

```
USER "John Q. Public"
```

18.0 Keyword Language Syntax

Each line of a keyword data file is parsed into numeric and character data. These are interpreted to set up control information and define input parameters. An input line can contain up to 2048 characters of information. Individual quote strings are limited to 200 characters in length.

Every line of the input data file is considered a keyword record, continuation record, or a comment record. Keyword records contain a keyword beginning in column 1. The keyword is used to determine the purpose of the subsequent data. Continuation records are used when a keyword record requires too much data to be placed on one line. Comment lines are ignored by the reading software but are useful for annotating the input file.

The information from each keyword record and subsequent continuation lines is moved into storage arrays. Data that can be deciphered as numeric values are placed into a numeric array. Other data are classified either as "secondary keywords" (called "modifiers") or "quote strings." Secondary keywords are stored as character images in an array. All such keywords or modifiers read from the input file are changed to uppercase before being stored. Quote strings are text strings that are enclosed in double quotation marks. These are stored exactly as they are read from the input file.

18.1 Keyword Records

Keyword records start in column 1 with any letter from A to Z, in either upper- or lowercase. The first eight letters of a keyword are stored in a variable and are used by the modeling software to determine the actions desired by the program user. All subsequent lines of text that do not have an alphabetic character or comment character in column 1 are treated as continuation lines. The following is an example keyword record (where SAMPLEKEY starts in column 1):

```
SAMPLEKEY 2 0 500 1 100
```

The word SAMPLEKEY is the keyword. The numbers 2, 0, 500, 1, and 100 are numeric data.

18.2 Continuation Records

Continuation records start with any valid separator character (except a double quotation mark). These are treated as additional data to the previous keyword record. Section 18.4.2 identifies valid separator characters. The combined data on a keyword line and on the subsequent continuation line(s) are treated as a single block of information. All numeric values and character strings on those lines are used as input data relevant to the keyword of the keyword line. The two following keyword entries contain the same information:

```
SAMPLEKEY 2 0 500 1 100
SAMPLEKEY 2 0
   500 1 100
```

18.3 Comment Records

Any line with the characters $, ! or / in column 1 will be treated as a comment record. These lines are ignored by the input data record reader. Both the $ and the ! can also be used to signify in-line comments

(not in column 1). Any information that follows a $ or a ! will be ignored. The / character indicates a comment only if it is the first character on the input line. The following are some examples of comment lines:

```
$This is a comment line
/This is a comment line
!This is a comment line
```

The following are some examples of in-line comments:

```
SAMPLEKEY 3 4.0 5.0 !Trailing information is ignored after the !
SAMPLEKEY 3 4.0 5.0 $Trailing information is ignored after the $
```

18.4 Input Data Handling

Each line of the input is read and parsed into numeric and character values. All numeric values are converted to real numbers (as opposed to FORTRAN integer). All data that cannot be interpreted as numeric information are stored as character values.

Numeric data can include a leading sign (+ or -), integer characters 0 through 9, a decimal point, and an exponent indication ("E" or "e"). The FORTRAN "double precision" exponent indicator "D" is not valid. A maximum of 10 digits is allowed when entering numeric data.

Secondary keywords, or modifiers, are character strings that could not be interpreted as numeric values. These are converted to uppercase, where necessary, and stored in an array. The number of secondary keywords that are moved into the array is stored for internal use.

Only the first eight characters of any keyword are significant. Keywords fewer than eight characters long are left justified and blank-filled.

18.4.1 Quote Strings

Quote strings are strings of literal text that must be used exactly as given in the input line. They are enclosed by double quotation marks and are typically used for passing file names into a program. Only the first 200 characters of a quote string are saved. Each quote string must begin and end on a single line of the input file. When an unclosed quote is encountered, an implied quote is created at the end of that line. The following is an example of quote string usage:

```
FILE "c:\apps\human\test.dat"
```

18.4.2 Data Separators

Keywords, numeric data, and secondary keywords must be separated by any one of the following data "separators": space character, comma, equal sign, colon, semicolon, left parenthesis, right parenthesis, single quotation mark, double quotation mark, and tab character.

Also, any character with a ASCII character storage code of less than 10 is treated as a separator character. This is used mainly to identify the ASCII tab character as a data separator. Double quotation marks are used differently than the other separators. They indicate text strings that are stored without conversion by

the program. As an illustration of the use of separator characters, the following keyword records all contain and convey the same information:

```
SAMPLEKEY 3 4.5 5.6 6.7
SAMPLEKEY 3 (4.5,5.6,6.7)
SAMPLEKEY 3 ( 4.5=5.6'6.7 )
SAMPLEKEY 3:4.5  5.6:6.7
```

19.0 Stochastic Variable Generation

Many of the codes in the TIIA generate values for stochastic variables. All of the codes use the same suite of statistical routines. The following are some major considerations for this process:

- Each distribution is generated using the Probability Integral Transformation method (Mood et al. 1974, p. 202).
- The uniform number generator uses a linear congruential method (Lewis et al.1969).
- Stratified sampling is used when the number of values to be generated is greater than 1.
- Most distributions may be truncated between two limits that are specified as limits in the uniform domain on the interval 0 to 1.
- The user may specify a cumulative distribution function in the form of a table of values.
- Information about a stochastic variable is linked to a unique character ID. Access to all information about the variable is available through use of the variable ID.

The following are the available statistical distributions:

- Constant value
- Uniform distribution between two limits
- Discrete uniform distribution on a set of contiguous integers
- Loguniform (base 10) distribution between two limits
- Loguniform (base e) distribution between two limits
- Triangular distribution defined using a lower limit, mode, and an upper limit
- Normal distribution with a mean and standard deviation
- Lognormal (base 10) distribution specified by the mean and standard deviation of the logarithms of the data
- Lognormal (base e) distribution specified by the mean and standard deviation of the logarithms of the data
- User-specified cumulative distribution function input as a table of probabilities and exceedance values
- Beta distribution that can be shifted and scaled from the standard (0,1) interval
- Log-ratio from a normal distribution
- Hyperbolic arcsine from a normal distribution.

19.1 Keywords Defining Stochastic Variables

Depending on the utility code, stochastic variables can be defined for STOCHAST, KDSOIL, DILUTE and INFILTRA keywords. The following general description is presented for STOCHAST(IC) keyword, although it applies to each of the other keywords. The following is this keyword's syntax:

```
STOCHASTIC [{ID=}"Quote1"] [Dist_Index Parameters] {TRUNCATE U1 U2}
{{LABEL=}"Quote2"} {UNITS="quote3"}
```

- The entry for Quote1 must be a unique character string of up to 20 characters that will be used to identify this stochastic variable in subsequent uses. It is case sensitive, and embedded spaces are significant. It is sometimes useful to make the character string some combination of a variable name and other data so that it can be recreated easily when stochastic data is needed.

- The entry for Quote2 is an optional description for the stochastic variable that can be up to 64 characters long and is used for output labeling purposes.
- The entry for Dist_Index must be an integer in the range 1 to 13 that identifies the index of a statistical distribution. The statistical distributions are defined in Table 19.1.
- The word Parameters in the general syntax statement indicates the numerical values of parameters required for defining the statistical distribution.
- The additional modifier TRUNCATE can be used for all distribution types except 1, 3, and 10. If TRUNCATE is entered, it must be followed by two values in the interval 0 to 1, inclusive. The lower value must be less than the upper value. These two values specify the tail probabilities at which to impose range truncation for the distribution. Truncation data must be entered after all of the other parameters that define the distribution.

Table 19.1 Common Statistical Distributions Available in TIIA Codes

Index	Distribution	Truncate	Parameters Required
1	Constant	No	Single value.
2	Uniform	Yes	Lower limit, upper limit.
3	Discrete Uniform	No	Smallest integer, largest integer.
4	Loguniform (base 10)	Yes	Lower limit, upper limit.
5	Loguniform (base e)	Yes	Lower limit, upper limit.
6	Triangular	Yes	Lower limit, mode, upper limit.
7	Normal	Yes	Mean, standard deviation.
8	Lognormal (base 10)	Yes	Mean, standard deviation of logarithms.
9	Lognormal (base e)	Yes	Mean, standard deviation of logarithms.
10	User Defined	Yes	Number of pairs, data for pairs of values ($Prob(X_i),X_i$).
11	Beta	Yes	Alpha, beta, lower limit, upper limit. The mean of the distribution would be alpha/(alpha+beta) if the limits were 0 and 1.
12	Log ratio	Yes	Mean, standard deviation (of normal), lower limit, upper limit.
13	Hyperbolic arcsine	Yes	Mean, standard deviation (of normal).

The following is an example STOCHASTIC keyword for a variable assigned a constant of 234.432:

```
STOCHASTIC "Unique1" 1 234.432 "Define a constant distribution"
```

The constant can take any value.

The following is an example STOCHASTIC keyword for a variable assigned a uniform distribution on -2 to 7:

```
STOCHASTIC ID="Unique2" 2 –2.0 7 "Uniform distribution on –2 to 7"
```

The two limits can take any values as long as the second value is strictly greater than the first value. The following is an example stochastic keyword for a variable assigned a discrete uniform distribution on the integers 6 to 70:

```
STOCHASTIC "Unique3" 3 6 70 "Discrete uniform distribution on 6 to 70"
```

The two limits must be integers where the second integer is strictly greater than the first integer.

The following is an example STOCHASTIC keyword for a variable assigned a loguniform (base 10) distribution on the interval 10^{-7} to 10^{-3}:

```
STOCHASTIC ID="Unique4" 4 1.0E-7 1.0E-3
   LABEL="Define a loguniform (base 10) variable on 0.0000001 to 0.001"
```

The two limits must both be greater than zero, and the second limit must be greater than the first limit.

The following is an example STOCHASTIC keyword for a variable assigned a loguniform (base e) distribution on the interval 10^{3} to 10^{6}:

```
STOCHASTIC "Unique5" 5  1.0E3  1E+6
   "Define a loguniform (base e) distribution on 1000 to 1000000"
```

The two limits must both be greater than zero, and the second limit must be greater than the first limit.

The following is an example STOCHASTIC keyword for a variable assigned a triangular distribution with a minimum of 2, a mode of 3, and a maximum of 7:

```
STOCHASTIC "Unique6" 6  2 3 7  "Triangular distribution on (2,3,7)"
```

The three values that define the triangular must all be different, and they must be entered in increasing order.

The following is an example STOCHASTIC keyword for a bioconcentration factor that is normally distributed with a mean of 125 and a standard deviation of 5 for a frog exposed to ^{14}C:

```
STOCHASTIC "BCFC14Frog" 7  125.0  5.0  "Example normally distributed frog"
```

The mean value can be any number, but the standard deviation must be greater than zero.

The following keyword would define a different stochastic variable from the one just entered because the identification string (Quote1) is case sensitive:

```
STOCHASTIC "BCFC14FROG" 7  125.0  5.0  "Example normally distributed frog"
```

The following keyword entry would define a lognormal (base 10) distribution where the mean and standard deviation (of the logarithms) are –2.0 and 0.5:

```
STOCHASTIC "Unique8"  8  –2  0.5 "Lognormal (base 10) variable"
```

The mean value can be any number, but the standard deviation must be greater than zero.

The following keyword entry would define a lognormal (base e) distribution where the mean and standard deviation (of the logarithms) are –2.0 and 0.5. In addition, the lognormal distribution will be truncated between the lower 0.025 and upper 0.99 probabilities.

```
STOCHASTIC "Unique9" 9 –2 .5 TRUNCATE 0.025 0.99
   "Example for a truncated lognormal variable"
```

The mean value can be any number, but the standard deviation must be greater than zero.

The following keyword entry illustrates the use of the user-defined distribution (distribution type 10). This example entry uses seven pairs of values. The first pair of numbers uses a probability of 0 to define the lower limit of the distribution at 8.4E-7. The last pair of numbers uses a probability of 1 to define the upper limit of the distribution at 1.73E-6. The other values are associated with the probability levels of

.025, .167, .5, .833, and .975. The probability data and distribution percentiles must be entered in strictly increasing order.

```
STOCHASTIC "Sr90Con" 10  7
   0  8.40E-7
   2.50E-02  9.20E-7
   1.67E-01  1.06E-6
   5.00E-01  1.21E-6
   8.33E-01  1.37E-6
   9.75E-01  1.58E-6
   1  1.73E-6
```

The first pair of numbers uses a probability of 0 to define the lower limit of the distribution. The last pair of numbers uses a probability of 1 to define the upper limit of the distribution. The intervening pairs define probability levels and the associated data values. The probabilities and data values must be entered in strictly increasing order.

The following keyword entry would define a beta distribution with parameters 1.1 and 2.1 on the interval (0,1):

```
STOCHASTIC "Unique11-1"  11  1.1  2.1  0.0  1.0
   "Beta (1.1,2.1) on the interval 0,1"
```

Let the first parameter be denoted by α and the second parameter be denoted by β. The mean of the beta distribution would be α /(α +β) if the limits were 0 and 1. Both α and β must be greater than zero. The lower limit must be less than the upper limit.

The following keyword entry would define a beta distribution with parameters 1.1 and 2.1 but on the interval –2 to 4:

```
STOCHASTIC "Unique11-2"  11  1.1  2.1  -2.0  4.0
   "Beta (1.1,2.1) on the interval (-2,4)"
```

The following keyword entry would define a log ratio distribution from a normal (-1.459,1.523) distribution on the interval -5.756 to 4.33:

```
STOCHASTIC "Test1203" 12 -1.459  1.523 -5.756 4.330
   "Log ratio from Normal(-1.4,1.5) on (-5.756,4.330)"
```

The entry for the normal standard deviation (a value of 1.523 in this example) must be greater than zero. The last two numerical values define the interval for the generated values, so the lower limit must be smaller than the upper limit.

The following keyword entry would define a hyperbolic arcsine distribution from a normal (0.189,0.146) distribution:

```
STOCHASTIC "Test1302" 13 0.189  0.146
   "Hyperbolic Arcsine from Normal(0.189,0.146)"
```

The entry for the normal standard deviation (a value of 0.189 in this example) must be greater than zero.

19.2 Probability Concepts

The distribution of a continuous random variable X (the term *continuous* indicates that the random variable is defined over a continuum of values) is completely described by its probability density

function, f(x). The interpretation of the probability density function is that the area under f(x), for an interval a<x<b, equals the probability that the random variable, X, will fall in the interval (a,b), denoted P[a<X<b]. One cannot make the statement P[X=t], because there is no area under the probability density function at any given point. Two axioms of probability theory (Mood et al. 1974, p. 22) are that the probability of any event is between zero and one, and the integral of the probability density function over the entire support (the interval [L,U]) of X equals 1. The integral of the probability density function from the lower bound L to some value x (suppose it is less than the upper bound U) represents the probability that X will be observed in the interval (L,x). This integral operation defines the cumulative distribution function for the random variable X. The cumulative distribution function is denoted by F(x) (the capital F for the cumulative distribution function corresponds to the lowercase f for the probability density function) and mathematically is represented by the following:

$$F(x) = \int_{L}^{U} f(s)ds$$

The inverse cumulative distribution function, $[F^{-1}(\bullet)]$, is single-valued if x is in the interval (L,U). Hence if p'= F(x') is known, in theory x'= F^{-1}(p') can be obtained.

19.3 Probability Integral Transform Method

Generation of a random variable from a given distribution typically involves the use of information either about f or F. There are two philosophical approaches to generating random numbers: exact methods and approximate methods. The algorithms embedded in TIAA employ exact methods. Exact methods can be further categorized into probability integral transform methods and functional methods. The probability integral transform method is employed in the TIIA.

In the probability integral transform method, the random variable of interest is expressed as a function of a U(0,1) random variable, where U(0,1) denotes the continuous random variable ranging uniformly over the interval (0,1). The probability density function of the uniform random variable is g(u)=1 if u0(0,1) and is zero elsewhere. The cumulative distribution function for this random variable takes the exceedingly simple form G(u)=u. It can be shown that any cumulative distribution function evaluated at a random value X (instead of being evaluated at a known value x as in the previous discussion) is distributed uniformly over the interval (0,1) (Mood et al. 1974, p. 202). Therefore, given a realization u of the U(0,1) random variable and a selected statistical distribution (known cumulative distribution function), one can set u=F(x) and solve to obtain x=F^{-1}(u). The value x thus obtained is a random realization from the selected statistical distribution.

In principle, one can obtain an exact solution for x given any specific cumulative distribution function and value u. In reality, there exist some distributions, such as the normal and beta distributions, for which no closed-form analytical expression for F^{-1} exists, and hence approximation methods must be applied.

The probability integral transform method allows efficient sampling from a subregion of the interval (L,U), such as (c,d), where L<c<d<U. In this case one would find the corresponding interval in the uniform domain, say (c',d'), and sample uniformly over that interval, by sampling from the rescaled uniform distribution [for example, u'=(d-c)u+c] and then obtaining x as usual using x=F^{-1}(u'). The rescaled uniform distribution takes the form g(u)=1/(d'-c') for u0(c',d') and is zero elsewhere. For any distribution with probability density function f(x) and cumulative distribution function F(x), the

probability density function, under truncation to the interval (c,d), is $f_T(x) = f(x)/[F(d)-F(c)]$. The divisor ensures that $f_T(x)$ integrates to unity.

19.4 Stratified Sampling

Stratified sampling can easily be implemented when generating random deviates using the probability integral transform method. This is accomplished by dividing the uniform interval (0,1) into subintervals, or strata, and sampling a specified number of times within each stratum, each time obtaining the corresponding value of x. Within TIIA, the strata intervals are assigned equal probability, and exactly one value is sampled within each stratum. The method generates samples from each stratum and then randomly shuffles the entire set of realizations using a variation of the Quicksort algorithm (Hoare 1961). The primary purpose of stratified sampling is to achieve more evenly spaced (in a probability sense) samples from the distribution of a random variable than would result from randomly sampling over the whole range of the distribution. Iman and Conover (1982) have shown that stratified sampling can result in more efficient estimation of simulation results for a variety of estimators than when using simple random sampling.

Two steps are used to obtain a stratified sample $\{s_i, i = 1, 2, ..., N\}$ of size N for the uniformly distributed variable S. First, generate values for s_i using the following equation:

$$s_i = \frac{(n-1) + u_i}{N}$$

where u_i is a uniformly distributed number between 0 and 1 generated using simple random sampling. These values satisfy the relationship $0<s_i<s_{i+1}<1$. In the second step, the s_i are reshuffled to a random order. This reshuffling can be achieved by generating a new sequence of uniformly distributed random numbers, a_i, i = 1, 2, ..., N using simple random sampling. The set of values $\{s_i\}$ are then reordered so they have the same rank order as the corresponding a_i.

19.5 Generation Algorithms

Table 19.1 summarizes the statistical distributions available in the TIIA codes. The following paragraphs describe the generation algorithms.

19.5.1 Algorithm for the Uniform Distribution

Algorithms that generate truly random uniform numbers do not exist, although many algorithms generate pseudo-random deviates (hereafter loosely referred to as random numbers). The selection of a random number generator is based on four considerations: 1) computer implementability, 2) degree of independence within a sequence of deviates, 3) periodicity or cyclic length of a sequence, and 4) uniform coverage of sequences (occurrence) over the interval (0,1), the square (0,1) X (0,1), etc., up to the hypercube (0,1) in k dimensions.

Commonly used random number generation techniques are linear congruential methods (Park and Miller 1988). The TIIA codes use a linear congruential random number generator. The linear congruential generator generates random integers from an algorithm of the form $S_i = (A \cdot S_{i-1} + C) \bmod M$. where S_i is the ith generated random integer, A and C are constants, M is the modulus of the generated integers, and

mod denotes the remainder function. These integers are converted to approximate uniform (0,1) numbers by the division $U_i = S_i / M$.

The period of a sequence $\{U_i\}$ of generated deviates is the minimal value k such that $U_i=U_{i+k}$ (this occurs independent of i for linear congruential generators). It can be shown that the period of any congruential generator does not exceed M. Therefore, if one is generating many uniform deviates, it is desirable that M be large. The performance of each congruential generator (each choice of A, C, and M) can thus be examined with respect to criteria proceeding from the four considerations given above.

Generation Algorithm: The TIIA implementation for generating uniform random variables uses a linear congruential generator with A=16807, C=0, and M=2147483647. These choices yield a sequence $\{U_i\}$ that 1) is implementable on a 32-bit computer without machine language coding, 2) is sufficiently independent on an element-by-element basis, 3) possesses a long cycle (period), and 4) has a reasonable degree of coverage over all hypercubes of dimension less than k. These conclusions proceed from results from tests described in Fishman and Moore (1986). The generation algorithm uses two steps;

$$S_i = A \times S_{i-1} \ \text{Mod}(M)$$
$$U_i = S_i / M$$

Any value, x, generated from the uniform (a,b) distribution in the TIIA codes makes use of a value, y, from the U(0,1) distribution. The value y is first generated, and then x is evaluated as x=a+(b-a)y. The uniform (a,b) distribution will be denoted by U(a,b).

Cumulative Distribution Function: The CDF for a U(a,b) random variable takes the form:

$$F(x) = \begin{cases} 0 & x < a \\ \left[\dfrac{x-a}{b-a}\right] & a \le x \le b \\ 1 & x > b \end{cases}$$

Expected Value: The expected value of a U(a,b) random variable is (a+b)/2

Variance: The variance of a U(a,b) random variable is $(b-a)^2/12$

Median: The median of a U(a,b) random variable is (a+b)/2.

19.5.2 Algorithm for the Discrete Uniform Distribution

Generation Algorithm: The probability density function for the discrete uniform distribution is f(x)=1/N for each of the N integers ranging in the interval L to U. The generation algorithm for the discrete uniform distribution is

$$F^{-1}(u) = L + \text{int}[u(U - L + 1)]$$

where the int(·) function returns the integer portion of its argument.

Cumulative Distribution Function: The cumulative distribution function of a discrete uniform random variable on the interval (a,b) is

$$F(x) = \begin{Bmatrix} 0 & x < a \\ \dfrac{1}{(b-a+1)} \sum_{i=a}^{b} I(a \le i \le x) & a \le x \le b \\ 1 & x > b \end{Bmatrix}$$

Expected Value: The expected value of a discrete uniform random variable on the interval (a,b) is

$$E(X) = \frac{b(b+1) - a(a+1)}{2(b-a+1)}$$

Variance: The variance of a discrete uniform random variable on the interval (a,b) is

$$V(X) = \frac{x(x+1)(2x+1) - (a-1)a(2a+1)}{6(b-a+1)} - \left[\frac{b(b+1) - a(a+1)}{2(b-a+1)} \right]^2$$

Median: The median of a discrete uniform random variable on the interval (a,b) is the integer closest to (a+b)/2.

19.5.3 Algorithm for the Loguniform Distribution

Generation Algorithm: The probability density function for the loguniform random variable of base b is

$$f(x) = \frac{I(b^c < x < b^d)}{x(d-c)\ln(b)}$$

for $-\infty<c<d<\infty$, where I is an indicator function (0 if false, 1 if true), b is the logarithm base (either 10 or the natural constant e), and ln(b) denotes the natural logarithm of b.

The inverse cumulative distribution function algorithm used to generate a value, x, from the loguniform distribution first generates a value, y, from the U(c,d) distribution and then evaluates the expression $x=b^u$.

Cumulative Distribution Function: The CDF algorithm for a loguniform (c,d) random variable is

$$F(x) = \begin{Bmatrix} 0 & x < b^c \\ \left[\dfrac{\ln(x) - c\ln(b)}{(d-c)\ln(b)} \right] & x \in [b^c, b^d] \\ 1 & x > b^d \end{Bmatrix}$$

Expected Value: The expected value of a loguniform (c,d) random variable is

$$E(X) = \frac{b^d - b^c}{(d-c)\ln(b)}$$

Variance: The variance of a loguniform (c,d) random variable is

$$V(X) = \frac{b^{2d} - b^{2c}}{2(d-c)\ln(b)} - \left[\frac{b^{d} - b^{c}}{(d-c)\ln(b)}\right]^2$$

Median: The median of a loguniform (c,d) random variable distribution is $b^{(c+d)/2}$.

19.5.4 Algorithms for the Triangular Distribution

Generation Algorithm: The triangular distribution has probability density function:

$$f(x) = \begin{cases} 2(x-a)/[(b-a)(c-a)] & \text{for} \quad a < x \le b \\ 2(c-x)/[(c-b)(c-a)] & \text{for} \quad b \le x < c \end{cases}$$

and takes the value 0 elsewhere.

The following equation provides the generation algorithm for the triangular distribution:

$$F^{-1}(u) = \begin{cases} a + \sqrt{u(c-a)(b-a)} & \text{for} \quad 0 \le u \le (b-a)/(c-a) \\ c - \sqrt{(1-u)(c-a)(c-b)} & \text{for} \quad (b-a)/(c-a) \le u \le 1 \end{cases}$$

Cumulative Distribution Function: The CDF algorithm for the triangular distribution takes the following form:

$$F(x) = \begin{cases} 0 & x \le a \\ \dfrac{(x-a)^2}{(c-a)(b-a)} & a < x \le b \\ 1 - \dfrac{(x-c)^2}{(c-a)(c-b)} & b < x \le c \\ 1 & x \ge c \end{cases}$$

Expected Value: The expected value of a random variable with the triangular distribution is (a+b+c)/3.

Variance: The variance of a random variable with the triangular distribution is

$$V(X) = \left[\frac{a^4c - a^4b + ab^4 - ac^4 - b^4c + bc^4}{6(b-a)(c-a)(c-b)}\right] - \left[\frac{a+b+c}{3}\right]^2$$

Median: The median of a random variable with the triangular distribution depends on the location of the mode b. The median is:

$$M(X) = \begin{cases} a + \sqrt{(b-a)(c-a)/2} & \text{for } b \ge (a+c)/2 \\ c - \sqrt{(c-b)(c-a)/2} & \text{for } b \le (a+c)/2 \end{cases}$$

19.5.5 Algorithms for the Normal Distribution

Generation Algorithm: A normal (μ,σ^2) random deviate, y, is obtained by generating a N(0,1) deviate, x, band then transforming that value using the equation $y=\mu+\sigma x$. The normally distributed random variable with mean μ and variance σ^2, denoted as $N(\mu, \sigma^2)$, has the probability density function:

$$f(x) = \frac{e^{-(x-\mu)^2/(2\sigma^2)}}{\sigma\sqrt{2\pi}}$$

for $-\infty<x<\infty$, $-\infty<\mu<\infty$ and $\sigma>0$.

The inverse cumulative distribution function for the N(0,1) random variable does not have a closed form expression. It is approximated by:

$$F^{-1}(p) = \begin{Bmatrix} q\,A(q^2)/B(q^2) & \text{for } |q| < 0.42 \\ \text{sgn}(q)\,C(r)/D(r) & \text{otherwise} \end{Bmatrix}$$

where $q=p-0.5$, and $r=\sqrt{\ln(0.5-|q|)}$. The quantity $(0.5-|q|)$ is formed as p or, to avoid cancellation if p is small, as (1-p). The letters A, B, C, and D represent polynomials of order 3, 4, 3, and 2, respectively, whose coefficients are given in Beasley and Springer (1985), and $\text{sgn}(q)=1$ if $q>0$ and -1 if $q<0$.

Cumulative Distribution Function: There is no closed form analytic expression for the CDF of a random variable with the normal distribution. Algorithm AS 66 (Hill 1985) can be used to generate an accurate numerical approximation.

Expected Value: The expected value of a random variable with the $N(\mu,\sigma^2)$ distribution is μ.

Variance: The variance of a random variable with the $N(\mu,\sigma^2)$ distribution is σ^2.

Median: The median of a random variable with the $N(\mu,\sigma^2)$ distribution is μ.

19.5.6 Algorithms for the Lognormal Distribution

Generation Algorithm: The logarithm of a random variable that is lognormally distributed is distributed as a normal $N(\mu,\sigma^2)$ random variable (thus the name lognormal). The probability density function of the lognormal distribution is:

$$f(x) = \frac{A}{x\sigma\sqrt{2\pi}} e^{-[\log(x)-\mu]^2/2\sigma^2}$$

for $x>0$ and $\sigma>0$. Because this distribution is available in both base 10 and natural logarithm base form, the constant A is $1/\log_e 10$ for base 10 and 1 for the natural logarithm base. The logarithm log(x) is also evaluated in terms of the chosen base.

A lognormal random variable, x, is generated using a two-step process. First, a value, y, is generated from the $N(\mu,\sigma^2)$ distribution. This value is then used in the expression $x=b^y$, where the base b is either 10 or the natural constant e, as desired.

Cumulative Distribution Function: There is no closed form analytic expression for the CDF of a random variable with the lognormal distribution. However, a closed form expression can be accomplished by generating the CDF of the logarithm of the random variable. Algorithm AS 66 (Hill 1985) can be used to generate an accurate numerical approximation.

Expected Value: The expected value of a random variable with the lognormal(μ,σ^2) distribution is

$$E(X) = e^{\left(\mu+0.5\sigma^2\right)}$$

Variance: The variance of a random variable with the lognormal(μ,σ^2) distribution is

$$V(X) = e^{\sigma^2}\left(e^{\sigma^2}-1\right)e^{2\mu}$$

Median: The median of a random variable from the lognormal(μ,σ^2) distribution is e^{μ}.

19.5.7 Algorithms for the User-Defined Distribution

Generation Algorithm: In addition to selecting from parametric families of distributions, the user may implement any other distribution by supplying a table of data pairs corresponding to the pairs [F(x),x]. Thus, the user provides the code with discrete evaluations of the cumulative distribution function. The algorithm linearly interpolates between these points to solve for F^{-1} when generating a random deviate. The interpretation of the table of data is that the CDF takes on values on a continuum of values rather than a discrete set of values.

19.5.8 Algorithms for the Beta Distribution

Generation Algorithm: The beta random variable, x, is described by the probability density function:

$$f(x) = \frac{x^{p-1}(1-x)^{q-1}}{B(p,q)}$$

for $p>0$, $q>0$, and $0<x<1$. This variable can be transformed to the interval (a,b), and the resulting probability density function for the random variable, y, takes the form:

$$f(x) = \frac{(b-a)^{-(p+q+1)}(y-a)^{p-1}(b-y)^{q-1}}{B(p,q)}$$

for $p>0$, $q>0$, and $a<y<b$. The second expression for the probability density function can be obtained from the first by the change of variable $y=(b–a)x+a$.

A closed form expression for the beta inverse cumulative distribution function does not exist. The algorithm implemented is provided in Algorithm AS 64/AS 109 (Griffiths and Hill 1985, p. 121). Algorithm AS 64/AS 109 requires the logarithm of B(p,q). Using the relationship between the beta and gamma functions (Mood et al. 1974, p. 535), B(p,q)=G(p+q)/{G(p)G(q)}, where G(·) denotes the gamma function, the logarithm of B(p,q) is computed using Algorithm ACM 291 (Pike and Hill 1966). Algorithm AS 64/AS 109 uses approximate starting values and a Newton-Rhapson iterative method to achieve a final solution.

Cumulative Distribution Function: There is no closed form analytic expression for the CDF of a random variable with the beta distribution. Therefore, the numerical approximation specified in Algorithm AS 63 (Mujamder and Bhattacharjee 1985) is used. This algorithm is based on the reduction method first published by Soper (1921).

Expected Value: The expected value of a random variable with the Beta distribution is a+(b-a)p/(p+q)

$$E(X) = a + (b - a)\frac{p}{p + q}$$

Variance: The variance of a random variable with the Beta distribution is

$$V(X) = \frac{pq(b - a)^2}{(p + q + 1)(p + q)^2}$$

Median: No analytically tractable expression is available for the median of a random variable with the Beta distribution.

19.5.9 Algorithms for the Log Ratio Distribution

Generation Algorithm: Let y denote a random variable from the log ratio distribution on the interval (a,b). The probability density function for y is:

$$f(y) = \frac{(b - a)e^{-(\ln\{(y-a)/(b-y)\}-\mu)^2/(2\sigma^2)}}{\sigma(y - a)(b - y)\sqrt{2\pi}}$$

where a<b and a<y<b.

A random variable, y, from the log ratio distribution is generated using a two-step process. First, a value, x, is generated from the $N(\mu,\sigma^2)$ distribution. This value is then used in the expression:

$$F^{-1}(x) = \frac{a + be^x}{1 + e^x}$$

Cumulative Distribution Function: There is no closed form analytical expression for the CDF of a random variable with the log ratio distribution.

Expected Value: There is no closed form analytical expression for the expected value of a random variable with the log ratio distribution.

Variance: There is no closed form analytical expression for the variance of a random variable with the log ratio distribution.

Median: There is no closed form analytical expression for the median of a random variable with the log ratio distribution.

19.5.10 Algorithms for the Hyperbolic Arcsine Distribution

Generation Algorithm: Let the random variable x be a normally distributed random variable with mean μ and variance σ^2. Then, let y be a random variable defined as $y = \sinh^{-1}(x)$. The probability density function for y is:

$$f(y) = \frac{0.5(e^{u} + e^{-u})e^{-(\sinh(y)-\mu)^2/(2\sigma^2)}}{\sigma\sqrt{2\pi}}$$

for $-\infty<y<\infty$, $-\infty<\mu<\infty$ and $\sigma>0$.

A random variable, y, from the hyperbolic arcsine distribution is generated using a two-step process. First, a value, x, is generated from the $N(\mu, \sigma^2)$ distribution. This value is then used in the expression:

$$F^{-1}(x) = \sinh(x)$$

Cumulative Distribution Function: There is no closed form analytical expression for the CDF of a random variable with the hyperbolic arcsine distribution.

Expected Value: There is no closed form analytical expression for the expected value of a random variable with the hyperbolic arcsine distribution.

Variance: There is no closed form analytical expression for the variance of a random variable with the hyperbolic arcsine distribution.

Median: There is no closed form analytical expression for the median of a random variable with the hyperbolic arcsine distribution.

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