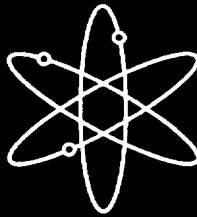


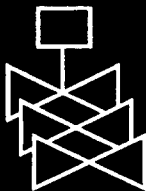
Residual Radioactive Contamination From Decommissioning



User's Manual
DandD Version 2.1



Sandia National Laboratories



U.S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
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Residual Radioactive Contamination From Decommissioning

User's Manual DandD Version 2.1

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ABSTRACT

The Decommissioning and Decontamination (DandD) software package developed by Sandia National Laboratories for the Nuclear Regulatory Commission (NRC) provides a user-friendly analytical tool to address the technical dose criteria contained in NRC's Radiological Criteria for License Termination rule (10 CFR Part 20 Subpart E). Specifically, DandD embodies the NRC's screening methodology to allow licensees to convert residual radioactivity contamination levels at their site to annual dose, in a way consistent with both 10 CFR Part 20 and the corresponding implementation guidance currently under development by NRC. The screening methodology and DandD are part of a larger decision framework that allows and encourages licensees to optimize decisions regarding alternative actions at their site, including the collection of additional data and information. The screening methodology employs reasonably conservative scenarios, fate and transport models, and default parameter values and parameter distributions to allow the NRC to quantitatively estimate the risk of terminating a license given only information about the level of contamination. A licensee has the option of specifying only the level of contamination and running the code with the default parameters or, if site-specific information is available, modifying scenario pathways or providing site-specific parameter distributions and then calculating dose. The original draft of Volume 2 of the NUREG/CR-5512 series documented a User's Manual for the deterministic Version 1.0 of the DandD software. This final version of Volume 2 provides an entirely new User's Manual for the Version 2.1 release of DandD, thus superceding and replacing DandD Version 1.0 and its draft User's Manual. The latest version of the software allows probabilistic (Monte Carlo) dose assessments and incorporates a new and improved Microsoft® Windows® standard user interface.

CONTENTS

ACRONYMS	x
FOREWORD	xi
ACKNOWLEDGMENTS	xii
1 INTRODUCTION	1-1
1.1 Background	1-1
1.1.1 Origin of Deterministic Methods for Decommissioning	1-1
1.1.2 Nuclear Regulatory Commission Decommissioning Guidance	1-1
1.1.3 Evolution of Probabilistic Evaluations	1-2
1.1.4 Decision Framework for License Termination	1-2
1.2 DandD Version 2.1 Overview	1-5
1.2.1 Summary of Requirements for Version 2.1	1-5
1.2.2 Features of DandD Version 2.1	1-6
1.2.3 Comparison to Version 1.0	1-8
1.3 User Manual Overview	1-8
2 INSTALLATION OF DandD	2-1
2.1 System Requirements	2-1
2.2 Installing from CD-ROM	2-1
2.3 Installing by Downloading from the Internet	2-1
2.4 Troubleshooting Installation Problems	2-1
2.5 Uninstalling DandD	2-1
3 WELCOME TO MONTE CARLO DandD	3-1
3.1 The DandD Group	3-1
3.2 Run a Simple Screening Analysis	3-1
3.3 Run a Site-Specific Analysis	3-3
4 USER INTERFACE REFERENCE GUIDE	4-1
4.1 Common Interface Operations	4-1
4.1.1 On-Line Help	4-1
4.1.2 Parameter Viewing Window	4-1
4.1.3 Parameter Modification Window	4-3
4.1.4 Graphics Windows	4-4
4.2 Scenario Tabs and Their Controls	4-6
4.2.1 Edit Exposure Pathway Button (Site-Specific)	4-6
4.2.2 Add Contaminants	4-7
4.2.3 Add Concentrations	4-11
4.2.4 Modify Parameters (Site-Specific Analysis)	4-14
4.2.5 Correlate Parameters (Site-Specific Analysis)	4-16
4.2.6 Execute Simulation	4-18
4.2.7 Sample Size Analysis	4-18
4.3 Main Menu Operations	4-20
4.3.1 File Management Menu Options	4-20
4.3.2 File/Restore Parameters to Default Value	4-22
4.3.3 File/Export as Zip for Submittal	4-22
4.3.4 File/Print	4-22
4.3.5 File/Properties	4-23
4.3.6 Edit/Copy	4-23
4.3.7 View/Reports	4-24

4.3.8	View/Tables	4-27
4.3.9	View/Graphics	4-29
4.3.10	Advanced/Report Template Editor	4-29
4.3.11	Advanced/Sensitivity Analysis	4-32
4.3.12	Window Menu Options	4-37
4.3.13	Help Options	4-38
5 FREQUENTLY ASKED QUESTIONS		5-1
6 REFERENCES		6-1
APPENDIX A DIFFERENCES BETWEEN VOLUME 1 AND RELEASE 1.0 OF DandD		A-1
A.1	Introduction	A-1
A.2	Nomenclature	A-1
A.3	Corrections and Changes to Equations	A-7
A.3.1	Ingestion Dose from Food Grown in Contaminated Soil	A-7
A.3.2	Dose Due to Food Grown with Contaminated Irrigation Water	A-8
A.3.3	Secondary Ingestion of Soil	A-8
A.3.4	Surface Water Pond Decoupling	A-8
A.3.5	Water Balance Model - Drinking Water Scenario	A-9
A.3.6	Water Balance Model - Residential Scenario	A-10
A.3.7	Including Initial Soil Concentration Twice in Dose Calculations	A-10
A.3.8	Separation of Irrigation and Drinking Water Dose Equation into Components	A-12
A.3.9	Multiple Layering in the Unsaturated Zone	A-12
A.3.10	Addition of Root Uptake and Resuspension to the C-14 in Water Special Model	A-13
A.3.11	Modification of the Irrigation Rate Parameter	A-13
A.3.12	Corrections to Equations	A-14
A.4	Corrections and Changes to Data Tables in Volume 1	A-14
A.4.1	Changes to the CHAIN.TXT File	A-15
A.4.2	Changes to BIOACCUM.TXT	A-16
A.4.3	Changes to CEDE.TXT	A-16
A.5	References	A-16
APPENDIX B SAMPLE PROBLEMS		B-1
B.1	Introduction	B-1
B.2	Reference Facilities	B-1
B.3	Nuclear Fuel Cycle Facilities	B-1
B.3.1	Nuclear Power Reactors	B-1
B.3.2	Non-Power Reactors	B-3
B.3.3	Uranium Fuel Fabrication Plants	B-6
B.3.4	Uranium Hexafluoride Plants	B-7
B.3.5	Uranium Mill Facilities	B-8
B.3.6	Independent Spent Fuel Storage Installations	B-8
B.4	Non-Fuel-Cycle Nuclear Facilities	B-9
B.4.1	Sealed Sources	B-9
B.4.2	Short-Lived Radionuclides	B-11
B.4.3	Rare-Metal Ore Processors	B-12
B.5	References	B-13
APPENDIX C FORMAT OF IMPORT CONCENTRATION FILE		C-1
APPENDIX D DandD DATABASE TABLE DESCRIPTIONS		D-1
D.1	Introduction	D-1
D.2	Table Descriptions	D-1
D.2.1	Application Tables (app tables)	D-1

D.2.2	Scenario Specific Tables (bld/res tables)	D-17
D.2.3	Model Result Tables (dat tables)	D-22
D.2.4	Error Information Tables (err tables)	D-27
D.2.5	Sampling Result Tables (par tables)	D-28
D.2.6	Sensitivity Analysis Tables (sen tables)	D-29
D.2.7	User Settings Tables (usr tables)	D-31
D.2.8	Other Tables	D-31
D.3	References	D-31
APPENDIX E TABLES OF TECHNICAL DATA		E-1
E.1	Introduction	E-1
E.2	Radioactive Decay Data	E-1
E.3	Dose Equivalent Factors	E-1
	E.3.1 External Dose Rate Conversion Factors	E-1
	E.3.2 Inhalation and Ingestion Dose Conversion Factors	E-2
E.4	Residential Soil Characteristics	E-2
E.5	Residential U.S. Bureau of Reclamation Percolation Fractions	E-3
E.6	References	E-3

LIST OF FIGURES

1.1	Decommissioning and license termination framework	1-4
1.2	Information flow in DandD Version 2.1	1-7
3.1	Creating a session file	3-2
3.2	Residential default pathway settings	3-2
3.3	Three site contaminants present	3-4
3.4	Adding concentration of Co60	3-4
3.5	Result summary of Case1 analysis	3-5
3.6	Limit area of contamination	3-6
3.7	Sample Size Analysis window for Case1	3-6
3.8	Dose distribution for Case 2	3-8
3.9	Select parameters for analysis	3-8
3.10	Detailed data for H2, unsaturated zone	3-9
3.11	Modifying distribution	3-10
4.1.1	Viewing a parameter value	4-2
4.1.2	Parameter modification window	4-3
4.1.3	Empirical distribution grid	4-5
4.1.4	Modify a grid entry	4-5
4.1.5	Typical graphics window	4-5
4.1.6	Modifying the Axis Scale	4-6
4.2.1	Session window	4-8
4.2.2	Change exposure pathways	4-8
4.2.3	Modify Pathways window	4-9
4.2.4	Add Contaminant window	4-9
4.2.5	Contaminant input modes	4-12
4.2.6	Import contaminant and concentration data	4-12
4.2.7	Nuclide concentration window	4-13
4.2.8	Parameter modification window for contaminant	4-13
4.2.9	General parameter viewing window (residential)	4-15
4.2.10	Modify parameter window for general and element parameters	4-15
4.2.11	Residential Element Parameters window	4-17
4.2.12	Residential Correlate Parameters window	4-17
4.2.13	Run Simulation window - in progress	4-19
4.2.14	Run Simulation window - complete	4-19
4.2.15	Advanced Execution Parameters window	4-19
4.2.16	Sample Size Analysis window	4-21
4.3.1	Open a session	4-21
4.3.2	Save a session as a zip file	4-23
4.3.3	Print function with respect to parameter viewing window	4-24
4.3.4	Session properties dialog box	4-25
4.3.5	Path of report shown in location text box in Netscape.	4-25
4.3.6	Paste a graphic into a document using Microsoft®Word® or Corel®WordPerfect®	4-26
4.3.7	Adjust size of window in Paintbrush	4-26
4.3.8	View Reports window	4-27
4.3.9	View data table window	4-28
4.3.10	Dose distribution	4-30
4.3.11	Time distribution	4-30
4.3.12	Dose history	4-31
4.3.13	Selecting a custom report to edit or delete	4-31
4.3.14	Report template editor	4-32
4.3.15	Data Influence Evaluation window	4-33
4.3.16	Three parts of the sensitivity analysis window	4-35
4.3.17	Histogram of parameter selected for sensitivity analysis	4-35
4.3.18	Iconizing main session window	4-38

LIST OF TABLES

4.2.1 Excerpt from Chain Data Table, contaminant 225Ac 4-10

ACRONYMS

ALI	Annual limit on intake
ALARA	As low as reasonably achievable
AMCG	Average member of the critical group
BWR	Boilingwater reactors
CCDF	Complementary cumulative distribution function
CEDE	Committed effective dose equivalent
CFR	Code of Federal Regulations
CI	Confidence Interval
DAC	Derived air concentration
DandD	Decontamination and decommissioning (software)
DCF	Dose conversion factor
DLL	Dynamically-linked library
EPA	Environmental Protection Agency (U.S.)
FGR	Federal guidance report
FRC	Federal Radiation Council
GUI	Graphical user interface
HTML	Hypertext markup language
ICRP	International Commission on Radiological Protection
K-S	Komolgorov-Smirnov (statistical test)
LHS	Latin Hypercube Sampling
MDAC	Microsoft Data Access Components
mrem/y	millirem/year
MS	Microsoft [®] Corporation
NRC	Nuclear Regulatory Commission (U.S.)
ORNL	Oak Ridge National Laboratory
P.O.	Performance objective
PDF	Probability distribution function
PNL	Pacific Northwest Laboratories
PWR	Pressurized water reactors
R&D	Research and development
SNL	Sandia National Laboratories
SRP	Standard Review Plan
TEDE	Total effective dose equivalent
UOM	Units of measurement
USBR	U.S. Bureau of Reclamation
USDA	U.S. Department of Agriculture

FOREWORD

This technical contractor report, NUREC/CR-5512, Volume 2, was prepared by Sandia National Laboratories under their DOE Interagency Work Order (JCN W6804) with the Radiation Protection, Environmental Risk and Waste Management Branch, Division of Risk Analysis and Applications, Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission. The report is a user's manual for version 2 of the DandD software, which implements the modeling methodology described in Volume 1 of NUREG/CR-5512 "Residual Radioactive Contamination From Decommissioning: Technical Basis for Translating Contamination Levels to Annual Total Effective Dose Equivalent" issued October 1992.

The purpose of the DandD software is to provide a simple screening approach for demonstrating compliance with 10 CFR 20, Subpart E. Version 2 of the software described in this report supercedes the earlier version described in the draft of this volume. Volume 2 of the software supports both a simple screening using generic scenarios and default parameter values or default probabilistic parameter distributions, as well as allowing input of site-specific parameters and modification of scenarios by changing or eliminating pathways. This software may be used to demonstrate compliance with the dose criterion in 10 CFR 20, Subpart E, as described in NUREG-1727 "NMSS Decommissioning Standard Review Plan" issued in September 2000.

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1 INTRODUCTION

1.1 Background

The Nuclear Regulatory Commission (NRC) is responsible for evaluating requests from facility owner/operators for the partial or total termination of NRC operating licenses for their facilities. This evaluation is based on radiological criteria defined in 10 CFR Part 20 Subpart E (NRC, 1998a). These criteria establish limits on the annual total effective dose equivalent (TEDE) received during the year to the average member of the critical group (AMCG). The critical group is "the group of individuals reasonably expected to receive the greatest exposure to residual radioactivity for any applicable set of circumstances" (10 CFR 20.1003).

NRC recognized that licensees who must decontaminate lands and structures would require assistance and guidance in determining the extent of decommissioning required to allow unrestricted release of their property. In making such a determination, the NRC must first ensure that public health, safety, and the environment are protected by determining that the total dose to an individual in the public from licensed operations is less than the public dose limit of 100 mrem/y. However, the NRC has set the goal for public doses attributable to residual contamination after decommissioning at a fraction (25 mrem/y) of the public dose limit (for the case of unrestricted release). The estimate of dose reduction is accomplished by first judging the potential future uses of the lands and structures as described by NRC-defined scenarios and exposure pathways, and then evaluating levels of radioactivity through modeling equations to arrive at a reasonable expectation of dose. The modeling and scenarios involved in this determination can become extremely complicated depending upon the level of detail and complexity required. Therefore, a methodology and associated analytical tools were developed in support of license termination.

1.1.1 Origin of Deterministic Methods for Decommissioning

In 1987, Pacific Northwest Laboratories (PNL) began developing the NUREG/CR-5512 methodology to translate residual radioactive contamination levels at sites licensed by the NRC into potential radiation doses to the public. Volume 1 documenting the methodology was issued in 1992 (Kennedy and Strenge, 1992).

During 1993, Sandia National Laboratories (SNL) calculated dose conversion factors (DCFs) using the NUREG/CR-5512 methodology to support the NRC's draft regulatory guidance in NUREG-1500 (Daily et al., 1994) and the draft generic environmental impact study on radiological criteria for decommissioning, NUREG-1496 (NRC, 1994). SNL developed and used four stand-alone Fortran computer codes to perform those calculations for the four exposure scenarios defined in Volume 1. These codes were not designed for external release or use.

In 1994, SNL began developing the Decontamination and Decommissioning (DandD) Version 1.0 code, a user-friendly software product that implements the NUREG/CR-5512 methodology. DandD Version 1.0 integrates the Fortran scenario modeling codes with a graphical user interface designed to run under Microsoft® Windows® with a minimal hardware configuration. DandD Version 1.0 is a deterministic code using default scenarios, exposure pathways, and constant parameter values. Version 1.0 of DandD was released in July 1998 and the user's manual for the program was published in draft as Volume 2 of the NUREG/CR-5512 series (Wernig et al., 1999).

DandD assists NRC licensees who have requested termination of their license and who, in some cases, must decontaminate lands and structures as part of the decommissioning process. The software does this by providing a tool that allows licensees to translate residual radioactive contamination levels at their site to TEDE values by analyzing and modeling the set of NRC-prescribed scenarios of future land use. DandD contains models of the transport and exposure pathways associated with each of the scenarios, and default values for most parameters. The software only requires information on source concentration from the user. Within strictly defined limits, the user may supply site-specific parameter values if available and defensible. The user may also modify or eliminate exposure pathways.

1.1.2 Nuclear Regulatory Commission Decommissioning Guidance

In support of the July 1998 release of the final rule on Radiological Criteria for License Termination (NRC, 1998a) as 10 CFR Part 20 Subpart E, NRC was required to draft and publish implementing guidance to interpret rule provisions and evaluate actions licensees would need to take to comply with license termination

processes. In March 1998, NRC staff completed development of Draft NUREG-1549, "Decision Methods for Dose Assessment to Comply with Radiological Criteria for License Termination" (NRC, 1998b). NUREG-1549 was intended to provide an overall framework for dose assessment and decision-making at sites undergoing decommissioning. In July 1998, the Commission approved publication of draft guidance DG-4006 for the License Termination Rule (NRC, 1998c) for a two-year interim use period and instructed the NRC staff to maintain a dialogue with the public through the use of a web site and public workshops. The Commission also directed the NRC staff to develop a Standard Review Plan (SRP) that incorporates the risk-informed iterative approach in NUREG-1549. (The NMSS Decommissioning Standard Review Plan (NUREG/SR-1727) is accessible through: <http://www.nrc.gov/NRC/NUREGS/SR1727/index.htm> 1.) The goal of the SRP is to enable NRC staff to evaluate information submitted by licensees in a timely, efficient, consistent manner and in such a way that the public health and safety is protected and the facility can be released in accordance with NRC's requirements.

1.1.3 Evolution of Probabilistic Evaluations

DandD Version 1.0 includes constant default parameter values and thus only allows deterministic analyses. However, all dose assessments are uncertain due to uncertainty about the processes and parameters that control exposure. The range of possible dose values given this uncertainty must be considered in order to support decisions based on dose. A tendency for a screening calculation to produce a dose value in the upper end of the range of possible doses allows that calculation to be used in decision making. The scenarios, models, and parameter values defined in Volume 1 (and embodied in DandD Version 1.0) were intended to have this tendency, but the supporting arguments were qualitative. NRC directed SNL to develop probability distribution functions (PDFs) for parameters, based on the information in Volume 1 and on any newer published studies, and to identify default values for those parameters suitable for screening calculations. Volume 3 of NUREG/CR-5512 provided the parameter analysis (Beyeler et al., 1999).

In March 1999, NRC directed SNL to develop an improved version of DandD based on the parameter analysis that would allow formalized treatment of parameter uncertainty through implementation of probabilistic features and that would provide an improved, updated graphical user interface. Section

1.2 discusses the capabilities embodied in the Monte Carlo Version 2.1 of the DandD code.

1.1.4 Decision Framework for License Termination

NRC guidance in support of the license termination rule provides a useful context for licensees using the DandD code for dose assessments related to decommissioning decisions. NUREG-1549 documents use of a decision framework to implement a phased approach in conducting dose assessments. The decision framework can be used throughout the decommissioning and license termination process for more simple sites to the most complex or contaminated sites. The framework allows iterative (phased) development and treatment of the uncertainties associated with regulatory decisions. As such, a licensee can begin with existing (and often very limited) knowledge about the site, conduct screening assessments, update the state of knowledge with site-specific information (thus reducing uncertainty), and refine the screening assessments, if necessary. By following this approach, the licensee is able to optimize resources and decisions related to site characterization, remediation, and potential land-use restrictions.

The decision framework methodology is based on the premise that screening dose assessments are performed with little site-specific information. An initial analysis using DandD Version 2.1 and default DandD Version 2.1 parameter distributions, along with a simple representation of contamination at the site, will produce generic dose assessments that are unlikely to be exceeded. The scenarios and models in DandD Version 2.1 were defined to be "reasonably conservative" so that they would not be "bounding" or unrealistic, while still generally overestimating (rather than underestimating) potential dose. The physical parameter distributions were defined to represent real conditions and expected variability across the United States. Behavioral and metabolic parameters were defined to represent the average individual within the defined screening group (or generic critical group).

Beginning with the simple screening assessments, the methodology ensures that as more site-specific information is incorporated, the uncertainty is reduced (state of knowledge is increased), and the estimate of the resulting dose generally decreases. DandD Version 2.1 can be used to incorporate new knowledge based on site characterization that may lead to eliminating certain exposure pathways or reducing parameter uncertainty. DandD used in the context of the decision framework provides assurance that obtaining additional site-specific information is worthwhile because it is

probable that a more “realistic” dose assessment will not result in a dose higher than that estimated using a simple screening analysis.

Steps in the Decision Framework

NUREG-1549 provides a summary of the decision framework and methodology for conducting dose assessments in support of license termination decisions. It also provides three separate discussions to illustrate the phased and iterative nature of assessments as increasing complexity occurs. The following provides a summary of the decision framework steps that provide the overall context for use of the DandD software within the NRC license termination decision process. Refer to Figure 1.1 (taken from NUREG-1549) while reviewing the following steps of the framework.

- Step 1: The first step in a dose assessment involves gathering and evaluating existing data and information about the site, including the nature and extent of contamination at the site. Often, minimal information is all that is needed for initial screening analyses (e.g., a simple representation of the source of contamination). However, licensees should use all information about the site that is readily available. This step also defines the performance objectives that must be met in order to demonstrate compliance with decommissioning criteria.
- Step 2: This step involves defining the scenarios and pathways that are important and relevant for the site dose assessment.
- DandD contains two generic exposure scenarios: residential and building occupancy.
- Step 3: Once scenarios are defined and exposure pathways identified, a basic conceptual understanding of the system is developed, often based on simplifying assumptions regarding the nature and behavior of the natural systems. System conceptualization includes conceptual and mathematical model

development and assessment of parameter uncertainty. DandD includes predefined conceptual models for the scenarios along with default parameter distributions (based on Kennedy and Streng, 1992 and Beyeler et al., 1999).

- Step 4: This step involves the dose assessment or consequence analysis, based on the defined scenario(s), exposure pathways, models, and parameter distributions. For generic screening, the licensee can accept and use the generic models and default parameter PDFs simply by running DandD with the appropriate site-specific source term, leaving all other information in the software unchanged. Site-specific assessments allow the user to change pathways and parameter distributions based on data and information obtained from the site. DandD provides various plots and reports of the dose distribution based on Monte Carlo sampling of the input distributions.
- Step 5: This is the first major decision point in the license termination decision process and involves answering the question of whether the dose assessment results from Step 4 demonstrate compliance with the dose criterion in 10 CFR Part 20, Subpart E (for unrestricted release, this is 25 mrem/y). NRC establishes the confidence required when interpreting the results from the probabilistic dose assessment. For instance, licensees may need to demonstrate that the 90th percentile value of dose is less than 25 mrem/y. If the results are below the limit, the licensee proceeds with Steps 6 and 7 to demonstrate As Low As Reasonably Achievable (ALARA) requirements and initiate the license termination process defined by NRC in other guidance documents. Note that DandD does not involve or automate these steps.

If the results exceed the performance objective, the user should proceed to Steps 8 and 9.

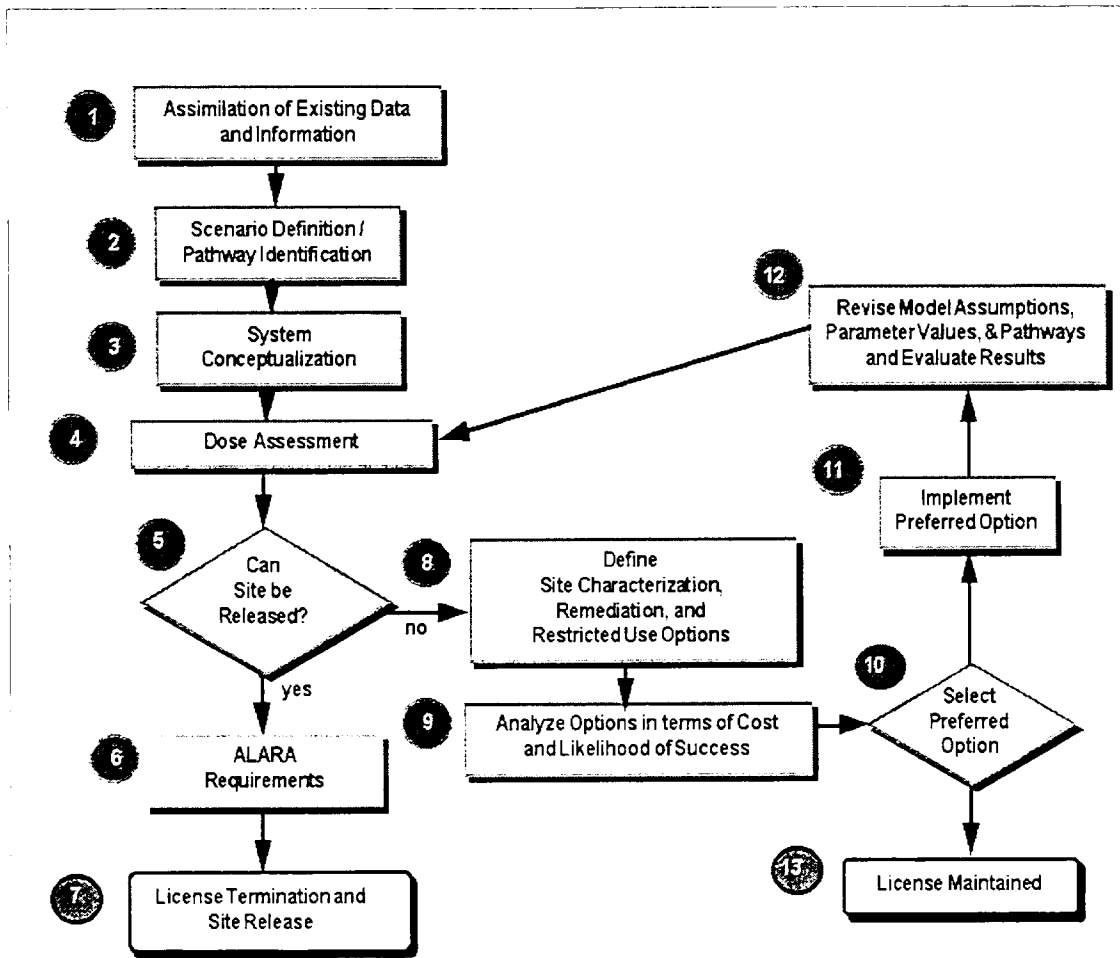


Figure 1.1 Decommissioning and license termination framework

Step 6: If the result in Step 5 is that the calculated dose is less than 25 mrem/y, the Licensee can proceed to satisfy NRC requirements to demonstrate dose is As Low As Reasonably Achievable (ALARA) (see NRC, 1998c).

Step 7: Following ALARA determination, Licensees would proceed with license termination procedures as outlined in applicable NRC guidance documents.

Step 8: Full application of the decision framework involves defining all possible options the licensee might address in order to defend a final set of actions needed to demonstrate compliance with license termination criteria. Options may include acquiring more data and information about the site and source(s) of contamination in order to reduce uncertainty about the pathways, models, and parameters

and thus reduce the calculated dose; reducing actual contamination through remediation actions; reducing exposure to radionuclides through implementation of land-use restrictions; or some combination of these options.

DandD provides a sensitivity analysis module to identify sensitive parameters (e.g., those having the greatest impact on dose assessment results) and to explore potential reductions in the uncertainty associated with those parameters. Note that one option may include elimination of exposure pathways due to site-specific considerations.

Step 9: All of the options identified in Step 8 are analyzed and compared in order to optimize election of a preferred set of options. This options analysis may consider cost of implementation, likelihood of success (and the

expected costs associated with success or failure to achieve the desired results when the option is implemented), timing considerations and constraints, and potentially other quantitative and/or qualitative selection criteria. At this time, the DandD software is limited to evaluating the potential impact on the dose results through selective truncation of the uncertainty bounds of the input parameters.

Step 10: The activities in Steps 8 and 9 provide information for the licensee to choose the preferred options based on considerations of cost, likelihood of success, timeliness, and other considerations. Based on the results of the DandD sensitivity analysis, for example, a licensee may identify one or more parameters that may be modified based on acquisition of site-specific information and data. If new data could reduce the uncertainty associated with sensitive parameters, the licensee may be able to defend a new calculated dose that meets the license termination criteria.

Step 11: Under Step 11, the preferred option is implemented. The licensee commits resources to obtain the information necessary to support revisions to the parameters identified in Steps 8 and 9.

Step 12: Once data are successfully obtained, the affected parameters for the predefined models are revised, as appropriate. Also, data may support eliminating one or more of the exposure pathways in the predefined scenarios. DandD provides for very simple and straightforward modification of the pathways and parameters of interest. The software also includes in the Help menu full documentation of the original basis for the parameter distributions, references, and sources of information the licensee might use in order to defend modifications based on their site-specific data and circumstances.

Once the pathways and parameters are revised, the licensee would revisit Steps 4 and 5 to determine the impact of the revisions on demonstrating compliance with the performance objectives. If met, the licensee proceeds to Steps 6 and 7. If the performance objective is still exceeded, the licensee returns to Steps 8 and 9 to analyze remaining options.

Step 13: If no viable options exist at this time, the

licensee may decide to defer actions at this site until circumstances allow revisiting license termination actions.

1.2 DandD Version 2.1 Overview

DandD Version 2.1 updates, improves, and significantly enhances the capabilities of Version 1.0. As such, this final Volume 2 of the NUREG/CR-5512 series documents the User's Manual for DandD Version 2.1, superceding and replacing the original draft of Volume 2 (Wernig et al., 1999) that documented DandD 1.0. In particular, Version 2.1 allows full probabilistic treatment of dose assessments, whereas Version 1.0 only allowed deterministic analyses. DandD Version 2.1 implements the methodology and information contained in NUREG/CR-5512, Volume 1, the methodology modifications described in Wernig et al. (reproduced as Appendix A), as well as the parameter analysis in Volume 3 that established the PDFs for all of the parameters associated with the scenarios, exposure pathways, and models embodied in DandD.

1.2.1 Summary of Requirements for Version 2.1

The most prominent new feature of DandD Version 2.1 is the incorporation of a Monte-Carlo simulation capability, a significant enhancement to the deterministic approach embodied in Version 1.0. This new capability was designed to be simple to use, while allowing more knowledgeable users to take full advantage of the Monte Carlo capability.

The completed system allows the user to perform an initial default screening analysis using the default parameter distributions defined in the parameter analysis. As with the existing deterministic code, only a source-term estimate is required for this calculation. The result of the Monte Carlo calculation is summarized by the dose at a default selected quantile value, which the user may compare against the 25 mrem/year standard to assess compliance. An original requirement was that this default operation should have a similar look and feel to that in Version 1.0.

Requirements for additional capabilities included:

- The user should be able to view the complete dose distribution functions, as well as the distribution functions for the time of peak dose and for the individual pathway doses.

- The user should be able to view the default distribution functions for each of the input parameters and to access the portions of Volume 3 documenting the basis for each default distribution.
- The user should be able to specify new distribution functions (or deterministic values) for each parameter based on site conditions and to record the justification for these distributions or values.
- The user should be able to request a ranking of parameters based on the sensitivity of dose to the parameter value.
- The user should be able to access pertinent information about the decision methodology for guidance on options for achieving compliance.

1.2.2 Features of DandD Version 2.1

Two scenarios are implemented in DandD: building occupancy and residential. The building occupancy scenario relates surface contamination levels in existing buildings to estimates of the TEDE received during a year of exposure with the conditions defined in the scenario for unrestricted commercial or light industrial use. The exposure pathways for this scenario include external exposure, inhalation exposure, and secondary ingestion.

The more complex residential scenario is meant to address sites with contamination in soils. The residential scenario considers more exposure pathways, including external exposure, inhalation, and the following ingestion pathways: drinking water, food grown from irrigation water, land-based food, soil, and fish. The types of land-based food considered are leafy vegetables, other root vegetables, fruit, grain, beef, poultry, milk, and eggs. Three types of animal feeds are considered: forage, stored grain, and stored hay.

A generic water-use model was developed to permit evaluation of the annual TEDE from drinking water from wells and from multiple pathways associated with irrigation water. This simple water-use model accounts

for radionuclide decay, progeny ingrowth, and environmental transport. The three boxes (or layers) in the water-use model are the surface soil, unsaturated soil, and the aquifer. Appendix A describes a modification to the three-box water-use model that allows up to 50 boxes in the unsaturated zone. The generic treatment of potentially complex groundwater systems provides a conservative analysis that may only suggest when additional site data and more sophisticated modeling are warranted.

The default input parameter distributions for each scenario and exposure pathway are consistent with conducting screening dose assessments, and represent large uncertainty about site conditions. To accommodate site-specific conditions the DandD software allows a simple, straightforward approach to modify scenario selection, exposure pathways, source, and many of the modeling parameters.

Figure 1.2 shows the overall information flow that takes place in the DandD code and the major processes that are involved. A Microsoft® Access® database is the repository for all of the information used by the system. It contains initial default values for all parameters, current parameter settings, sampled parameter values generated by the Latin Hypercube Sampling (LHS) code (Iman and Shortencarier, 1984), dose model results, and report templates.

- The graphical user interface (GUI) controls the overall information flow, at the user's direction, and invokes the supporting components to generate parameter samples and run the dose model. An important design goal for this interface was to quickly step through a default analysis, while allowing any aspect of the calculation to be adjusted to site-specific conditions, if required.
- The LHS pre/post processor builds the input file for the LHS program based on the current parameter distributions in the database, invokes LHS to generate the samples, and processes the LHS output file. The resulting parameter values are stored in the database and are checked against any limits that have been defined.

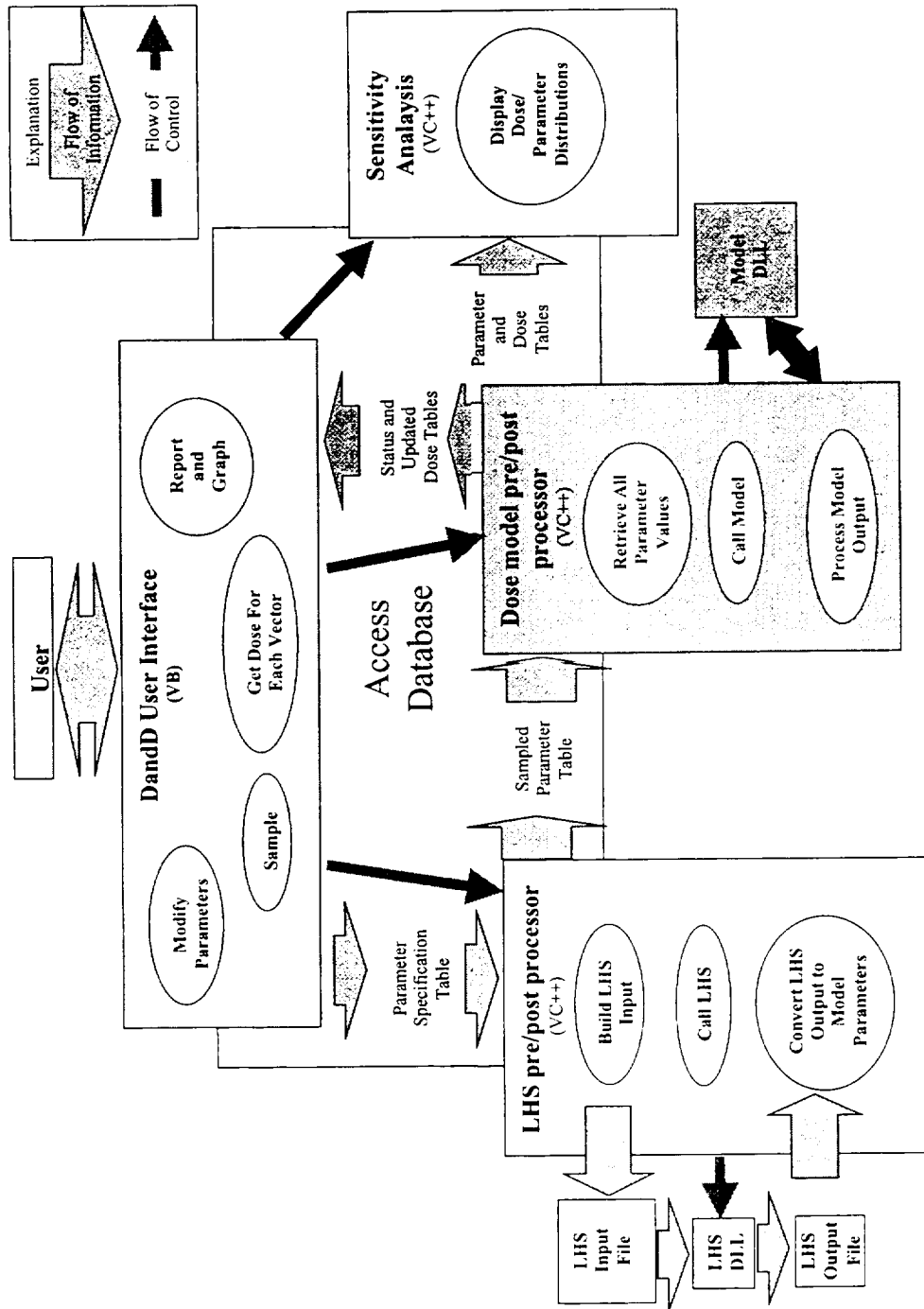


Figure 1.2 Information flow in DandD Version 2.1

- The LHS program performs the parameter sampling. The system uses the official version of LHS, which is maintained by SNL for general distribution.
- The dose model pre/post processor retrieves the simulation options and parameter values for a specified simulation (sample vector) from the database and invokes the appropriate scenario model to calculate dose. The resulting dose values are appended to output tables in the database.
- The dose model dynamically-linked libraries (DLLs) perform the dose calculations. For each realization in a simulation, an annual TEDE is calculated for every year in the exposure period.
- The peak TEDE over the exposure period is then identified from the set of annual TEDEs. This will yield a set of peak TEDE values, one for each realization. From this set, statistics such as percentiles may be determined, along with associated confidence intervals.
- Finally, DandD Version 2.1 includes a sensitivity analysis module that assists licensees and NRC users to identify those parameters in the screening analysis that have the greatest impact on the results of the dose assessment. Armed with this information and the guidance available in NUREG-1549, licensees are able to make informed decisions regarding allocation of resources needed to gather site-specific information. When cost and likelihood of success associated with acquisition of this new knowledge are considered, licensees are better able to optimize the decisions to acquire site data that allow more realistic dose assessments that, in turn, may lead to demonstrated and defensible compliance with the dose criteria for license termination.
- Version 2.1 provides direct capability to select or exclude exposure pathways.
- Limits on the area of contamination can be specified in Version 2.1 and are appropriately reflected in the calculated dose values.
- The Help features have been significantly updated to incorporate information pertinent to probabilistic analysis. NRC references and guidance (including NUREG-1549), and the new features presented in the GUI.
- Extensive parameter help has been added based on the NUREG/CR-5512, Volume 3 parameter analysis. This information has been integrated as HTML documents to facilitate maintenance.
- Version 2.1 elicits and tracks user justification for any modifications to pathways, parameters, or parameter correlations.
- Following execution of the models and depending on the results, Version 2.1 provides guidance for increasing sample size to reduce sampling error.
- A parameter sensitivity analysis capability was added.
- The output reports and plots have been improved consistent with the reporting and display requirements of a probabilistic dose assessment.
- Standard file management features have been incorporated.
- Version 2.1 provides window printing capabilities throughout the GUI to allow screen capture documentation of important aspects of an analysis.
- Version 2.1 can save a compressed version of the session for submittal to NRC.

1.2.3 Comparison to Version 1.0

DandD Version 2.1 provides many useful improvements on Version 1.0 of DandD:

- The GUI was significantly enhanced and upgraded to both incorporate the added features of Version 2.1 as well as to use standard Microsoft® Windows® features and conventions.
- Version 2.1 performs probabilistic dose assessments while maintaining ease of use; Version 1.0 only allowed deterministic analyses.

- The application has been redesigned to facilitate separate maintenance of the interface, the initial session file containing default settings, the parameter documentation, and the dose models.

1.3 User Manual Overview

Section 2 summarizes system requirements to install and successfully operate DandD Version 2.1. Installation instructions are provided to install the software from CD-ROM, Web, or FTP location and includes troubleshooting notes. The installation

package includes all necessary installation notes in online documentation.

Section 3 introduces the user to the basic capabilities of DandD Version 2.1 and its documentation. All of the online documentation and selections in the DandD program group found from the Microsoft® Windows® Start menu are summarized. Finally, this section provides a quick tour of DandD and the sensitivity analysis module using example problems.

Section 4 is the heart of the User's Manual. This reference guide provides comprehensive descriptions of all features incorporated in the Version 2.1 user interface. Common interface features and operations are summarized first (Section 4.1), followed by summaries of all the features and controls on the main session window. This latter set of instructions in Section 4.2 provides the procedure users will generally follow to

execute DandD. Section 4.3 describes each of the menu options, ranging from file menu operations, to viewing reports and plots, to utilizing the advanced features including the sensitivity analysis module.

Finally, Section 5 provides responses to a set of frequently asked questions based, in part, on past NRC training and workshop experience and on questions users may have with the new features of DandD Version 2.1.

A set of Appendices supplements the discussions provided in the main body of the User's Manual, including the presentation of additional sample problems and technical background information on data tables underlying the DandD software. The design of the DandD database file is explained, and the requirements for specifying and setting up import concentration files are summarized.

2 INSTALLATION OF DandD

2.1 System Requirements

The DandD software requires the following

- a personal computer with Microsoft® Windows® 95/98 or NT 4.0 installed;
- a VGA monitor (recommended desktop set to minimum of 800 × 600 pixels);
- a mouse or other pointing device;
- 40 MB of free disk space;
- a printer to use the print functions included with DandD;
- a floppy drive, network, or Internet connection to submit session files for review;
- a frame-enabled browser such as Internet Explorer or Netscape Navigator to allow access to the DandD reports and an online version of NUREG/CR-5512, Volume 3.

2.2 Installing from CD-ROM

To install DandD, run Setup.exe as follows:

- Click on the Microsoft® Windows® Start button and select the Run command.
- Click on the Browse button, and locate Setup.exe on the installation CD.
- Click Open.
- Click OK in the Run dialog box.

The DandD installation procedure should now execute.

On certain installations, DCOM95 and MDAC (Microsoft® Data Access Components) will automatically install before DandD installs. Some system files will be updated. This is necessary for the correct installation of DandD. This is a Microsoft® update related to the feature that DandD session files are

stored as database files. This procedure has been automatically built in the DandD installation process. This update should not affect the Microsoft® Windows® desktop or other applications that are installed.

2.3 Installing by Downloading from the Internet

Users may access the DandD code for installation at the NRC site: <http://www.nrc.gov/RES/rescodes.htm>. Scroll down to the "Radionuclide Transport and Decommissioning Codes" section. Select "Click here to Download" to access the setup.exe file. Also, select "Click here for Installation and Setup of DandD on your Computer" for additional installation instructions.

Proceed to run the file Setup.exe as described in Section 2.2.

2.4 Troubleshooting Installation Problems

When installation is completed, the user can access the files 'Read Me,' 'Getting Started with DandD,' and 'Introduction to DandD' from the DandD program group off the Microsoft® Windows® Start menu under the Programs group.

If difficulty is experienced installing DCOM95 or MDAC, users should contact their system administrator for assistance. Users may also contact NRC technical support at DandD@nrc.gov with questions regarding installation and use of DandD.

2.5 Uninstalling DandD

Select 'Uninstall DandD' from the DandD program group off the Microsoft® Windows® Start menu under the Programs group. When executed, the DandD files will be removed from the user's system. However, existing session files in the DandD_Docs directory will not be removed. There is no uninstall for DCOM95 or MDAC. Microsoft® considers these to be system upgrades and does not offer an uninstall procedure.

3 WELCOME TO MONTE CARLO DandD

3.1 The DandD Group

The DandD installation will create a program group that can be accessed from the Microsoft® Windows® Start menu.

From the Start button, select Programs, then select DandD. The first menu level includes a subgroup called Documents. This subgroup contains the following:

- Getting Started with DandD - a document that describes the items in the DandD group and the database metaphor used to manage session files.
- Introduction to DandD - a summary of the DandD decision process, with three example problems. New users should step through these problems to become familiar with DandD features and the interface.
- NRC References - on-line browser-based reference materials on the DandD scenarios and general technical concepts. Users will need a browser such as Internet Explorer or Netscape installed to view this file.
- Readme - notes and information regarding the installation of DandD, including precautions.

Following the Documents entry are:

- DandD - An alternative to the desktop shortcut for launching the DandD application.
- DandD Help - This provides direct access to the Help topics in DandD without launching the software.
- Uninstall DandD - This menu option should be used to remove DandD from user's computers.

3.2 Run a Simple Screening Analysis

Note to users: Refer to Section 4.2 for detailed instructions and illustrations for conducting a dose assessment with the DandD code. Sections 4.1 and 4.3 provide additional guidance and illustrations for common and main menu operations, respectively. Finally, Appendix B provides a breadth of example problems for a wide

range of user facilities.

To start the application, either double-click the icon on the desktop or select DandD from the DandD group on the Microsoft® Windows® Start menu.

Press F1 at any time if help is needed for a window.

In the following example, a site with shallow-soil contamination seeks license termination. Preliminary survey data, site operational records, and leakage and spill events show localized contamination from Co-60, Sr-90, and Cs-137 in the soil. Measured contamination levels for each radionuclide averaged over the site area of interest are 3 pCi/g, 2 pCi/g, and 1.2 pCi/g, respectively.

None of the default parameter values are modified in this screening analysis.

Creating a Session File:

1. After opening DandD Version 2.1, select *File/New* and type in a unique file name: Simple Case 1, and click it *Open*.
2. In the *Site Name* field of Session Properties, enter: Site X - Analysis of Co-60, Sr-90, and Cs-137.
3. In the *Analysis Description* field, enter: General Contamination of Soils - Analyzed Today! as shown in Figure 3.1. Click *OK*.
4. Note the *Site Name* in the title bar of the main window and the file name at the bottom of the window. This information can also be reviewed by selecting *File/Properties*. This information will be copied to the summary reports.

Defining Site Contamination (Source Term):

5. Select the tab for the Residential scenario, which applies to this case. For this initial screening assessment, leave all pathways operative (checked). Click the *Edit Exposure Pathway* button to view default pathway settings as shown in Figure 3.2. Click on *Cancel* to return to the main screen.

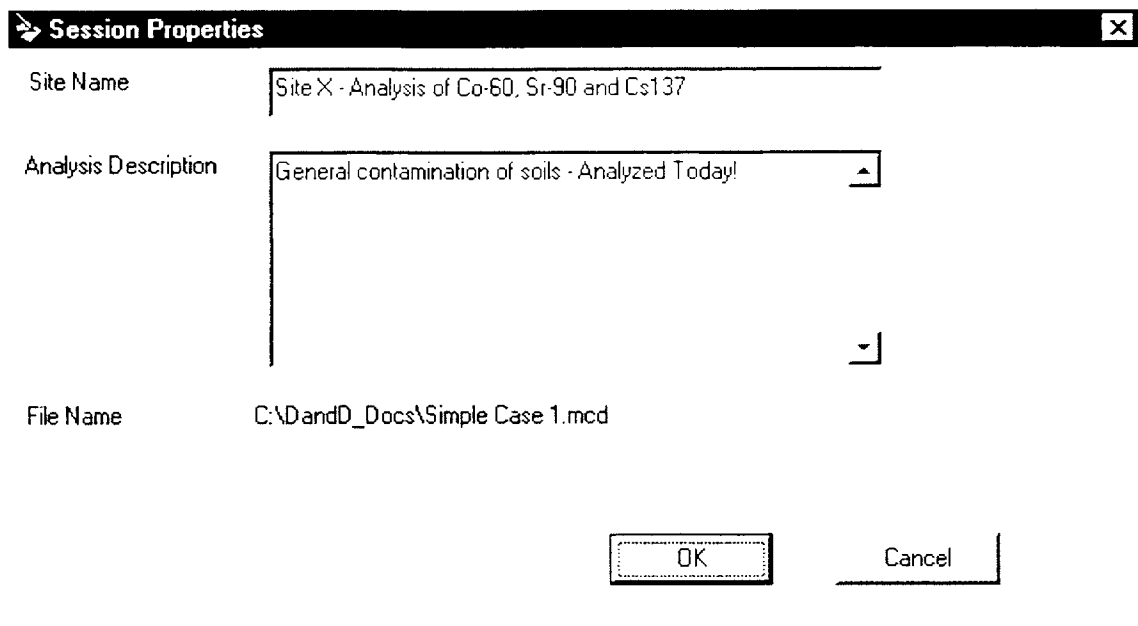


Figure 3.1 Creating a session file

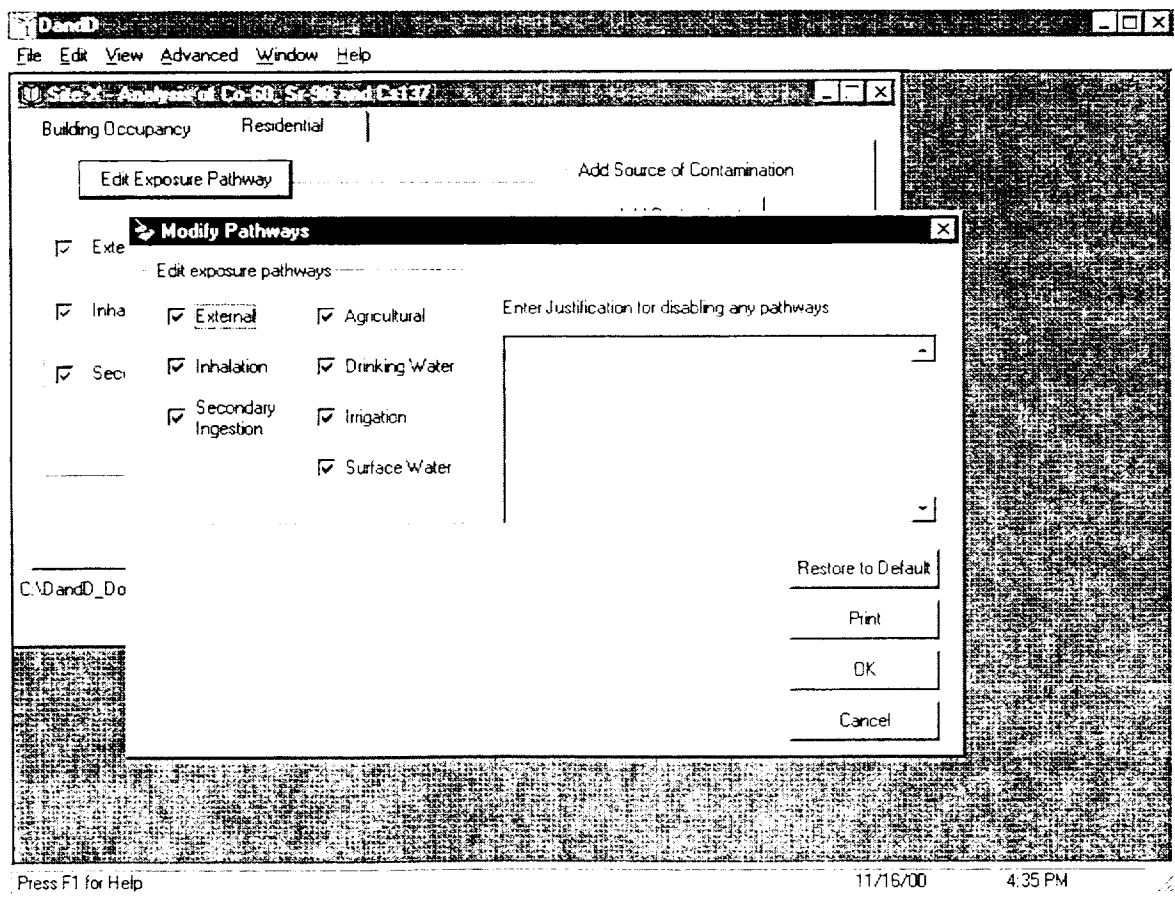


Figure 3.2 Residential default pathway settings

6. In the *Add Source of Contamination* Panel, click on *Add Contaminants*.
7. In the *Potential Contaminants* list (Figure 3.3), scroll down, select ^{60}Co , and click on the right arrow or double-click on the radionuclide to add this nuclide to the *Site Contaminants* list.
8. Repeat #7 to add ^{90}Sr and ^{137}Cs to the list of contaminants at the site as shown in Figure 3.3.
9. Do not change the output or calculation options; click *OK*.
10. Click *Add Concentrations* button and note that Co-60 is selected by the dark arrow head to the left of Co-60, but no value has been added.
11. Click *Modify Value*. For Co-60, do not change the *Distribution* or *Units of Measure* (ensure units are pCi/g). In the *Value* field, enter 3 (Figure 3.4).
12. To justify this value, enter "Site survey data" in the justification field as shown in Figure 3.4. Note that the justification field must be completed. Do not change the *Area of Contamination*. Click *OK*.
13. Select ^{90}Sr .
14. Click on *Modify Value*. Enter 2 in the *Value* field, and enter the justification "Site survey data." Click *OK*.
15. Select ^{137}Cs .
16. Click on *Modify Value*. Enter 1.2 in the *Value* field, and enter the justification "Site survey data." Click *OK*, then *Close*.
17. In this screening analysis, do not change any parameters.

Executing DandD:

18. To run this screening assessment, click on *Execute*.
19. Click on *Run Simulation*; progress can be viewed in the adjoining panel or aborted at any time.

20. When the simulation is completed, the 90th percentile of the peak TEDE distribution $4.89\text{E}+01$ mrem/year with a 95% confidence interval (CI) of $4.53\text{E}+01$ to $6.25\text{E}+01$ mrem/year, is displayed as shown in Figure 3.5.
21. If the result had fallen below the 25 mrem/y NRC dose standard, the licensee might have elected to proceed with the NRC license termination process. In this case, the licensee instead decides to explore options for reducing uncertainty regarding the site, potential remediation actions, and/or restricted release provisions.
22. Click on *Close*.

Viewing Results:

23. Before proceeding, more information is desired about the current analysis. Select *View* on the main menu bar, and click on *Reports*. In the *View Reports* window, select *Detail*, then select *Create Report* to view a brief report of the user input to this analysis (this may take a minute or two to generate in the browser). In the *Detail* report, take note of the various sections of the report, including the *Detailed Results* following the *Summary Results* near the end of the report.
24. Note that 90% of the simulated TEDE values are less than $4.89\text{E}+1$ mrem/y. Also note in the *Detailed Results* tables that the agricultural pathway for ^{90}Sr and the external pathway for Co-60 dominate the results. Close the browser window and click *Close*.
25. Select *View/Graphics/Dose Distribution* from the main menu bar. Clicking an item under both *Pathways* and *Radionuclides* will allow additions or deletions from the plot to depict those contributions to dose. Note that the agricultural pathway for ^{90}Sr and external pathway for Co-60 dominate the results. Click *Done* to close the *Dose Distribution* plot.

3.3 Run a Site-Specific Analysis

After running a simple screening analysis described in the previous section, the licensee discovers an error in the survey data and is able to justify reductions in the levels of contamination at the site. A re-analysis is performed based on this new information.

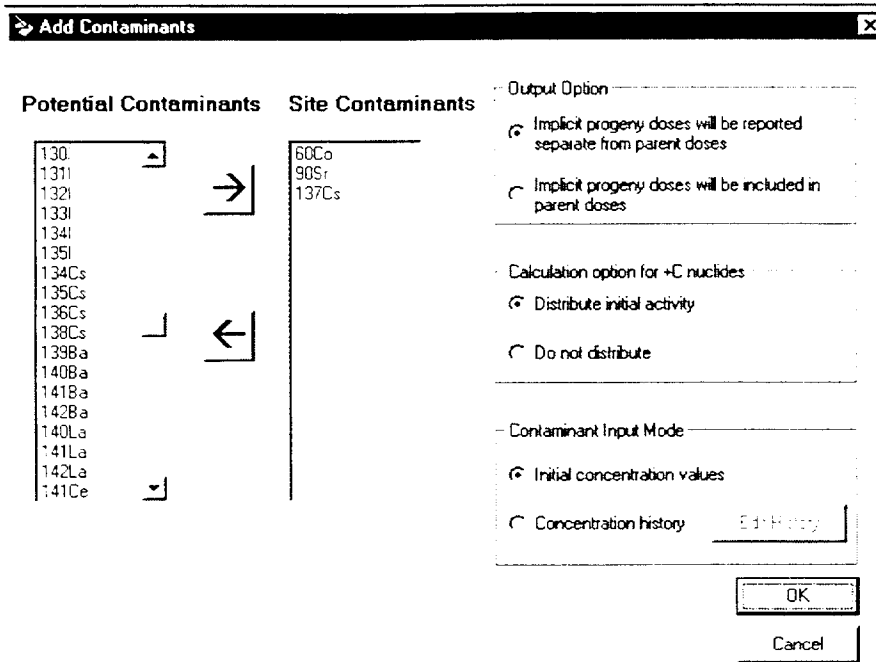


Figure 3.3 Three site contaminants present

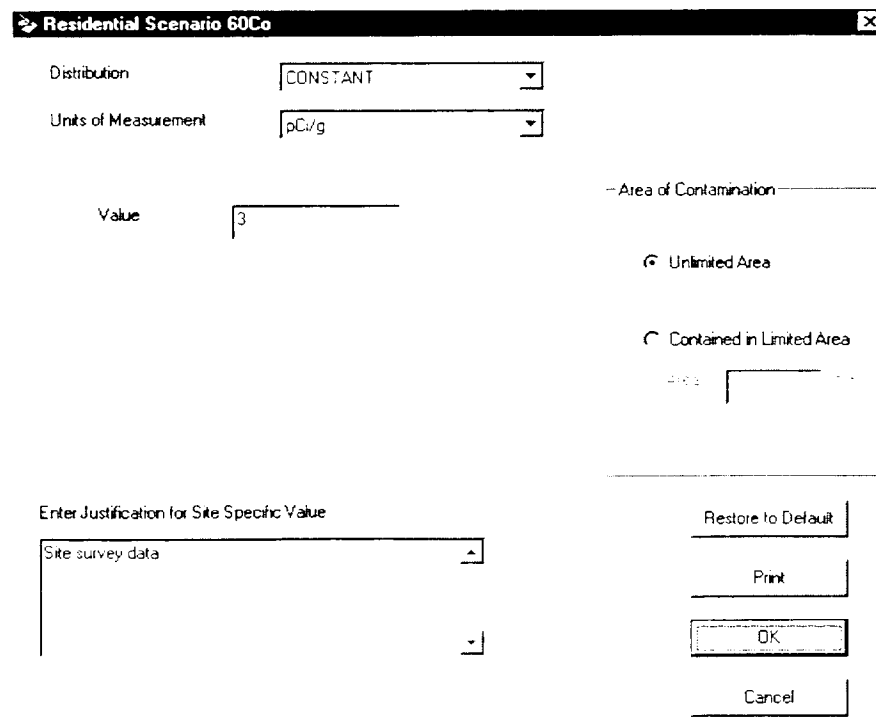


Figure 3.4 Adding concentration of Co60

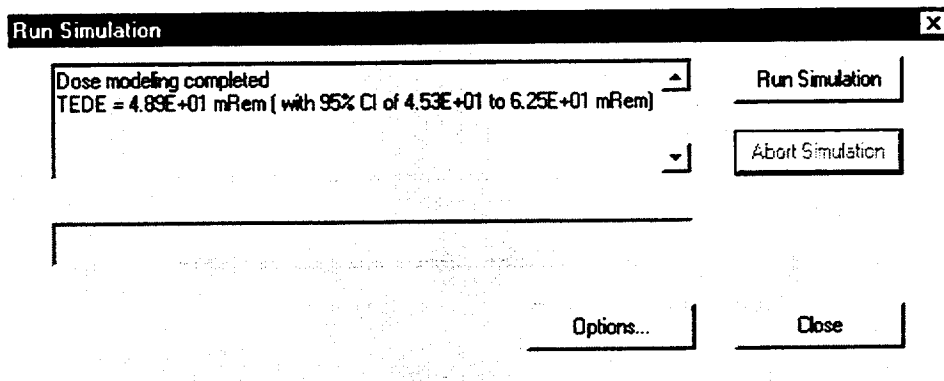


Figure 3.5 Result summary of Case1 analysis

Updating Source Term Information:

1. In the main window, save a new session for the reanalysis by selecting *File/Save As* and naming the new analysis Simple Case 2. Click the *Open* button. If desired, change the *Site Name* and/or *Analysis Description* under *File/Properties* and click the *OK* button.
2. In the main window under the Residential tab, leave all pathways selected for this iteration.
3. In the main window, click on *Add Concentrations*, verify that Co-60 is selected, and click on *Modify Value*. Enter a new constant value of 1. Change the *Area of Contamination* to *Limited Area* and enter 40 m². Supplement the justification text that this new information is based on new site survey data as shown in Figure 3.6. Click *OK*, and *OK* regarding deletion of the existing calculations.
4. Select Sr-90 and click *Modify Value*. Enter a new value of 1.5. Supplement the justification text that this new information is based on new site survey data. Change the *Area of Contamination* to *Limited Area* and enter 30 m². Click *OK*.
5. Select Cs-137 and click *Modify Value*. Do not change the value for contamination; change the *Area of Contamination* to *Limited Area* and enter 20 m². Supplement the justification text that this new information is based on new site survey data. Click *OK*.
6. Click on *Close* to return to the main screen. No other changes to the original settings are needed (contaminants, general, or element parameters).

Executing DandD:

7. Click on *Execute*, and click *Options* to ensure the *Save Dose History* checkbox is selected, then click *OK*. Click *Run Simulation* to reanalyze the dose models with the reduced contaminant data.
8. The displayed results (27.5 mrem/y)* are still above the 25 mrem/y dose standard. When the confidence interval includes the performance objective, the Sample Size Analysis window opens as shown in Figure 3.7. This information allows the user, if desired, to determine the effect of increased sample size on the ability to demonstrate compliance and to rerun the simulation with a larger number of simulations.

Viewing Results:

9. Click *Close* on the Sample Size Analysis and Run Simulation windows.
10. Select *View* on the main menu bar, click on *Reports*, and double-click on *Detail* to create and view the report for this analysis iteration.

*If the displayed results are slightly different, the user did not necessarily make an error. In some cases, the random sample values of the parameters depend on the order the user defined and modified the parameters. This will result in a slightly different value of the TEDE and 95% confidence interval bounds. The program results are still valid. This order dependence is a bug and may be fixed in a future version. When this bug is fixed, users may not get the results reported above.

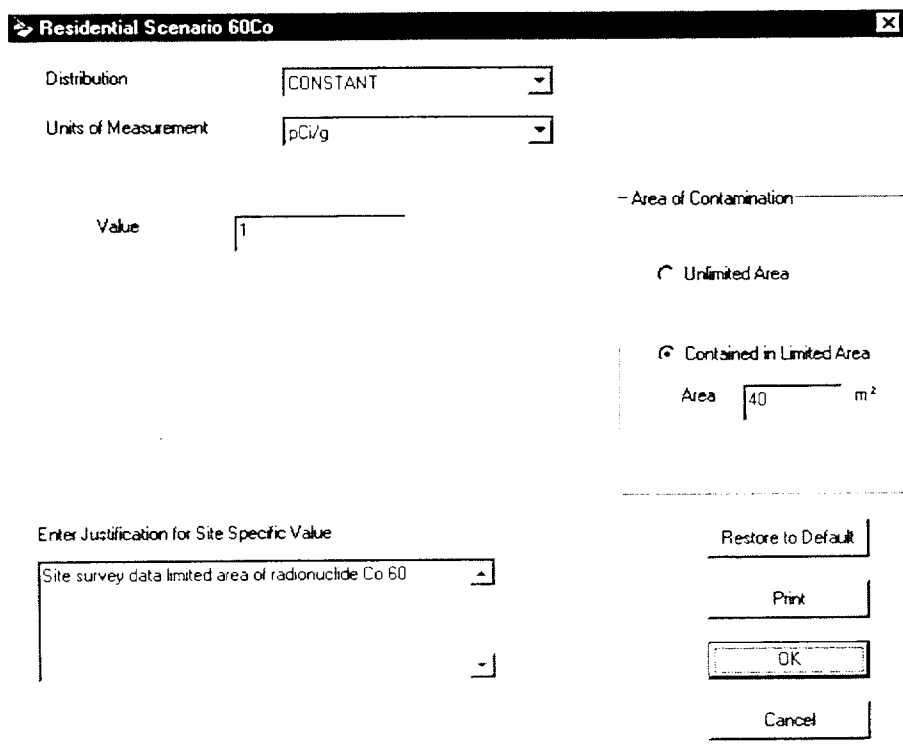


Figure 3.6 Limit area of contamination

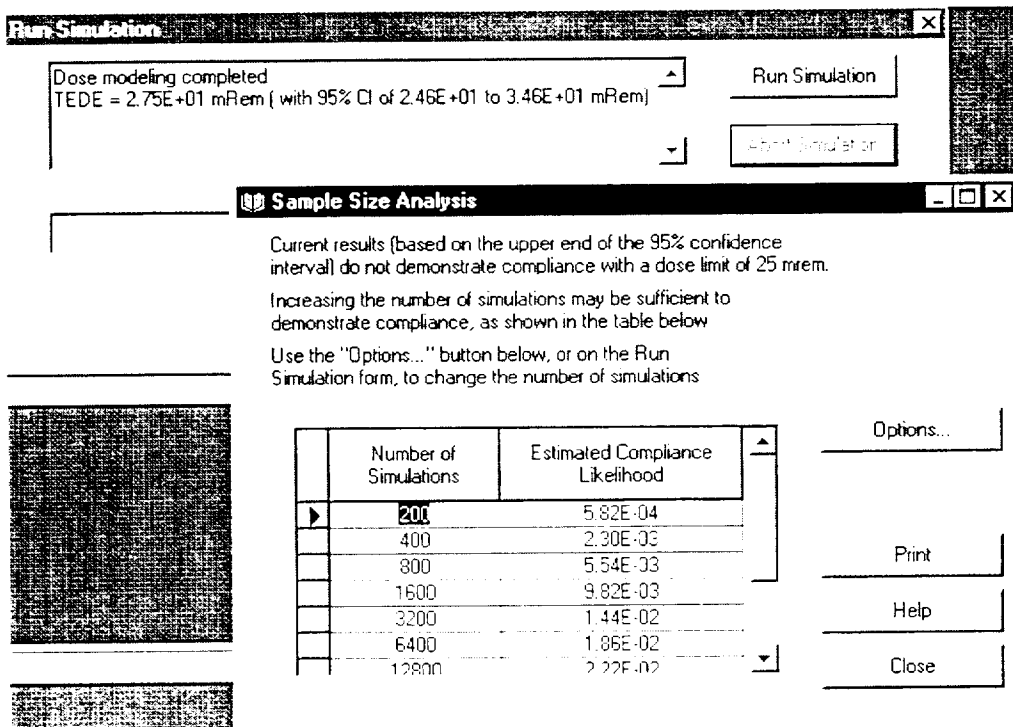


Figure 3.7 Sample Size Analysis window for Case1

11. Scrolling to the end of the report, note that 90% of the simulated TEDE values are less than 2.75 E+01 mrem/y. This result is above the 25 mrem/y standard. As such, the licensee elects to conduct an options identification and analysis process using the DandD sensitivity module. Also note in the detailed report that the external pathway for Co-60 and agricultural pathway for Sr-90 still dominate the results. Close the browser window and select Close to return to the main window.
12. Again, these contributions to dose can be verified: select *View/Graphics/Dose Distribution*. In the *Plot Scale* group of buttons, click *X Axis*, click the *Log* radio button, then click *OK* to change the x-axis to a log scale. Click *External* for *Co-60* and *Agricultural* with *Sr-90* to add those plots to the graph as shown in Figure 3.8. Click *Done* to close all graphs and reports.

Sensitivity Analysis:

DandD provides the capability to conduct sensitivity analysis to identify parameters that have the greatest impact on the dose distribution and those for which new information could impact on the compliance decision.

13. Select *Advanced/Sensitivity Analysis* from the menu bar. The Data Influence Evaluation window lists all uncertain parameters in this analysis and develops a preliminary list of the most sensitive parameters for analysis. The user is able to add or remove parameters from this list for further analysis. Note that the uncertain uptake rates for leafy plants, rooting plants, and fruit for Sr-90 are listed as the most sensitive parameters by the initial analysis.
14. Scroll down the *Available for Analysis* list, highlight CDO (average dust loading outdoors), and click on *Select Parameter for Analysis*. Repeat this process for AP (water application rate) and CDI (average dust loading indoors) to add these additional parameters to the lower list: *Selected for Analysis* as shown in Figure 3.9.
15. Click on the *Analyze* button; this launches a separate module that allows the user to investigate potential effects of parameter values from site-specific data. The overall objective in the greater context of the decision framework is to reduce the uncertainty associated with the parameter(s) via acquisition of supporting site data, update the

values for the parameter(s) based on defensible data, and rerun the analysis to determine the impact on the dose distribution. The sensitivity analysis package allows the user to manipulate the preliminary list of parameters by truncating their distributions to reflect either existing site knowledge or informed judgment about the probability of successfully acquiring site data that may support the new truncated distribution. See Section 4.3.11 for detailed instructions on use of the Sensitivity Analysis module.

16. Select either *File/Exit* or click the close window "X" at the upper right portion of the Sensitivity Analysis window. Click *OK* to close the Data Influence Evaluation window.

Reiteration of Dose Assessment:

Based on the sensitivity analysis and other site investigations, the site analyst embarks on the next course of action and analysis. Site land use studies and projections, along with site characterization data, suggest that this site owner can justify eliminating the agricultural pathway. Though drinking water wells and irrigation are still viable future possibilities at this site, the analyst is able to justify modification of the depth to the water table. The following analysis implements those changes.

1. In the main window, save a new session for the reanalysis by selecting *File/Save As* and naming the new analysis "Simple Case 3." Click the *Open* button. If desired, change the *Site Name* and/or *Analysis Description* under *File/Properties*.
2. In the main window under the *Residential* tab, click the *Edit Exposure Pathway* button to open the Modify Pathways window.
3. Click on the *Agricultural* checkbox to deselect this pathway, and enter a justification that this modification is based on current land-use studies and future land-use projections. Print this window, if desired, by clicking the *Print* button and then click *OK*. Click *OK* to acknowledge that current calculations will be overwritten.
4. Click on *General Parameters* to open the Residential Parameters window. Note the parameter category buttons along the top of this window. Scroll down the list included in the Basic group.

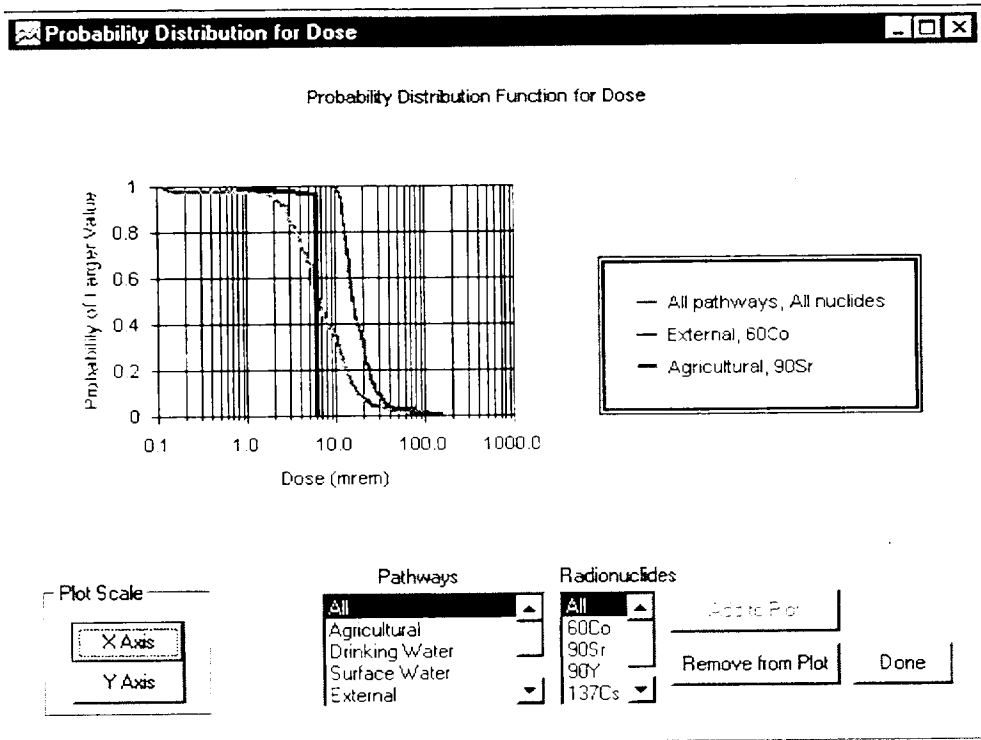


Figure 3.8 Dose distribution for Case 2

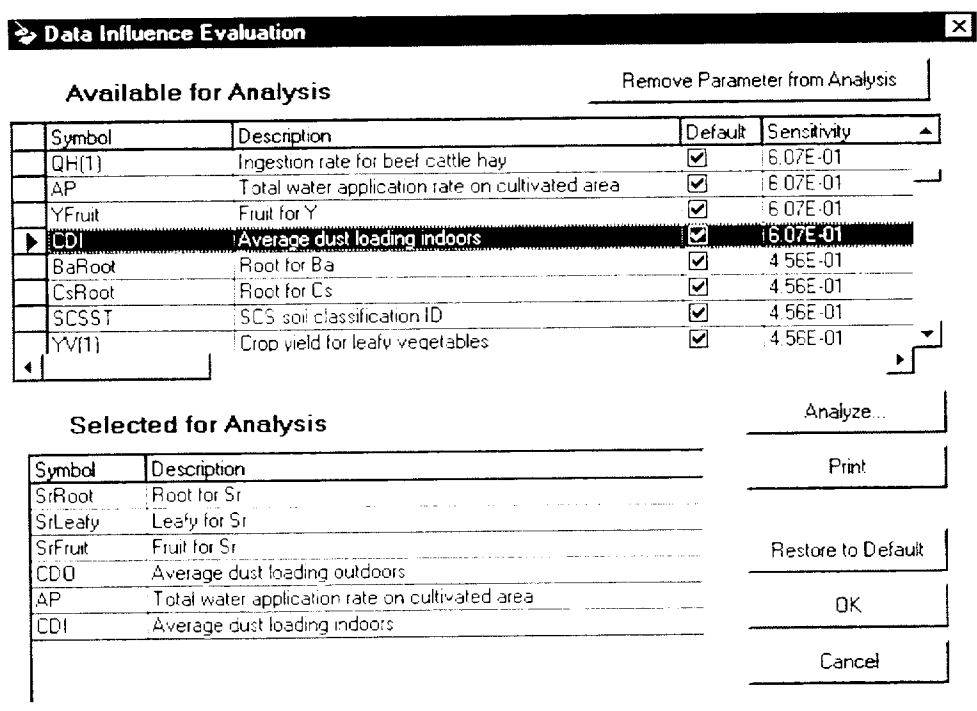


Figure 3.9 Select parameters for analysis

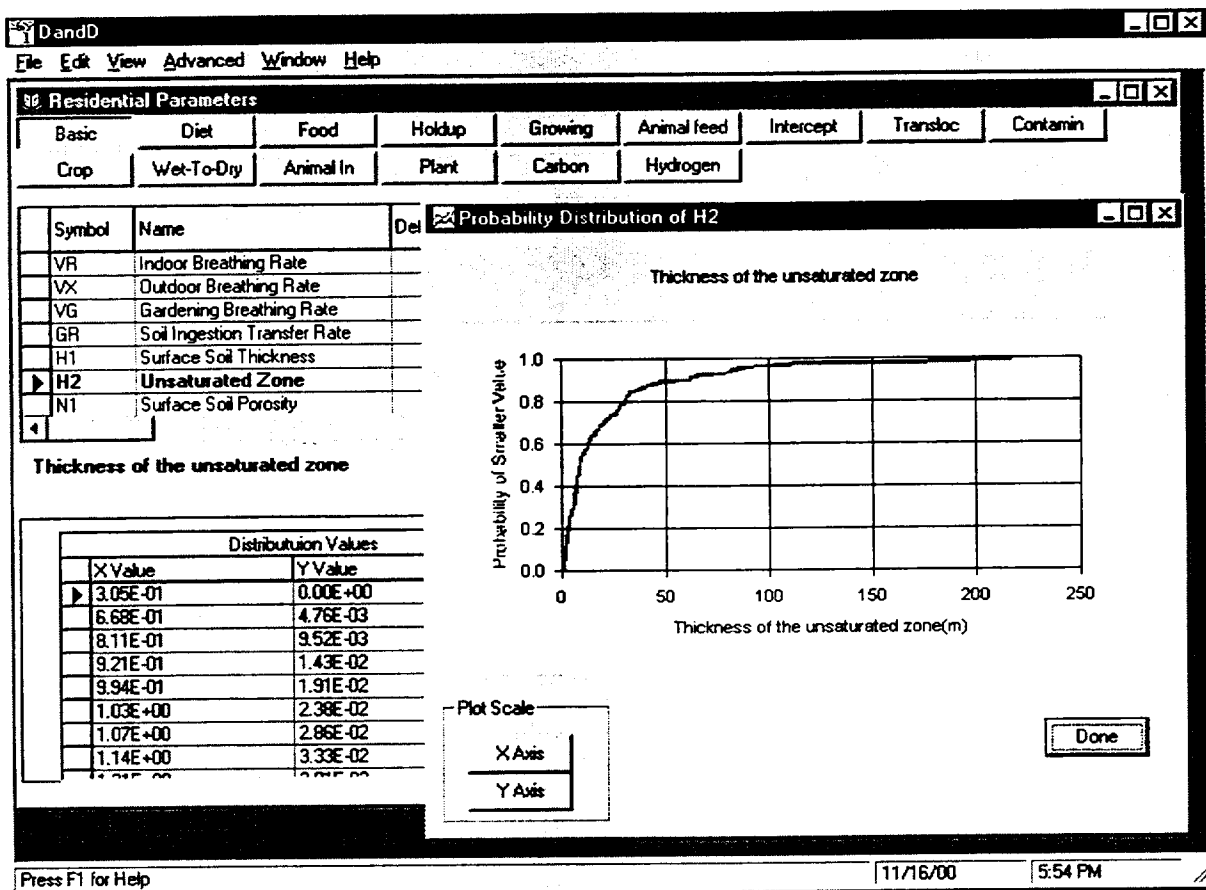


Figure 3.10 Detailed data for H2, unsaturated zone

- Locate and select H2, Unsaturated Zone Thickness, and click *Plot* to view the current default distribution for this parameter as shown in Figure 3.10. Click *Done* to close the plot. Click *Modify Value*.
- Change the distribution type to Uniform, leave units unchanged, and enter 100 m and 150 m as the lower and upper limits for the expected thickness of the unsaturated zone at this site. Enter justification text stating that this range of values is based on site characterization studies as shown in Figure 3.11. Click *OK*.
- Click *Plot* to review the new distribution, then click on *Done*. Click on *Close* to close the Residential Parameters window.
- To run this new simulation, select *Execute* followed by *Run Simulation*. When complete, the results of this new analysis—2.84 mrem/y—fall well below the 25 mrem/y performance objectives for this site. As such, the licensee elects to pursue the license termination process with NRC based on well-documented and supported information and analyses using the DandD code.
- To exit DandD, click the *Close* button in the Run Simulation window. Select *File/Exit* from the main menu.

Residential Scenario Unsaturated Zone Thickness [X]

Distribution: UNIFORM

Units of Measurement: m

Lower Limit: 100

Upper Limit: 150

Enter Justification for Site Specific Value

Based on site characterization studies

Restore to Default

Print

OK

Cancel

Figure 3.11 Modifying distribution

4 USER INTERFACE REFERENCE GUIDE

4.1 Common Interface Operations

4.1.1 On-Line Help

DandD was designed to provide an on-line user manual that reduces the need to refer to a hard-copy manual. It provides on-line documentation and software guidance using the Microsoft® Windows® Help system and HTML help that is available to view from the user's computer. The HTML help files are local to the user's computer. It is not necessary to have an Internet connection to view the HTML help, but the user will need a browser such as Internet Explorer or Netscape installed.

The Microsoft® Windows® Help facility is a hypertext system that allows the user to easily jump from one topic to another and back again. Hypertext is basically the same as regular text with one exception: hypertext contains connections within the text to other documents. These hypertext links, called hyperlinks, connect to other documents in the help system and appear as colored, underlined text. By clicking on the hyperlink text, the program will display a different help topic document.

The user can get help with the basic program usage by pressing the F1 function key, or by using the *Help/Contents* and *Help/Search For Help On* options from the main menu. Additionally, selecting *Help/NRC References* from the main menu will open a document that describes the models in more detail. The user can get context help on parameters by clicking the *Parameter Help* button. This button is displayed on the parameter viewing window.

The Help system includes Index and Find tabs that help locate particular topics, a Bookmark command that can flag topics of interest, an Annotate feature that lets the user add their own comments to the help text, a Copy command that copies selected information onto the clipboard, and a Print command. More information on Microsoft® Windows® help is available by selecting Help from the Microsoft® Windows® Start button, clicking *Help*, and searching for the keyword Help in the Index tab of the Microsoft® Windows® help window.

4.1.2 Parameter Viewing Window

The windows for viewing parameter values all have a similar design. Parameters are divided into three types: source concentrations, general parameters describing the physical properties of the site, and element parameters related to the chemical elements in the decay chains of the source radionuclides.

The source concentration parameter settings can be viewed by clicking the *Add Concentrations* button in the Session window. The general parameter settings can be viewed by clicking the *General Parameters* button in the Session window. If the residential scenario tab is the current scenario, the element parameter settings can be viewed by clicking the *Element Parameters* button in the Session window.

The general parameters and element parameters for the residential scenario are grouped into categories, as shown in Figure 4.1.1. Select the parameter category by clicking on one of the category buttons located at the top of the Parameter Viewing window. These buttons do not appear on the Add Concentrations form nor on the building occupancy parameter viewing forms.

A data grid summarizes information concerning the parameters in the chosen category. The general parameter grid entries have the following meaning:

- **Symbol:** symbol used in Kennedy and Strenge (1992) to identify a parameter.
- **Name:** user-friendly name used to identify the parameter.
- **Default:** check appears if the user has not modified the parameter. No check appears if the user has entered a site-specific value.
- **Read Only:** check appears if DandD does not allow this parameter to be modified.
- **Distribution Name:** name of probability distribution associated with the parameter. If name is CONSTANT, there is no associated distribution.

If name is DERIVED, the parameter value is calculated from other parameter values.

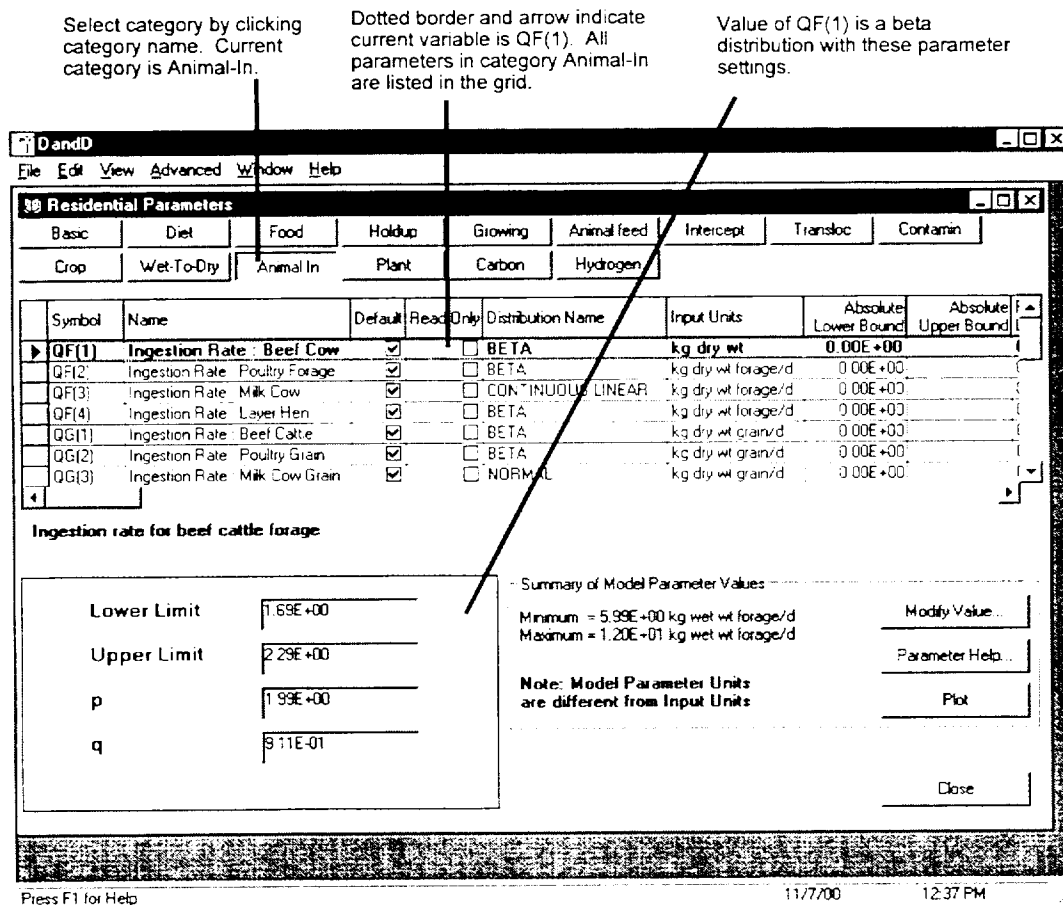


Figure 4.1.1 Viewing a parameter value

- **Input Units:** units of the site-specific or default parameter value. These units can be modified from the Parameter Modification window.
- **Absolute Lower Bound:** smallest value of the parameter that is allowed by the modeling code. DandD will prevent lower values from being used.
- **Absolute Upper Bound:** largest value of the parameter that is allowed by the modeling code. DandD will prevent higher values from being used.
- **Recommended Lower Bound:** DandD will warn about, but not prevent, parameter values smaller than the recommended lower bound.
- **Recommended Upper Bound:** DandD will warn about, but not prevent, parameter values larger than the recommended upper bound.

Select the parameter to view or modify by clicking the appropriate row on the data grid. After the parameter has been selected, the data defining the value or distribution for this parameter is shown on the lower left corner of the screen.

The amount of data needed to define the value depends on the associated distribution. If the parameter is a constant value, only one number is required. If the parameter value is defined by a probability distribution, several numbers may be needed to define the distribution. A normal distribution, for example, requires two numbers: a mean value and a standard deviation. If the parameter is a tabulated (or empirical) distribution, the parameter values will be a list of ordered pairs where the x value is a parameter value and the y value is related to the probability that the parameter has that value. Some parameters may be assigned a distribution called "Derived." This means that the value of the parameter is calculated from the values of other parameters. Unless the derived param-

eter is marked as “Read Only,” the user can modify the derived parameter value to a specified value. Beyeler et al. (1999) contains information describing the calculations used to derive parameter values from other parameters.

The actual values for the parameter used in the dose calculation are summarized in the lower right portion of the parameter viewing screen labeled *Summary of Model Parameter Values*. The summary information displayed on the right side of the Parameter Viewing window, and the plots of the parameter values, are presented in the units used by the model, which may be different than the input units.

To modify a parameter value, click on the *Modify Value* button on the right side of the screen or double-click the parameter row in the grid. If the parameter is not a read-only parameter, the Parameter Modification window will open (see Section 4.1.3). If the parameter is a read-only parameter, it cannot be modified and a pop-up box will notify the user of this.

Detailed information about the parameter can be obtained by clicking the *Parameter Help* button. This information includes the parameter definition, how the parameter is used in the dose model, what data was used to develop the default value or probability distribution, and information about assigning a site-specific value.

A probability distribution of the parameter value can be displayed by clicking the *Plot* button, which brings up the Parameter Plot window. This plot will not give any useful information if the parameter value is a constant.

4.1.3 Parameter Modification Window

Modify parameters by clicking on the *Modify Value* button in any Parameter Viewing window. A window similar to Figure 4.1.2 will open.

Select the type of distribution to associate with the parameter from the *Distribution* pull-down list at the top of the screen.

Modify the parameter units by selecting the appropriate entry from the *Units of Measurement* pull-down list. Only units that are appropriate for the parameter and that can be converted into the model input units are displayed. DandD saves the values entered and units used, even if those units are different from the units used by the model.

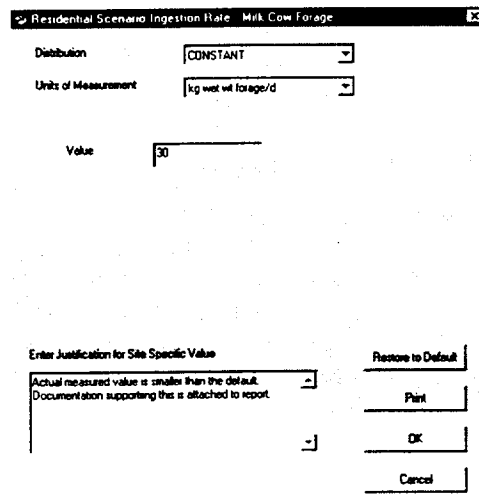


Figure 4.1.2 Parameter modification window

After selecting the units of measurement, enter the values that define the distribution. DandD provides a wide range of distribution types. Each distribution type can accept a wide range of values for its parameters. These values may either consist of a list of (x,y) pairs (known as tabulated data) or a list of specific distribution parameters (such as the mean and standard deviation of the normal distribution). If the parameter has no distribution, but is a single number, set the *Distribution* field to CONSTANT. Type the value in the field labeled *Value*.

It is possible to specify values for the distribution parameters that lead to invalid distributions, causing the LHS sampling to fail. The user will be notified and will need to modify the parameter distribution accordingly.

The distribution DERIVED has no numeric values to enter. This choice means that the parameter value is calculated from the values of other parameters by the model engine. Only some parameters have built-in functions for deriving values. If the parameter cannot be derived by the model engine, the distribution DERIVED will not be available for this parameter. If the user wants the model engine to calculate the parameter value, set the distribution type to DERIVED. The parameter values calculated by the model engine can be viewed from the Parameter Viewing window. A description of the derived parameters can be found in Beyeler et al (1999).

If the user selects an empirical distribution, a grid of tabulated data will be displayed, as shown in Figure 4.1.3. To delete a row of tabulated data, select the row by clicking on the left margin of the row. Press the

Delete key on the keyboard to delete the row. If the cursor has focus on a number in the grid and the pencil icon is present as shown in Figure 4.1.4, press the ESC key on the keyboard to undo typing. As long as the pencil icon is shown on the left margin of a row, click in a cell on that row and press the ESC key to undo changes. Use the arrow keys on the keyboard to go to the next cell.

If a parameter value is modified from the default value, the user will be required to enter text explaining why the value or distribution specified is appropriate (see Figure 4.1.2). This field is labeled *Enter Justification for Site Specific Value*.

To reset the parameter definition to the default value or distribution, click the *Restore to Default* button. It will still be necessary to click the *OK* button to accept the default values for the parameter.

To discard the changes made, click the *Cancel* button.

To save changes, click the *OK* button. This will close the Parameter Modification window and save any changes made to the parameter value. After any parameter values have been changed, DandD regenerates the set of parameter values that will be used in the dose calculation. This may take a few seconds.

If the value or distribution specified is not consistent with the absolute limits defined for the parameter, the user will be notified and required to change the parameter value before executing the dose model. If the parameter value or distribution falls outside of any recommended limits, the user will be notified. The dose model can be executed in this case, however, special justification may be needed for the value or distribution.

4.1.4 Graphics Windows

The Graphics windows can be accessed through the main menu *View/Graphics* after running a simulation. The Graphics windows can also be accessed to view distributions associated with individual parameters

through the *Plot* button on the Parameter Viewing windows. A typical graphics window is shown in Figure 4.1.5. For specific information on the meaning of the data, see the appropriate description in Section 4.3 under the associated menu selection (e.g., *View/ Graphics*).

Not all graphics windows will have all of the functions described below. In particular, windows displaying a parameter distribution and the *Time Distribution* will not have the *Pathways* and *Radionuclides* list boxes. If the parameter or result is a constant value, the graphics window will display a vertical line at the constant value.

PDFs for individual pathways and individual radionuclides can be added to the graph by selecting a specific pathway (or *All*) from the *Pathways* list box, selecting a specific radionuclide (or *All*) from the *Radionuclides* list box, and clicking the *Add to Plot* button.

Curves can be removed from the graph by selecting the curve and pressing the "Delete" key on the keyboard or clicking the *Remove from Plot* button on the form.

Three methods are available for selecting curves. A curve can be selected by clicking it on the graph. A curve can also be selected by clicking on the corresponding line in the legend. This feature can be used to find curves that overlap other curves on the graph or that fall along the y axis. Finally, a curve can be selected for deletion by selecting the appropriate entry in the *Pathways* and *Radionuclides* lists. If a curve is selected by clicking on an entry in the *Pathways* and *Radionuclides* list, and the curve has already been added to the graph, then only the *Remove from Plot* button will be enabled. Otherwise, only the *Add to Plot* button will be accessible to the user.

The plot area can be selected and resized using the resizing controls. The legend can also be selected, resized, and repositioned. If the legend or the plot area are moved or resized, the legend may not be automatically resized to include new curves added to the plot.

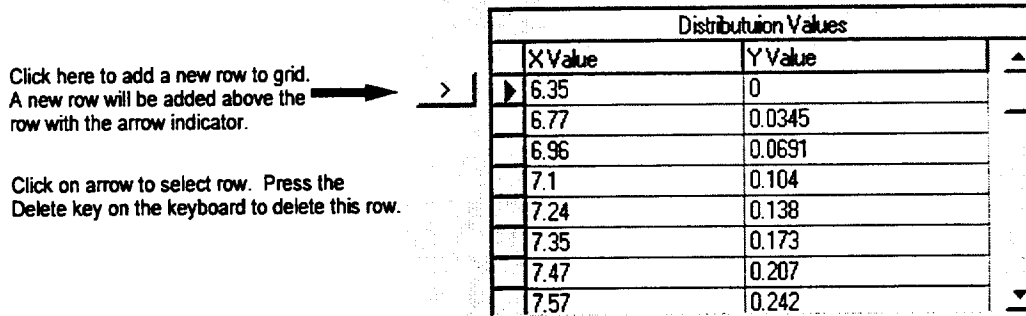


Figure 4.1.3 Empirical distribution grid

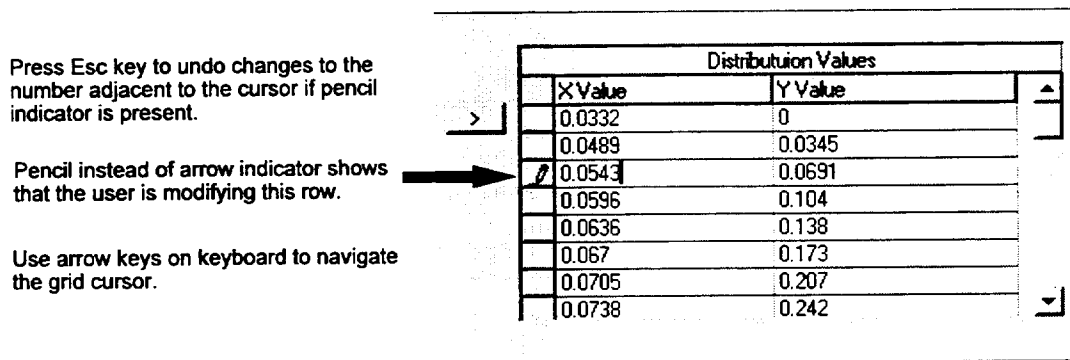


Figure 4.1.4 Modify a grid entry

1. Select a Pathway and a Radionuclide by selecting from the Pathways and Radionuclides list.

2. Click the Add to Plot button to add graph to plot. Click the Remove from Plot button to remove a selected graph from plot.

Click on white border of graph or legend to activate moving and resizing handles. Plot title can also be moved by selecting and dragging it.

Click the X Axis or Y Axis buttons to modify the scale of the x or y axis.

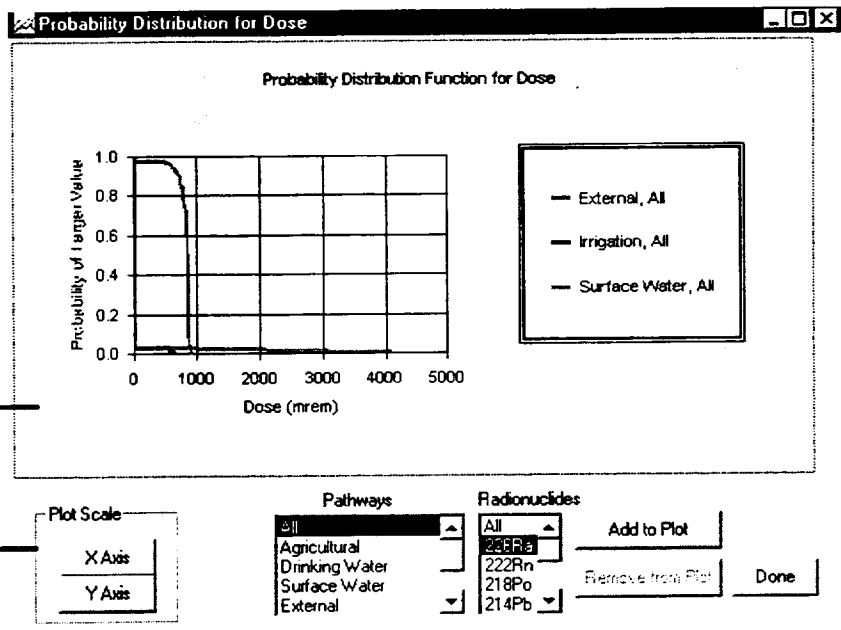


Figure 4.1.5 Typical graphics window

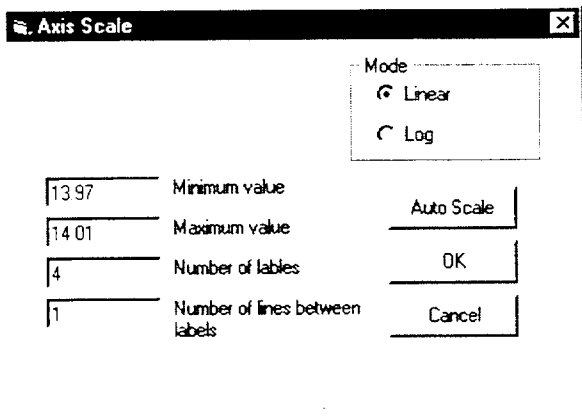


Figure 4.1.6 Modifying the Axis Scale

It may be necessary to manually resize the legend to see descriptions for all of the curves on the plot. The user can also select and move the plot title.

Click the *X Axis* or *Y Axis* buttons to modify the axis on the plot. An Axis Scale window, as shown in Figure 4.1.6, will open.

The scales for the x and y axes can be set using the *Minimum value* and *Maximum value* fields. All scales are initially set automatically based on the range of data in the plot. This automatic scaling can be restored using the *Auto Scale* button.

Minimum value and *Maximum value* determine the range of the plot axis. *Number of labels* determines the number of labeled lines, and *Number of lines between labels* sets the number of axis lines that are shown between labeled lines.

The *Linear/Log* radio buttons set the axis scaling mode. Both the minimum and maximum values must be positive if Log scaling is selected.

Click *OK* in the Axis Scale window when finished.

The plot can be printed using the *File:Print* command from the main menu.

The plot can be copied to the clipboard using the *Edit/Copy* menu commands. It can be pasted as a graphic image in a word-processing application using the *Paste Special* command in the word processor. By default, the x-y data pairs that define the curves (dose-probability, time of peak-probability, or dose history) will be pasted as text from the clipboard.

Click on the *Done* button to close the window. The graph created will not be saved by DandD.

4.2 Scenario Tabs and Their Controls

When a DandD session is opened (using the *File/Open* or *File/New* command), a window with two tabs is opened. This is called the Session window (see Figure 4.2.1). One of the two default scenarios NRC has included in DandD can be selected by clicking the *Residential* or the *Building Occupancy* tabs within the Session window. The underlying engine used for analysis is different between the two scenarios.

Depending on the tab selected, different options are available. The residential scenario includes more exposure pathways and has more site-specific parameters available than the building occupancy scenario. These parameters are accessible by clicking the *General Parameters* or *Element Parameters* button. The residential scenario also allows input of concentration data via a text file. The building occupancy scenario does not have the *Element Parameters* button available.

The building occupancy scenario data is stored independently from the residential scenario data. This allows the saving of data and results from both scenarios in the same session file. The user can also switch between scenarios by clicking the appropriate tab without any loss of data or results.

The following section describes the controls available to the user in the Session window.

4.2.1 Edit Exposure Pathway Button (Site-Specific)

The following exposure pathways are supported for the building occupancy scenario:

1. External: external radiation from inside building surfaces
2. Inhalation: exposure by breathing indoor air contaminated by resuspension of radionuclides from building surfaces
3. Secondary Ingestion: ingestion of contaminated dust inside building surfaces

The residential model supports the following pathways:

1. External: external radiation from inside building surfaces, outside soil, and garden soil
2. Inhalation: exposure by breathing inside air, outside air, and garden air
3. Secondary ingestion: consumption of contamination from dust on inside building surfaces, outside soil, and garden soil
4. Agricultural: consumption of agricultural products that do not use well water
5. Drinking Water: consumption of drinking water from a well
6. Irrigation: consumption of agricultural products that use well water
7. Surface Water: consumption of aquatic products from surface water sources

Detailed information about the meaning of these pathways is available by selecting *Help/NRC References* from the main menu.

By default for screening assessments, all pathways will be selected. Pathways should not be deselected unless users are conducting a site-specific analysis.

The current exposure pathways are shown in the Session window. Select or remove pathways by clicking the check boxes or the *Edit Exposure Pathway* button as shown in Figure 4.2.2. If this is done, the Modify Pathways window will open, as shown in Figure 4.2.3. Turn pathways on or off by clicking the check box adjacent to the pathway.

If a pathway is deselected from the analysis, dose calculations involving that particular pathway are not performed. Selecting or deselecting the various pathways does not change the values or distributions of any parameters, although some parameters may not be used when pathways are deselected.

Changing the values of some parameters can affect

doses that occur over more than one pathway. For example, modifying the Time Outdoors parameter changes the calculated dose due to the external, inhalation and secondary ingestion pathways. Parameter help accessed via the Parameter Viewing window (see section 4.1.2) and the online help accessed by selecting *Help/NRC/References* from the main menu will supply the user with specific parameter and pathway dependency information.

The user is required to justify disabling exposure pathways for a given scenario in the dose assessment. The screen including the user justification text may be saved as hard copy documentation using the *Print* button.

To restore all pathways to original settings, click the *Restore to Default* button. Alternatively, click *Cancel* to ignore all changes to the Modify Pathways window. Otherwise, click *OK* to save pathway settings and return to the main Session window.

4.2.2 Add Contaminants

4.2.2.1 Adding Contaminant Source

The first step in a screening analysis is to indicate the radionuclide contaminants present at the site. Until the source of contamination is specified, all other buttons (with the exception of the *Edit Exposure Pathway* button) in the Session window will not be accessible. Clicking the *Add Contaminants* button in the Session window opens the Add Contaminants window, as shown in Figure 4.2.4.

Add radionuclides to the source term by selecting a symbol from the list labeled *Potential Contaminants*. Click on the right arrow button to add the contaminant. Alternatively, the user can double-click on the symbol to move the radionuclide to the *Site Contaminants* list.

To remove the contaminant from the list labeled *Site Contaminants*, select a contaminant and click on the left arrow button. Double-clicking a symbol in the *Site Contaminants* list will also remove it from the source term.

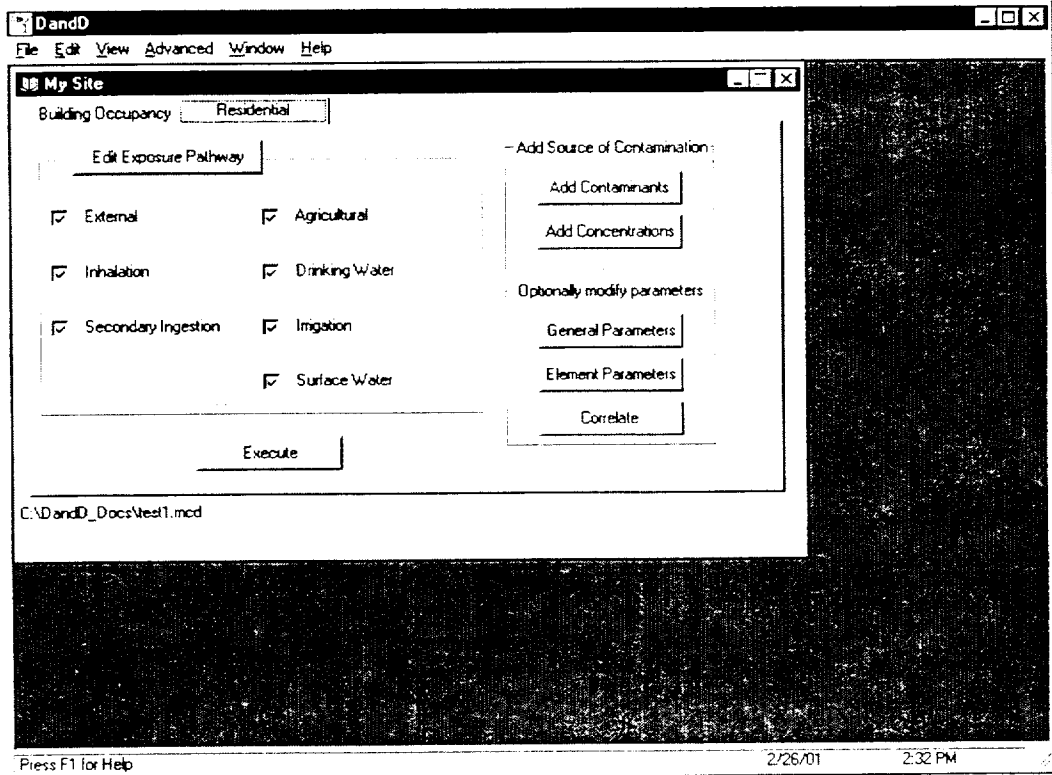


Figure 4.2.1 Session window

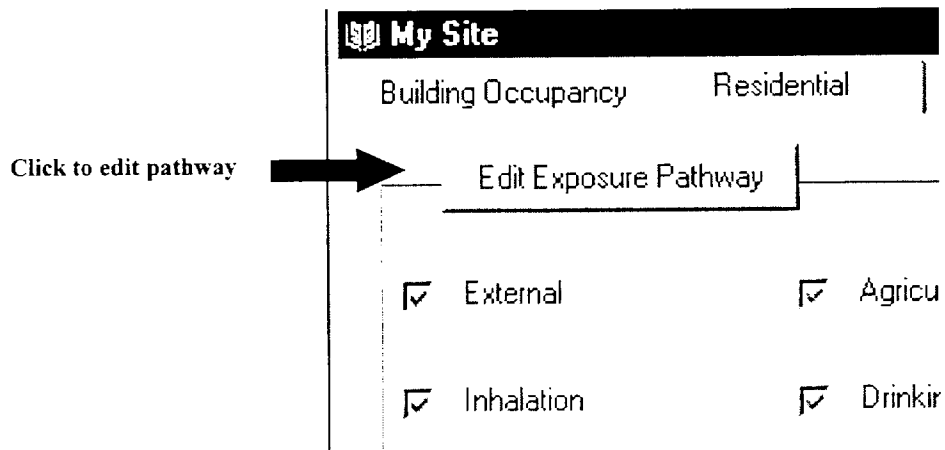


Figure 4.2.2 Change exposure pathways

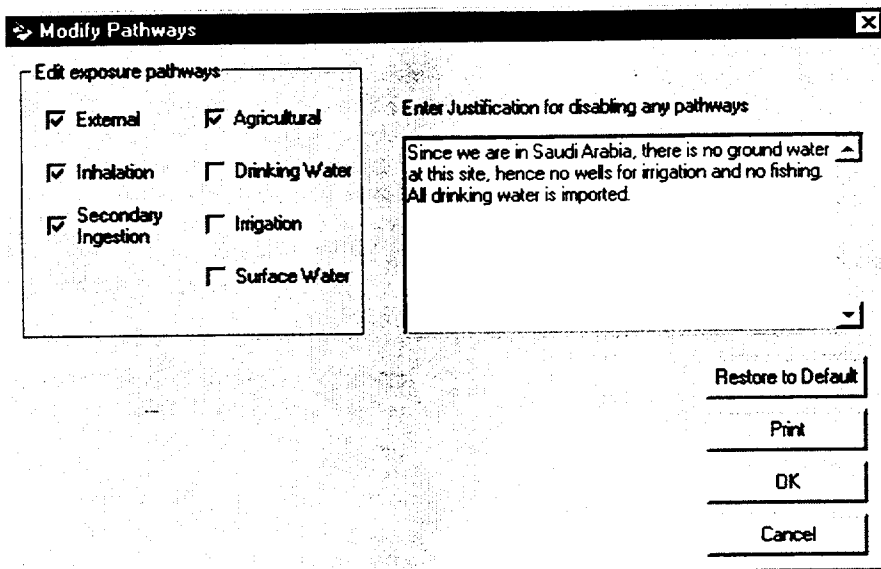


Figure 4.2.3 Modify Pathways window

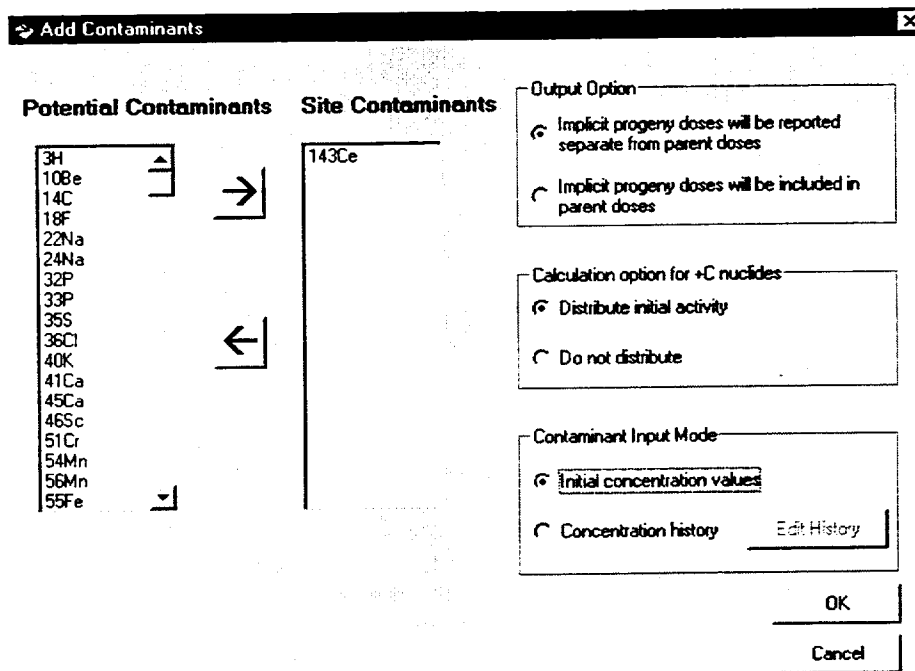


Figure 4.2.4 Add Contaminant window

4.2.2.2 Implicit Progeny Output Option

Some short-lived radionuclides are assumed to be in equilibrium with their parent radionuclides. These particular radionuclides, called *Implicit progeny*, are not in the *Potential Contaminants* list. The user can identify which nuclides are *Implicit* by noting that there

are no reported *Half Life* entries in the *Radioactive Decay Data* table. (The *Radioactive Decay Data* table can be viewed by selecting *View/Tables/ Radioactive Decay Data* from the main menu.)

By default, the dose from these radionuclides is not included with the parent dose, but is reported sepa-

rately. If the *Implicit Progeny doses will be reported separate from parent doses* is selected (default), these short-lived radionuclides will be listed in the *Chain Data* portion and the *Detailed Results* portion of the reports (see Section 4.3.7). In the *Chain Data* table from the *Detail* report, as shown in Table 4.2.1, the implicit nuclides have a *Chain Position* value of *Implicit* and no half-life reported.

Table 4.2.1 Excerpt from Chain Data Table, contaminant 225Ac

Nuclide	Chain Position	Half Life	Fractional Yield
225Ac	1	1.0E+01	
221 Fr	Implicit		1
213 Po	Implicit		0.9784
(many more implicit follow)			

Select the radio button *Implicit progeny doses will be included in the parent doses* to have implicit progeny doses included with the parent doses. In this case, the initial concentrations, chain data, and results section of the reports will not reference these radionuclides. No matter which radio button is selected, the dose from implicit radionuclides is always included in the dose calculations.

4.2.2.3 Distribute Option for +C Nuclides

Some radionuclide chains can decay in a state of transient equilibrium. This means that all progeny of a radionuclide chain parent have half-lives somewhat shorter than that of the parent and a long period of time has elapsed since the initial contamination. In essence, all the progeny exponential decay terms are removed from the calculations because they approach zero much faster than the parent exponential decay term. Therefore, after a period of time, all progeny of the chain parent decay at the same rate as the parent. A review of transient equilibrium is given in Kaplan (1962).

In DandD, there are 15 radionuclide chains (including Th_Nat, which is the same as 232Th in equilibrium) that can decay in a state of equilibrium. Except for Th_Nat, these chains are designated with a "+C" after their respective names. For example, the selection 232Th decays in the normal fashion while the selection 232Th-C decays in a state of transient equilibrium.

With respect to DandD, for a radionuclide chain that decays in the normal fashion, only the chain parent is

initially at the site; the initial condition is assigned to the parent only. Progeny are generated from the decay of the parent. For a chain in equilibrium, all radionuclides in the chain are initially at the site; the initial conditions for each radionuclide in the chain are assigned based on distributing the assigned initial condition for the chain and the equilibrium relationship among all the radionuclides in the chain.

There are two methods for distributing the initial condition assigned to a chain in equilibrium described, as follows.

Selecting the radio button *Distribute initial activity* means that the specified initial activity is divided among all explicit and implicit radionuclides in the chain based on the decay constants and fractional yields of the radionuclides in the chain (see Table 4.2.1). The initial activity assigned to the parent is always less than that input by the user. The calculated initial activity of all the radionuclides in the chain sum to the initial activity input by the user.

Selecting the radio button *Do not distribute* means that the specified initial activity is used to set the initial activities of all explicit and implicit radionuclides in the chain based on the decay constants and fractional yields of the radionuclides in the chain (see Table 4.2.1). The input initial activity is assigned to the parent and the initial activities of all progeny in the chain are based on the initial activity of the parent. The calculated initial activity of all radionuclides in the chain sum to an activity greater than that input by the user.

The default setting is *Distribute initial activity*. The selected distribution option is applied to all selected equilibrium chains in the Add Contaminants window.

For example, suppose 232Th+C is selected and assigned an initial activity of 10 pCi/g. The 232Th chain has five explicit progeny, including the parent radionuclide and six implicit progeny, for a total of 11 radionuclides. If the *Distribute initial activity* option is selected, each radionuclide is assigned an initial activity of 1 pCi/g except for 212Po and 208Tl, which are assigned initial activities of 0.6407 pCi/g and 0.3593 pCi/g, respectively, because of branching. The initial activities of all radionuclides in the chain sum to 10 pCi/g. If the *Do not distribute* option is selected, each radionuclide is assigned an initial activity of 10 pCi/g, except for 212Po and 208Tl, which are assigned initial activities of 6.407 pCi/g and 3.593 pCi/g, respectively, because of branching. The initial activities of all radionuclides in the chain sum to 100 pCi/g.

which is greater than the initial activity assigned.

4.2.2.4 Import Contaminant and Concentration Data (Residential Scenario Only)

If the current scenario is residential, the option of specifying the radionuclides and their concentrations from a text file is available. The Contaminant Input Mode is a toggle that will switch between manual and import modes.

By default, the *Initial concentration values* radio button will be selected. In this case, the user will be expected to manually specify the source in this form and enter the soil concentrations at the beginning of the scenario via the *Add Concentrations* form. However, site contaminants and time varying values for the concentrations can be specified via a text file by setting the *Concentration history* radio button (Figure 4.2.5).

The concentration history may already be present in the session file if a file has already been imported for this session. If it is present, the nuclides described in the file will be listed in the *Site Contaminants* list box. The user will be required to fill in the *Justification* field. In this case, it is not necessary for the user to enter any initial concentrations.

To replace the current data or specify a new concentration file, click the *Edit History* button, as shown in Figure 4.2.5.

To import a file, click the *Import File* button (Figure 4.2.6). Locate a concentration file (*.con file) and click OK in the *Import Concentration File* dialog box (see Appendix C for file format). The user can replace an imported file with another file by clicking the *Import File* button and specifying the desired replacement file.

At this point, the data in the concentration file should show in the grid, as demonstrated in Figure 4.2.6. A list of the parent nuclides imported will appear in the

Nuclides Imported list. This data cannot be edited directly through DandD.

If the data are satisfactory, click the *OK* button. The data will be loaded into the session file. Otherwise, click the *Cancel* button to disregard the imported data.

To complete the process of importing the concentrations, enter a justification in the field labeled *Enter Justification for using concentration history* in the *Add Contaminants* form. Click *OK* to save these settings. Notice that the *Add Concentrations* button in the *Session* form is dimmed. This is because the concentrations have already been specified in the concentration file.

4.2.3 Add Concentrations

Specify the initial concentration of the radionuclides at the site by clicking on the *Add Concentrations* button (Figure 4.2.1). This button will be available only if contaminants have been added. This button will not be available if the *Concentration History* toggle has been set from the *Add Contaminants* window.

The nuclide Parameter Viewing window, shown in Figure 4.2.7, is opened when the user clicks on the *Add Concentration* button. See Section 4.1.2 for a complete description of a Parameter Viewing window. Each nuclide shown in this window has the following grid entries:

- **Nuclide Symbol:** name of radionuclide, atomic weight followed by symbol (e.g., 235U means Uranium 235).
- **Area:** the characters UNLIMITED, meaning the contaminant is spread evenly over the exposure area for the scenario, or an area in square meters defining the contaminated area. The user can modify this value in the Parameter Modification Window.

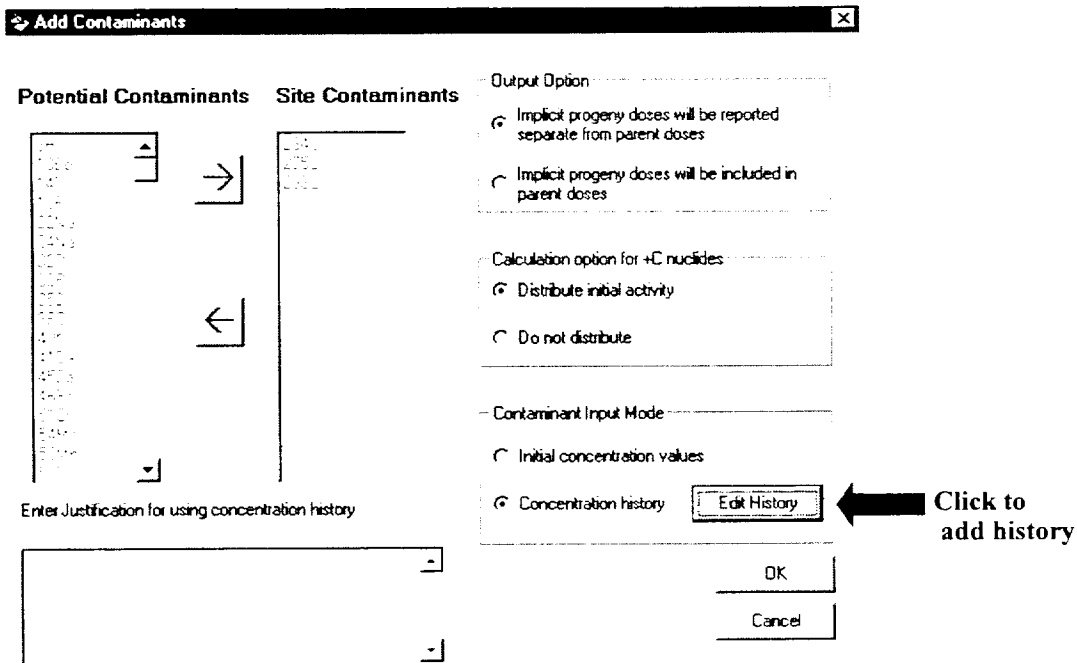


Figure 4.2.5 Contaminant input modes

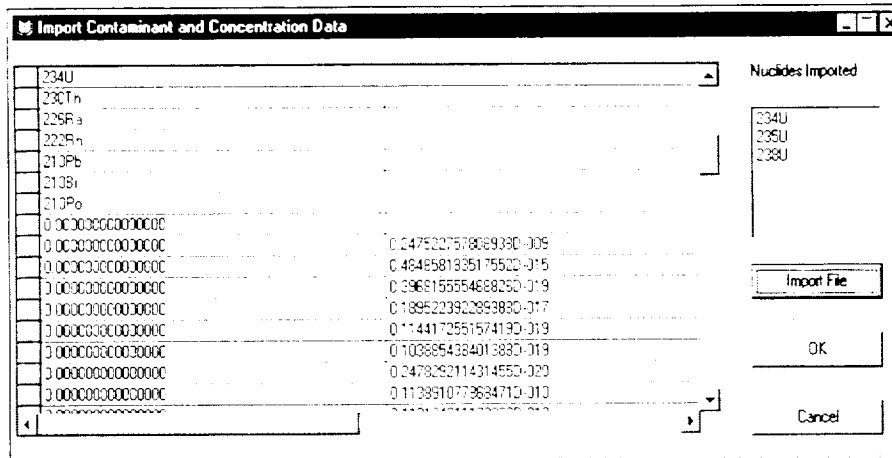


Figure 4.2.6 Import contaminant and concentration data

- **Distribution Name:** same meaning as discussed in Section 4.1.2.
- **Input Units:** Units of concentration. The default units for the building occupancy ($\text{dpm}/100\text{cm}^2$) are different than the units for the residential scenario (pCi/g).

To add a concentration of a nuclide, double-click on the nuclide symbol in the data grid. Alternatively, click once on the symbol in the data grid to select the nuclide. The value of the concentration is shown on

the lower left portion of the window. Then, click the *Modify Value* button to open the parameter modification window. See Section 4.1.3 for a complete description of a Parameter Modification window.

Once the Parameter Modification window opens, follow the six steps indicated in Figure 4.2.8. The *Restore to Default* button will restore the distribution to *Constant*, the concentration to zero, the units to the default units for the given scenario, the area to *Unlimited*, and the *Justification* to a blank field.

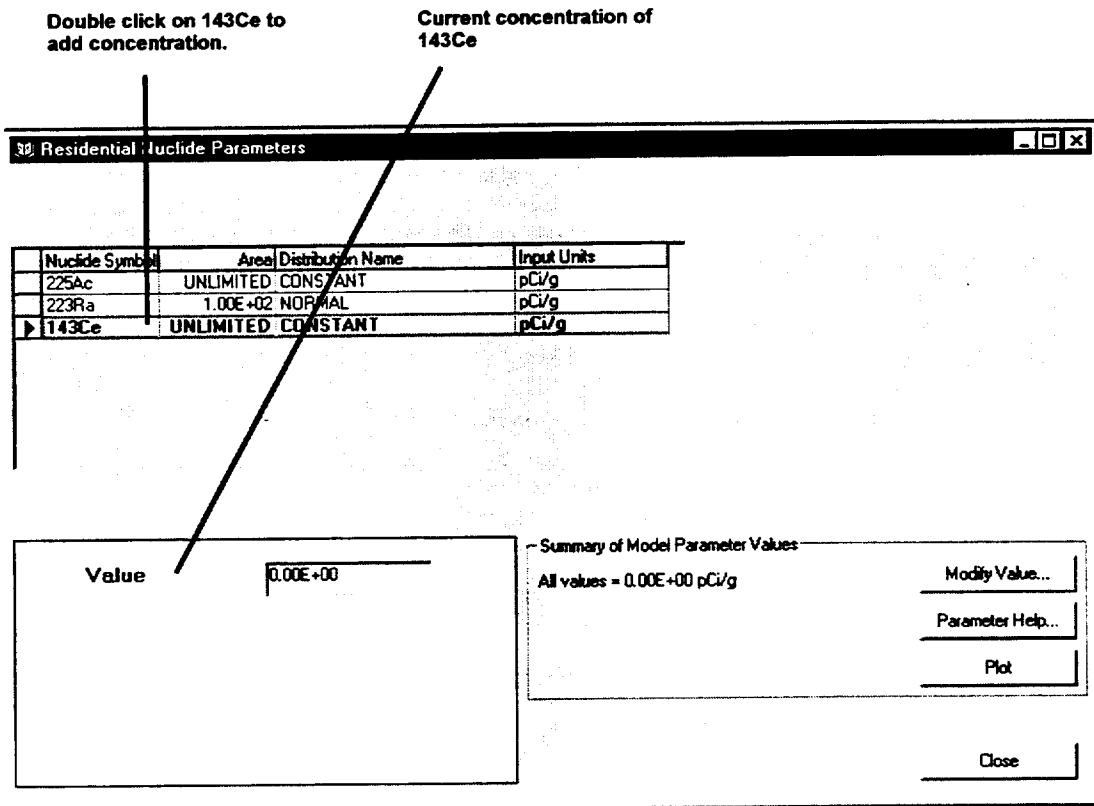


Figure 4.2.7 Nuclide concentration window

1. Select distribution. CONSTANT means no probability distribution.
2. Change Units of Measure (UOM) if needed.
3. Enter a concentration.
4. Specify the area of contamination if known.
5. Explain how the concentration was derived in the Justification Field.
6. Click OK when finished.

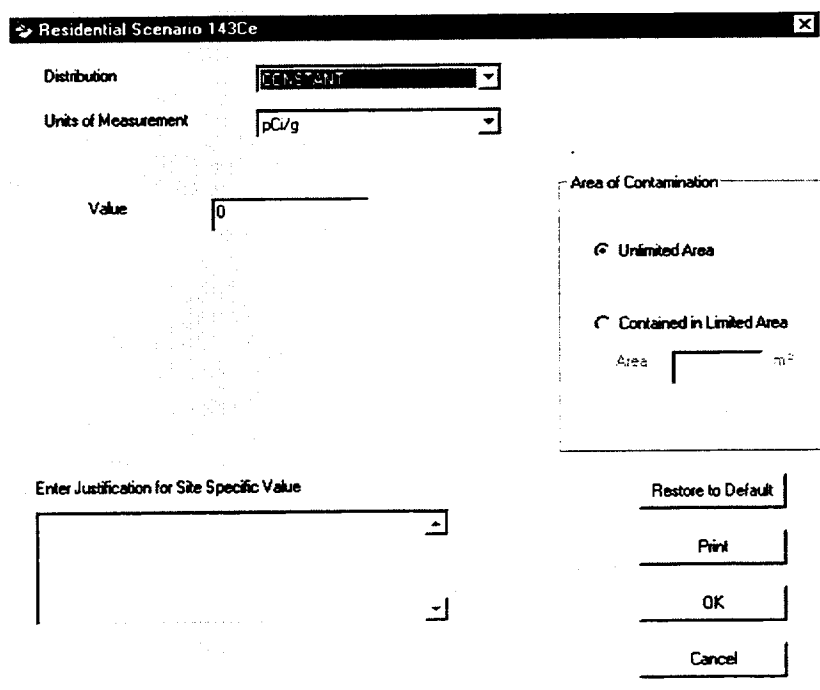


Figure 4.2.8 Parameter modification window for contaminant

The *Print* button will print a copy of the screen, and will print the contents of the grid separately if an empirical distribution (such as Continuous Linear) was specified.

Within the *Area of Contamination* panel, the user has the option of specifying either an unlimited area or a limited area based on site-specific knowledge about the spatial distribution of their site contamination. By default, DandD uses the specified concentration directly in the dose calculation. This usage is equivalent to assuming that all material contacted by the receptor during the duration of the exposure scenario is contaminated at the same concentration (regardless of site location). The specified concentration should be the largest spatially averaged concentration that is consistent with available information about the site. The averaging area should correspond to the smallest exposure area among the active pathways. This approach is selected by the *Unlimited Area* radio button.

Alternatively, if the user can demonstrate that contamination is limited to a particular area, and that no contamination occurs outside that area, then the user may specify the area of contamination by selecting the *Limited Area* radio button and providing the size of the contaminated area. Using this option, the concentration that the user specifies should reflect the average value over the contaminated area. DandD will then use this concentration and the contaminated area, along with the smallest exposure area among the active pathways, to calculate the concentration used in the dose calculations.

For more information on specification of source concentration and exposure area, the user is referred to the online help. Click on *Help/Contents/Reference* and select the items *Source Concentration* and *Exposure Area* for detailed information that can be viewed or printed, as desired.

4.2.4 Modify Parameters (Site-Specific Analysis)

In a site-specific analysis, parameters can be modified based on site information. Click the *General Parameters* button in the main Session window (Figure 4.2.1) to open the general parameters viewing window. See Section 4.1.2 for a complete description of a Parameter Viewing window.

General Parameters

Once the Parameter Viewing window (as shown in Figure 4.2.9) has been opened, select the parameter category (residential scenario only).

If a parameter has been selected in the Parameter Viewing window, clicking the *Parameter Help* button will display detailed information about the selected parameter. This can help the user understand the meaning of the parameter. The parameter distribution can also be viewed graphically by clicking on the *Plot* button in the parameter viewing window.

Double-click on the parameter symbol in the data grid to modify the value of the parameter. Alternatively, click once on the symbol in the data grid to select the parameter. The value of the parameter is shown on the lower left portion of the window. Then, click the *Modify Value* button to open the Parameter Modification window. See Section 4.1.3 for a complete description of a Parameter Modification window.

The Parameter Modification window should now open as shown in Figure 4.2.10. Follow the five steps as indicated in the figure to modify a parameter.

The *Restore to Default* button will restore the value of the parameter to the default probability distribution and value(s) as documented in Beyeler et al. (1999). In this case, the *Enter Justification for Site-Specific Value* field will be blank.

The *Print* button will print a copy of the screen, and will print the contents of the grid separately if an empirical distribution (such as Continuous Linear) was specified.

After a parameter has been modified and the *OK* button is clicked to commit the modification, all of the uncertain parameters are resampled by LHS. This may take a few seconds. This is necessary so dependant variables (such as variables of type Derived) are recalculated correctly and graphical data is current. In addition to resampling the data, if there are any existing data sets in the session corresponding to the results of a simulation, these data sets are deleted. This means that if the user modifies a parameter after running a simulation within the same scenario, the output results are nullified. Even reports will be deleted. This is done to ensure integrity between the results and the current parameter settings.

1. Select category.
(Only for residential)

2. Select parameter.
Left arrow indicates
WV(3) is selected.

3. Double click on
WV(3) or click on *Modify Value*
button to change
value of selected
parameter.

Residential Parameters

Basic	Diet	Food	Holdup	Growing	Animal feed	Intercept	Transloc	Contain
Crop	Wet-To-Dry	Animal In	Plant	Carbon	Hydrogen			
Symbol	Name	Default	Read Only	Distribution Name	Input Units	Absolute Lower Bound	Absolute Upper Bound	
WV(1)	Wet/dry : Leafy Vegetables	<input checked="" type="checkbox"/>	<input type="checkbox"/>	CONTINUOUS LINEAR	none	0.00E+00	1.00E+00	
WV(2)	Wet/dry : Other Vegetables	<input checked="" type="checkbox"/>	<input type="checkbox"/>	CONTINUOUS LINEAR	none	0.00E+00	1.00E+00	
WV(3)	Wet/dry : Fruit	<input checked="" type="checkbox"/>	<input type="checkbox"/>	CONTINUOUS	none	0.00E+00	1.00E+00	
WV(4)	Wet/dry : Grain	<input checked="" type="checkbox"/>	<input type="checkbox"/>	CONSTANT	none	0.00E+00	1.00E+00	
WFI(1)	Wet/dry : Beef Cow Forage	<input checked="" type="checkbox"/>	<input type="checkbox"/>	BETA	none	0.00E+00	1.00E+00	
WFI(2)	Wet/dry : Poultry Forage	<input checked="" type="checkbox"/>	<input type="checkbox"/>	DERIVED	none	0.00E+00	1.00E+00	
WFI(3)	Wet/dry : Milk Cow Forage	<input checked="" type="checkbox"/>	<input type="checkbox"/>	DERIVED	none	0.00E+00	1.00E+00	

Wet/dry conversion factor for fruits

Distribution Values	
X Value	Y Value
3.69E-02	0.00E+00
4.87E-02	3.45E-02
5.45E-02	6.91E-02
5.93E-02	1.04E-01
6.31E-02	1.36E-01
6.72E-02	1.73E-01
7.10E-02	2.07E-01
7.44E-02	2.42E-01

Summary of Model Parameter Values

Minimum = 3.69E-02
Maximum = 2.81E-01

Buttons: Modify Value..., Parameter Help..., Plot, Close

Figure 4.2.9 General parameter viewing window (residential)

1. Change the distribution if needed.
CONSTANT means no probability
distribution.

2. Change measurement units if
needed.

3. Modify distribution parameters.

4. Enter the reason parameters are
changed from their default values.

5. Click OK to retain new values,
Cancel to disregard.

Residential Scenario Grain concentration factor for Pr

Distribution: LOGNORMAL-N

Units of Measurement: pCi/kg dry-wt grain per pCi/kg sc

Mean of Ln(X): -5.52146091786225

Standard Deviation of Ln: 0.904218150639886

Enter Justification for Site Specific Value

Buttons: Restore to Default, Print, OK, Cancel

Figure 4.2.10 Modify parameter window for general and element parameters

See the main menu function *File/Restore Parameters to Default Values* to restore all site-specific values to screening, or default, values.

Element Parameters

For the residential scenario only, click the *Element Parameters* button to open the element parameters viewing window (Figure 4.2.11). These parameters are based on elements in the decay chain.

For each category (e.g., Partition Coefficient), the grid depicts an entry for each element present in the decay chains.

- **Element:** Name of element associated with the parameter. This is an element in the decay chain of one of the contaminants. Some elements in the decay chain (such as At) may not be listed because of their short half-lives.

The following grid entries have the same meaning as the entries described in Section 4.1.2:

- **Default**
- **Distribution**
- **Input Units**
- **Absolute Lower Bound**
- **Absolute Upper Bound**
- **Recommended Lower Bound**
- **Recommended Upper Bound**

4.2.5 Correlate Parameters (Site-Specific Analysis)

The user can specify linear rank correlations between any two parameters whose values are defined by probability distributions. Clicking the *Correlate* button in the main session window will open the Correlate Parameters window, as shown in Figure 4.2.12. In the window, there is a main grid that lists each correlation that is currently defined. For the building occupancy scenario, this table is initially empty. For the residential scenario, the default screening analysis includes two correlations.

It is possible to specify combinations of valid correlations that are not mutually consistent. For example, two parameters "A" and "B" can be assigned a correlation of 0.99, parameters "B" and "C" can also be given a correlation of 0.99, but parameters "A" and "C" can be assigned a correlation of -0.99. Each correlation is valid by itself but the three are incom-

patible. DandD does not check for this type of inconsistency. The parameter sampling may fail if the user defines inconsistent correlations.

Add a correlation in the table's insertion row (indicated by "**") by:

- Clicking in the "Parameter One" cell and selecting one of the uncertain parameters from the list-box;
- Clicking in the "Parameter Two" cell and selecting the second parameter from the list-box;
- Entering the desired rank correlation between the two selected parameters in the "Coeff" cell; and
- Entering an explanation of the correlation in the "Justification" cell.

The correlations specified apply to the ranks of the parameter values rather than to the values themselves. Specified correlations must be greater than -1 and less than 1. These limits are checked by the program. The user is required to enter a justification in the justification cell for every non-default (i.e., user-defined) correlation or modification of the coefficient from the default value.

If any two parameters are not correlated, they have a correlation coefficient of zero. However, this is not listed in the grid, but is an implied correlation.

Default correlations are those that are defined for a screening analysis. For example, in the building scenario, the default correlations are zero for all uncertain parameters. In the Correlate Parameters window, there will be no grid entries. In the residential scenario, there are two default correlations, as shown in Figure 4.2.12.

To remove a *default* correlation, the user must enter a zero for the correlation coefficient in the *Coeff* column in the *Correlation Coefficients* grid, as shown in Figure 4.2.12. The user can also change the correlation coefficient of a default correlation to reflect different correlation values.

User-specified correlations are new grid entries that the user entered for a site-specific analysis. To remove a user-specified correlation, the user should select the grid row by clicking on the row and press the delete key on the keyboard. This method does not work for removing a default correlation.

Select parameter name. There are 10 different parameters.

All elements in the decay chain of the contaminants (in this case Th227) are listed exactly once.

Detailed description of parameter.

Grain factor for Tl is a Lognormal-N distribution with the following value.

Element	Default	Distribution	Input Units	Absolute Lower Bound	Absolute Upper Bound	Recommended Lower Bound	Recommended Upper Bound
Tl	<input checked="" type="checkbox"/>	LOGNORMAL-N	pCi/kg dry-wt grain	0.00E+00	0	0	0
Pb	<input checked="" type="checkbox"/>	LOGNORMAL-N	pCi/kg dry-wt grain	0.00E+00	0	0	0
Bi	<input checked="" type="checkbox"/>	LOGNORMAL-N	pCi/kg dry-wt grain	0.00E+00	0	0	0
Po	<input checked="" type="checkbox"/>	LOGNORMAL-N	pCi/kg dry-wt grain	0.00E+00	0	0	0
An	<input checked="" type="checkbox"/>	CONSTANT	pCi/kg dry-wt grain	0.00E+00	0	0	0
Ra	<input checked="" type="checkbox"/>	LOGNORMAL-N	pCi/kg dry-wt grain	0.00E+00	0	0	0
Ac	<input checked="" type="checkbox"/>	LOGNORMAL-N	pCi/kg dry-wt grain	0.00E+00	0	0	0
Th	<input checked="" type="checkbox"/>	LOGNORMAL-N	pCi/kg dry-wt grain	0.00E+00	0	0	0

Figure 4.2.11 Residential Element Parameters window

Default correlations have a check mark in the Default field.

1. Define a new correlation by choosing two parameters from drop-down menu.
2. Enter coefficient between -1 and 1.
3. Enter a justification for the parameter correlation.
4. Click OK to save changes.

Default	Parameter One	Parameter Two	Coeff	Justification
<input checked="" type="checkbox"/>	KSDEV: Permeability Probability	BDEV: Parameter "b" Probability	-0.35	
<input checked="" type="checkbox"/>	NDEV: Porosity Probability	BDEV: Parameter "b" Probability	-0.35	
<input type="checkbox"/>	Bi: Beef	Ac: Beef	0.5	This is a new correlation to demonstrate this window
<input type="checkbox"/>		Ac: Coefficient		
		Ac: Eggs		
		Ac: Factor		
		Ac: Fruit		

Figure 4.2.12 Residential Correlate Parameters window

The user can move from cell to cell in the grid by using the keyboard arrow keys.

Click the *Restore to Default* button to restore the parameters to their default correlations. Click the *Print* button to print the contents of the grid of correlated parameters. Click OK to preserve changes in the session. Click Cancel to ignore changes made to the correlations.

4.2.6 Execute Simulation

Perform the dose calculations by selecting the *Execute* button from the Session window. The Run Simulation window will open.

Click the *Run Simulation* button to perform all of the calculations required to evaluate compliance with the dose standard. Execution status messages will appear in the text pane of the execution dialog, as shown in Figure 4.2.13. The progress of the dose calculations will be shown in the dialog status meter. Click the *Abort Simulation* button to abort the simulations. DandD will not interrupt the current simulation, but will abort after the current simulation has completed. Therefore, the user may not get an immediate response after clicking this button.

On successful completion, the estimated 90th percentile value of the TEDE distribution used for comparison against the dose standard will be displayed (as shown in Figure 4.2.14). (As noted in Section 1, the NRC dose limit for unrestricted use is 25 mrem/year.) The endpoints of a 95% confidence interval for this quantile value are also reported. The estimated quantile value for TEDE is uncertain because it is estimated using a finite number of parameter samples. The reported confidence interval reflects this uncertainty.

In some cases, the uncertainty due to sampling error can affect the comparison against the dose standard. In these cases, the sampling error can be reduced by increasing the number of simulations (using the advanced simulation *Options*). If comparison against the dose standard is influenced by sampling error, DandD will display the Sample Size Analysis form containing information about increasing the number of simulations (see Section 4.2.7).

Clicking the *Options* button on the *Execute* form will bring up a dialog box that allows the user to set advanced simulation options as follows (see Figure 4.2.15). Most users will not need to change these options from their default settings.

- *Number of Simulations* corresponds to the number of times the model will be executed. Each time the model is executed, the values of each of the uncertain parameters vary depending on the numbers generated from sampling (by LHS). The dose model is always executed using constant values of parameters. The *Number of Simulations* used in the analysis is automatically increased if DandD determines that more samples are needed to adequately control parameter correlations or to estimate the confidence interval for the 90th percentile value of TEDE. DandD will open a window to indicate when it increases the number of simulations. After executing the dose model, DandD performs a sample size analysis and may recommend that the number of simulations be increased.
- *Seed for Random Generation* is the random number seed used to generate the values for the parameters that have probability distributions associated with them. Changing this number will change the sampled values of the uncertain parameters used in the simulations. The seed should be more than five digits long for the best sampling results. Powers of two should be avoided. The value for the seed should be in the range of 1 to 2,147,483,647.
- The *Save Dose History Information* checkbox determines whether or not dose history information is generated and saved in the session file. This information is needed to create history plots. Note that selecting this option can increase the execution time for the dose model and will significantly increase the size of the session file. History plots can be accessed after execution by using the *View/Graphics/Dose History* option on the main menu (see Section 4.3.9).

4.2.7 Sample Size Analysis

The 90th percentile of the TEDE distribution, used for comparison against the regulatory limit of 25 mrem, is estimated in DandD Version 2.1 via Monte-Carlo sampling. The resulting estimate of this statistic is subject to sampling error. The error size can always be reduced by increasing the number of samples used to estimate the TEDE distribution. Sampling error is significant if the 25 mrem limit lies within the range of possible values of the 90th percentile.

The range of possible values is indicated by the 95% confidence interval reported on the *Execute* form and

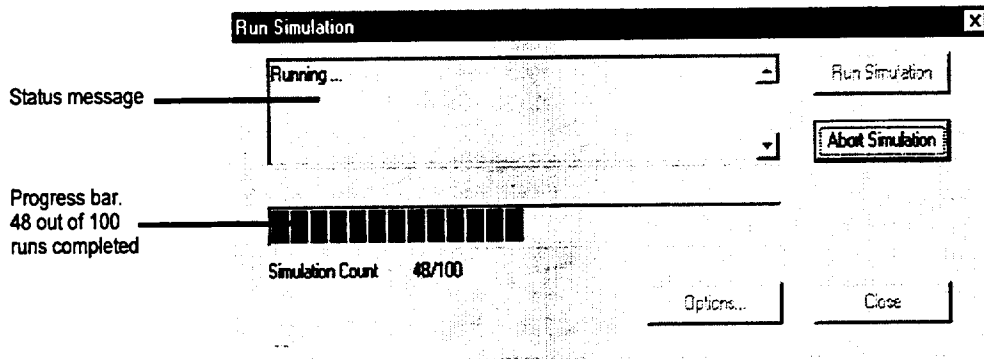


Figure 4.2.13 Run Simulation window - in progress

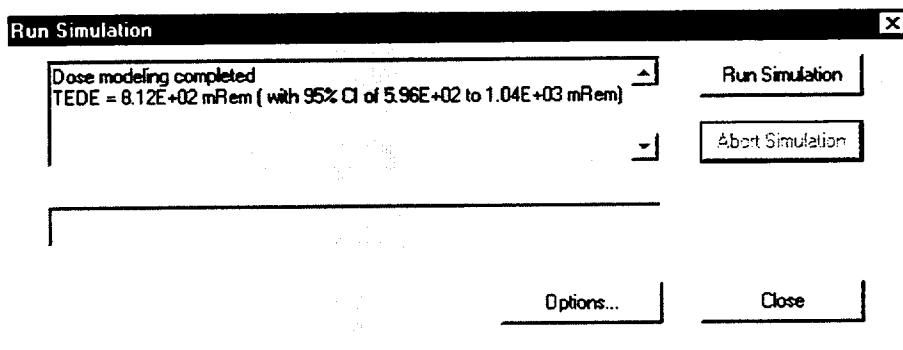


Figure 4.2.14 Run Simulation window - complete

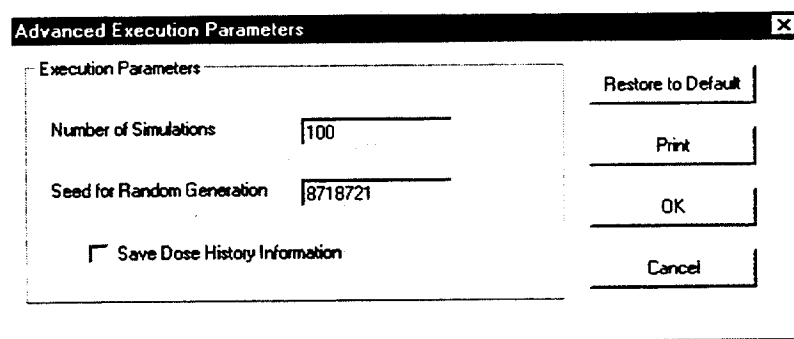


Figure 4.2.15 Advanced Execution Parameters window

in the output reports. To account for sampling error in the compliance determination, the upper endpoint of the confidence interval is the value that is compared to the regulatory limit of 25 mrem. This comparison allows for a defensible regulatory decision given the current estimate of the dose distribution, the number of samples used to estimate that distribution, and the

location of the estimate with respect to the 25 mrem limit.

The upper and lower limits of the confidence interval are reported for all calculations. If the upper limit is less than the regulatory limit, or if the lower limit is greater than the regulatory limit, then increasing the

number of samples is unlikely to affect the comparison with the dose limit, and no more information is presented.

When, however, the confidence interval includes the regulatory limit, then reducing the uncertainty due to sampling error may lead to dose estimates below the limit. In this case, the Sample Size Analysis form is automatically displayed (see Figure 4.2.16). Based on the location of the confidence interval compared to the regulatory dose limit, DandD estimates the likelihood that the upper endpoint of a narrower confidence interval, produced by increasing the number of samples, would fall below the regulatory dose limit. This estimate is made for several alternative values for the number of samples, as well as for an infinite number of samples, and is tabulated on the form.

This information can be used to decide whether increasing the number of samples is likely to be useful, and if so, how many samples to use.

For example, the Sample Size Analysis window shown in Figure 4.2.16 will open when a simulation is run resulting in a TEDE value where the 95% confidence interval straddles the performance objective of 25 mrem. In the example, the TEDE was 25.1 mrem with a 95% confidence of the TEDE values falling between 22.4 and 28.5 mrem. Because the upper and lower 95% confidence interval contains the performance objective of 25, increasing the number of samples may by itself be enough to reduce the upper endpoint of the confidence interval below the dose limit. The Sample Size Analysis window (see Figure 4.2.16) shows the effect of increasing the number of samples on the likelihood of this occurring.

The information in the Sample Size Analysis window helps the user decide how many simulations to run. To choose the sample size, the user needs to consider the real time it will take to run the model with the new value for the number of simulations. In the example shown in Figure 4.2.16, setting the number of simulations to 200 has only a 3% likelihood of demonstrating compliance. Setting the number of simulations to 6400 increases the likelihood of demonstrating compliance to approximately 23%. However, it will take 64 times as many model calculations as it takes with the number of simulations set to 100.

The user can change the number of simulations by clicking the *Options* button and entering the number of simulations in the Advanced Execution Parameters

window. Alternatively, the user could close the Sample Size Analysis window and click the *Options* button in the Run Simulation window to change the number of simulations in the Advanced Execution Parameters window. The model could then be executed by clicking the *Run Simulation* button in the Run Simulation window.

Clicking the *Print* button in the Sample Size Analysis window will create a hardcopy of this window.

4.3 Main Menu Operations

4.3.1 File Management Menu Options

The file management menu options are the *New*, *Open*, *Save As*, and *Close* commands. To execute any of these commands, click on *File* in the DandD main menu and select an option. The session file consists of a single file with an extension of "mcd" (Monte Carlo DandD).

When DandD is first started, there are no sessions opened. The first step is either:

1. Create a new session by selecting *New* from the File menu, or
2. Open an old session by selecting *Open* from the File menu.

If the user selects *New* from the File menu, a window similar to Figure 4.3.1 will open. The user should then type in a file name for the session and click the *OK* button in the Open Session dialog box.

A directory is created during installation to hold the user's files. This is the default location for all session files and reports. The name of this directory is "DandD_Docs," located on the drive where DandD was installed. However, the user can save or open the session files on any drive or directory desired.

After naming the new session in the Open Session window, a *Session Properties* form will then be displayed, and the user will be asked to enter a site name and description of the analysis. The user must enter the description and no more than 50 characters for the site name. Click the *OK* button on the *Session Properties* form to save this information. The site name and description can be modified at a later date by using the *File/Properties* feature (see Section 4.3.5).

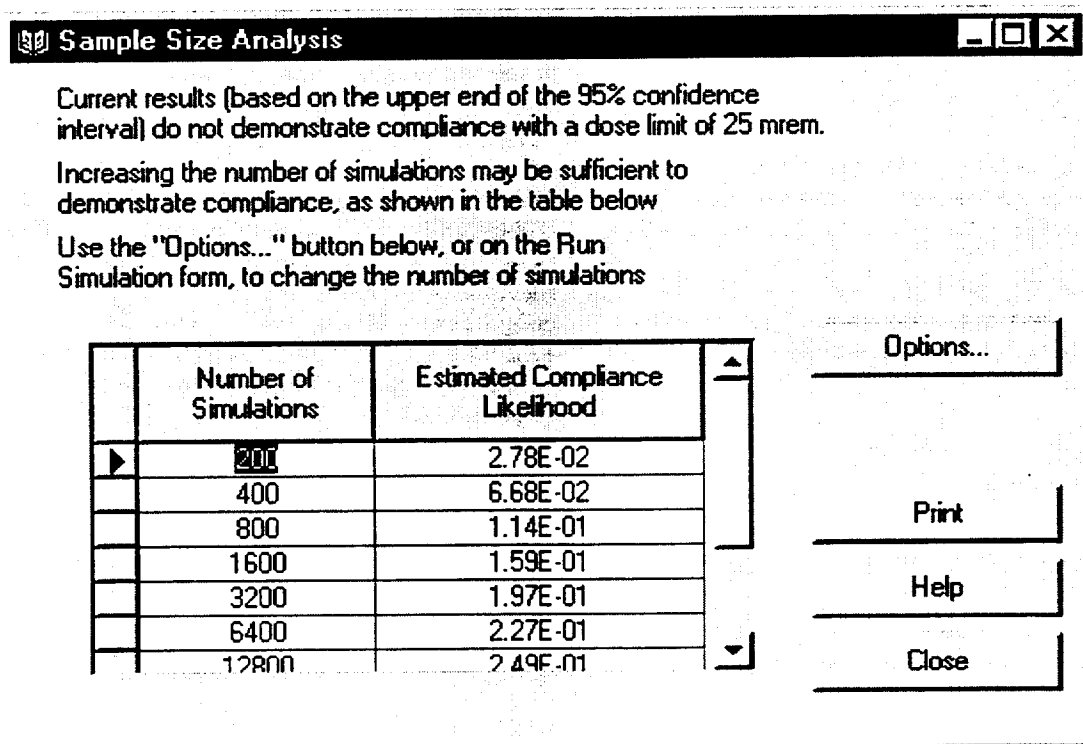


Figure 4.2.16 Sample Size Analysis window

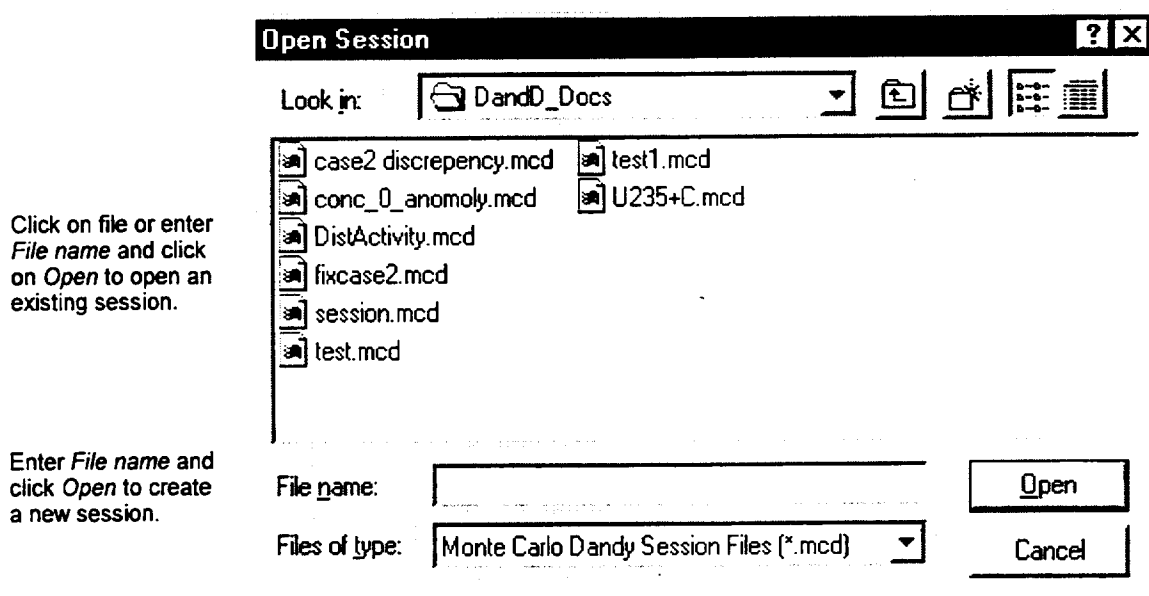


Figure 4.3.1 Open a session

If the user selects *Open* from the File menu, a window similar to Figure 4.3.1 will open. The user should then type in a file name for the session and click the *OK* button or double-click on the session file to open an existing session.

Unlike word processing applications, changes to the session file are automatically saved as they are made. This is why there is not a *File/Save* function available.

Additionally, only one session file may be opened at a time. If the user wants to use an existing session as a starting point for another session, the *File/Save As* command should be used.

See Appendix D for a complete description of the file structure developed for DandD Version 2.1.

If the user clicks *Close*, the session file is closed. All data from the simulation and any user settings will be retained.

4.3.2 File/Restore Parameters to Default Value

All site-specific parameters can be reset to the default (screening) value by using the *File/Restore Parameters to Default Value* option. This will set all parameters other than the contaminants and concentrations, including execution parameters, to their default values. This will also reset the correlations to their default values.

This option only applies to the current scenario. For example, if site-specific parameters have been specified for the residential scenario and the current scenario is building occupancy, then the command *File/Restore Parameters to Default Value* will only apply to the building occupancy scenario. Any modified residential (site-specific) values will be retained.

This option is only available if all parameter viewing windows are closed. Individual parameters can be reset to the default from their Parameter Modification window.

A checked box to the right of the parameter name in the parameter viewing screen (the window that opens when the user clicks the *General Parameters* or *Element Parameters* button; see Figure 4.1.1) indicates if the parameter is set to its default value. However, it is not reasonable to check each parameter for this in the residential scenario because there are too many parameters.

To discover which variables are set to site-specific values (i.e., a value other than the default value), create the report titled *ModelInputSummary* from the *View/Reports* menu selection (see Section 4.3.7).

4.3.3 File/Export as Zip for Submittal

The residential and building occupancy settings and simulation results are contained in a single file with an "mcd" extension (e.g., session.mcd). However, these files usually will not fit on a floppy disk. They are also bulky to email. Session files can be compressed for transmittal to the NRC using the *File/Export as Zip* command. These files can then be unzipped by using commercial packages WinZip or PkUnzip.

If the *File/Export as Zip* option is selected, a window similar to Figure 4.3.2 will open. Once a location has been selected for the new file and the user clicks the *OK* button, a copy of the session file will be compressed and saved with a zip extension. For example, if the session file is called x.mcd and the export function is executed, a new file called x.zip will be created. The file x.mcd will still be available.

It is not necessary to use the function *File/Export as Zip* to submit a session file to the NRC. This was added as a feature to easily transmit on floppy disks or to facilitate sending the session as a compact email attachment.

Using this function is also a convenient way to backup work onto a floppy disk.

4.3.4 File/Print

The *File/Print* option is used to create a hardcopy of the active window. This is only available for screens that allow concurrent interaction with other windows in the interface.

Screens that do not allow concurrent interactions (known as modal screens) will have a *Print* button in the lower right-hand corner of the screen. For example, all of the parameter viewing screens, such as the *General Parameters*, *Add Concentrations*, and *Element Parameters*, allow access to the *File/Print* option. The parameter modification form will have a lower right *Print* button.

For all screens, the print function will create a hardcopy of the window screen. In the example of a parameter viewing screen, this allows the user to identify which category and variable they have selected.

1. Choose the drive to place the compressed session.
2. Choose the directory to place the compressed session.
3. Click OK to save the compressed session.

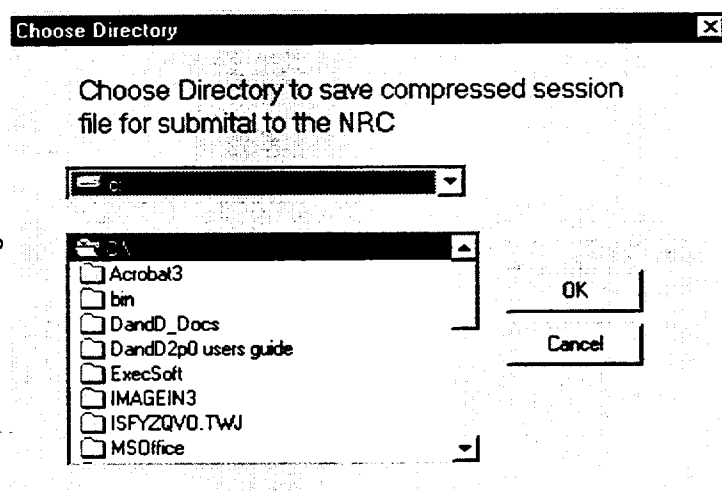


Figure 4.3.2 Save a session as a zip file

Some of the screens contain grid data that require the user to use the scroll bar to view the complete list. For example, the residential scenario *General Parameters* screen may contain two grids if the selected parameter has related empirical data, as shown in Figure 4.3.3. Following the screen shot, a dump of the primary grid will be printed. In the example of a parameter viewing screen, this will be a dump of all parameter information in the selected category. The values defining the probability distribution associated with the parameters will not be printed.

To print the data relevant to a single parameter, double-click the parameter name in the parameter viewing form. The parameter modification form should open. Within the parameter modification form, click the *Print* button. All the data relevant to the selected parameter will be printed.

Create a hardcopy of all site-specific parameter values by creating the report titled *ModelInputSummary* from the *View/Reports* menu selection. Print using the browser window print function.

Create a hardcopy of all values by running a simulation and creating the report titled *Detail* from the *View/Reports* menu selection. Print this information by using the browser window print function.

4.3.5 File/Properties

To modify the properties of a session (i.e., the session name and analysis description), select *Properties* from

the File menu. A window will open similar to Figure 4.3.4 that will allow these properties to be modified. Modify the site name and analysis description. Click *OK* to accept the changes and close the window.

When a new session is created, this window will open to allow the user to define the initial session properties. The user will be required to enter the site name and the analysis description (the site name must be no more than 50 characters). This information is used when the final reports are created via the *View/Reports* menu item (see Section 4.3.7).

4.3.6 Edit/Copy

The Edit/Copy function is available when the user has a graph opened. This function will put a copy of the graph and the data associated with the graph on the Microsoft® Windows® clipboard. It can be pasted as a graphic image in Microsoft® Word® or Corel® WordPerfect®, using the *Paste Special* command. If the Paste function in Microsoft® Word®, Corel® WordPerfect®, or Microsoft® Excel® is used instead, the x-y data pairs that define the curves on the plot will be pasted into the document.

The user can use the keyboard shortcuts Ctrl + V (press V while holding down the Control key) to paste, Ctrl + C to copy, and Ctrl + X to cut selected text from the justification and text fields of other windows. However, the *Edit/Copy* menu command is not available for text fields. An example of using the graphics copy feature to paste a copy of a graph into a report

File/Print will output a screen shot of current window.

File/Print will output all data in the selected category. In this example, the category is Wet-To-Dry.

To output all of the data corresponding to a variable, click on *Modify* and use *Print* button in the modify parameter window.

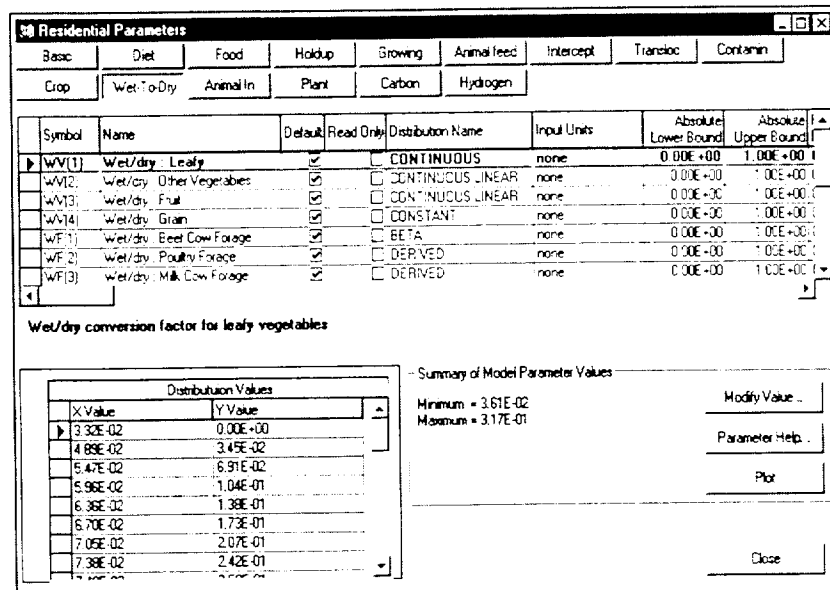


Figure 4.3.3 Print function with respect to parameter viewing window

created by DandD follows.

- Step 1: Create the report by using the *View/Reports* command. For example, create the report *Summary* under the building occupancy simulation. The default Internet browser will be started and the file containing the report *session_bld_Summary.htm* will be opened. Make note of the path and filename of this report from the Location field of the browser window, as shown in Figure 4.3.5.
- Step 2: Open up a word-processing program such as Microsoft[®] Word[®] or Corel[®] WordPerfect[®]. Open the report created in Step 1 in this application. Alternatively, the user could select *Communicator/Page Composer* from the Netscape main menu and open the report in this application.
- Step 3: Create the desired graph in DandD using the *View/Graphics* choices off the main menu or the *Plot* command from the Parameter viewing screen. Select the desired graphic elements, and then invoke *Edit/Copy* from the main menu to create a copy of the graphic on the clipboard.
- Step 4: If using Microsoft[®] Word[®] or Corel[®] WordPerfect[®], select the *Edit/Paste Special* function. A window similar to Figure 4.3.6

will open. Choose the *Paste* radio button, *As Picture*, and click *OK*.

If using *Composer*, first create a file that contains the graphic. The graphics are stored as separate files for web pages. To do this, start Microsoft[®] Windows[®] Paintbrush from the Microsoft[®] Windows[®] Accessories group. Select *Edit/Copy* from Paintbrush to paste the graphic into Paintbrush. Adjust the size of the paint window to minimize the bits to save by selecting *Image/Attributes* and setting the width and height to the actual width and height of the graphic, as shown in Figure 4.3.7. Save the graphic in the directory where the report is saved (this is, by default, DandD_Docs) as a 24-bit bmp file.

Within Netscape *Composer*, select *Insert/Image* from the main menu. On the *Image* tab, click the *Choose File* button. Select the file saved in Paintbrush. Click *OK* when prompted to convert the file to jpg format. The graphic will be inserted.

4.3.7 View/Reports

When the DandD dose calculations are completed (Section 4.2.6), the results can be used to generate reports that describe the input data and resulting dose

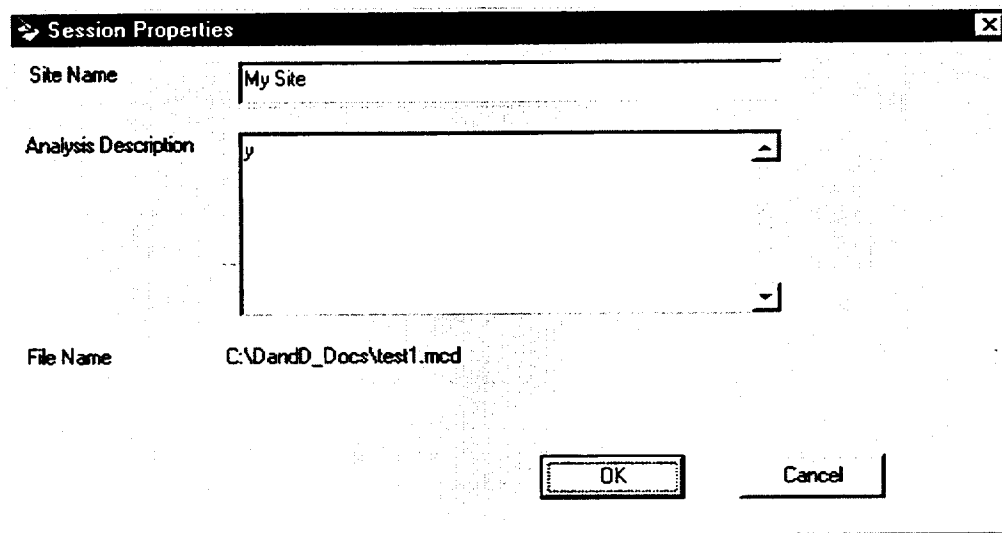


Figure 4.3.4.. Session properties dialog box

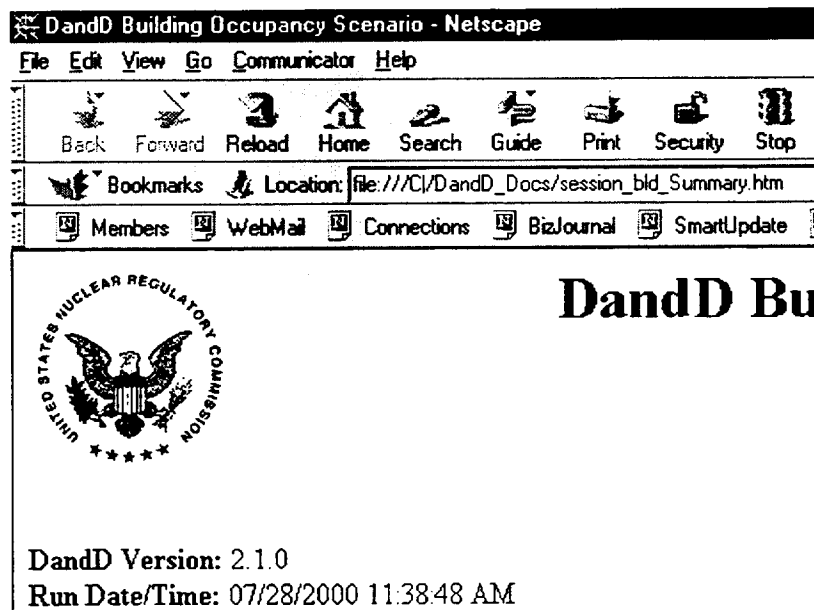


Figure 4.3.5 Path of report shown in location text box in Netscape.

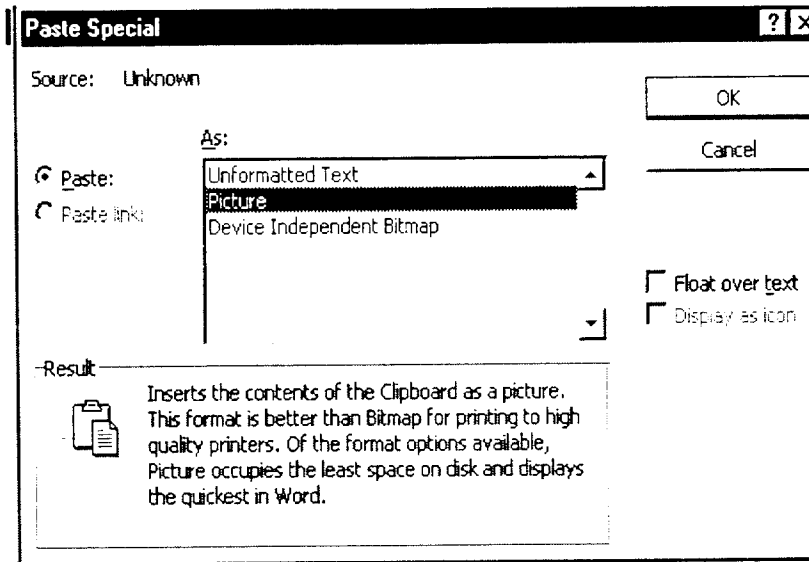


Figure 4.3.6. Paste a graphic into a document using Microsoft[®]Word[®] or Corel[®]WordPerfect[®]

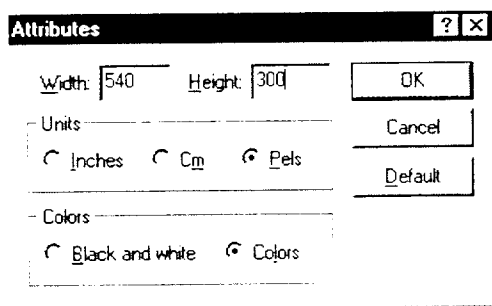


Figure 4.3.7 Adjust size of window in Paintbrush

value by selecting *View/Reports* from the main menu. These reports are generated as HTML files. A browser such as Internet Explorer or Netscape must be installed to view the reports from DandD. Because HTML is a standard format, reports may also be opened in a word-processing package such as Microsoft[®] Word[®] or Corel[®] WordPerfect[®]. Reports can also be opened in an HTML editor such as Netscape Composer.

The reports are created in the same directory as the session file. The report name is built using the scenario, the session name, and the template name. For example, the report Test_bld_Summary.htm was generated by a session titled Test.med from the building occupancy scenario (bld) using a template called Summary.

After a simulation is completed, reports are not automatically generated. Reports are generated on request by using the *View Reports* form, as shown in Figure 4.3.8. Once the report has been generated, it will be available on the hard drive.

To generate a new report file, click the radio button *Create a report based on current session*. Select the report template by clicking on the desired template. Either double-click on the template name or click on the *Create Report* button to generate a new report.

The first three template entries are default report templates. If any custom templates have been defined by using the *Advanced/Report Template Editor* option from the main menu, those template names will also be listed (see Section 4.3.10).

To view a previously created report, click the radio button *View a saved report*. A *File Open* dialog box will open. Select the desired HTML file to open. The default browser will start and the file will be loaded.

The reports can be opened with a word-processing program such as Microsoft[®] Word[®] or Corel[®] WordPerfect[®]. They can also be posted to web sites, saved as text files from the browser, or printed from the browser.

1. Choose to create a new report or view an existing report.
2. Select a report template if creating a new report.
3. Click on Create Report or View Report depending on the choice made at Step 1.

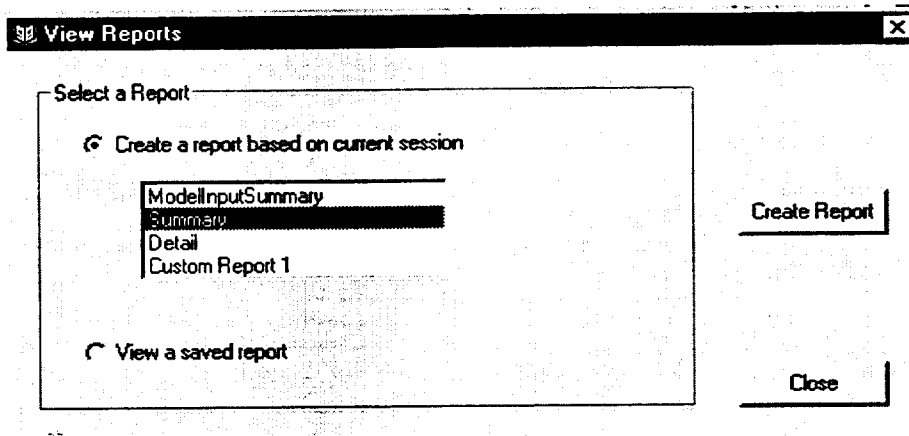


Figure 4.3.8 View Reports window

The following default report templates are always available:

1. *Model Input Summary* summarizes the model input and the site-specific parameter values. This option is available even when there are no output results.
2. The *Summary* report is a terse description of the session. It lists the major program options and describes any changes from the default parameter values or distributions. Parameters left at their default settings are not listed in the report. Output from the simulation is limited to the calculated dose value.
3. The *Detail* report is a comprehensive list of all of the program settings and parameter values, as well as detailed information that breaks down the calculated dose into pathway and nuclide components. The report lists the values or distributions for each parameter, whether or not it has been changed from the default value. Because of the large number of parameters in the residential scenario model, the *Detail* report can be quite lengthy and may take some time to generate.

Additionally, custom report templates can be defined by using the *Advanced/Report Template Editor* option from the main menu (Section 4.3.10).

If the site data are changed in any way, DandD will delete any associated report files that were generated. This allows the software to ensure that the data shown in the report are consistent with the data saved in the session.

4.3.8 View/Tables

There are four tables in DandD that the user is not permitted to edit. However, the user can view the data in these tables by selecting the table name from *View/Tables* in the main menu. A window will open displaying the data, as shown in Figure 4.3.9. When the user has finished viewing the data, the window may be closed by clicking the *Close* button or choosing the *File/Close* option from the main menu.

Appendix E contains an explanation of the data in these tables. The data are not listed in this document, but can be viewed or printed from DandD. The meaning of the columns within these tables is as follows.

Radioactive Decay Data

Parent refers to the original contaminant, not the immediate parent in the decay chain.

Progeny is a by-product in the decay chain of *Parent*.

HalfLife is half-life of *Progeny*.

PositionInChain is number of decay generations from *Parent*. A radionuclide directly descended from *Parent* will have a value of 2 for *PositionInChain*. If *Parent* and *Radionuclide* are equal, then *PositionInChain* will be equal to one.

FirstParentIndex indicates which radionuclide in the chain is the immediate parent of this nuclide.

Soil Class	Mean LN	SDev LN Ksat	KSat Minimum	KSat Maximum	KSat P
silt	-10.06	0.5259			
sandy clay	-11.7	1.706			
sandy clay loam	-8.782	1.22			
silty clay	-13.78	1.224			
loamy sand			0.000039	0.0134	0.79836133
clay	-11.36	1.509			
clay loam	-10.22	1.414			
silty clay loam	-11.96	1.327			
sand			0.00035	0.0186	1.31616284
sandy loam	-7.182	0.9292			
silt loam	-10.24	1.383			
loam	-8.81	1.159			

Figure 4.3.9 View data table window

FirstParentFraction is fraction of decays of the first parent that produce *Progeny*.

SecondParentIndex indicates alternate radionuclide that can decay to *Progeny*.

SecondParent is fraction of decays of the second parent that produce *Progeny*.

AtomicNumber is number of protons in the *Progeny*.

Dose Equivalent Factors

Parent is name of the parent radionuclide.

Radionuclide is name of the radionuclide.

ImplicitProgenyFraction is fraction of parent transitions that produce this radionuclide.

Ingestion is unit committed effective dose equivalent (CEDE) conversion factor for ingestion.

Inhalation is unit CEDE conversion factor for inhalation.

ExternalSurface is unit CEDE conversion factor for external surface exposure.

External15cm is unit CEDE conversion factor for external exposure at 15 cm.

Residential Soil Characteristics

This table holds the parameters that describe the hydrologic characteristics of 12 soil types defined by the United States Bureau of Reclamation (USBR) (see Appendix E). These characteristics can be used to derive interrelated values for the soil parameters of the residential scenario model. *Ksat* is the saturated conductivity, and "b" is the "b" parameter of the saturation/permeability model.

SoilClass is the name of the soil classification. *Mean Ln* is the mean value of the natural log of *Ksat*, in cm/sec, for soils with a lognormal distribution.

S Dev LN Ksat is the standard deviation of the natural log of *Ksat* for soils with a lognormal distribution.

K Sat Minimum is the minimum value of *Ksat* for soils with a beta distribution.

K Sat Maximum is the maximum value of *Ksat* for soils with a beta distribution.

K Sat P is the P parameter of the beta distribution of *Ksat* for soils with a beta distribution.

K Sat Q is the Q parameter of the beta distribution of *Ksat* for soils with a beta distribution.

Mean Ln B is the mean value of the natural log of parameter “b” for soils with a lognormal distribution.

Sdev LN B is the standard deviation of the natural log of “b” for soils with a lognormal distribution.

B Minimum is the minimum value of “b” for soils with a beta distribution.

B Maximum is the maximum value of “b” for soils with a beta distribution.

B P is the P parameter of the beta distribution of parameter “b” for soils with a beta distribution.

B Q is the Q parameter of the beta distribution of parameter “b” for soils with a beta distribution.

Mean NI is the expected value of porosity.

SDev NI is the standard deviation of porosity.

Residential USBR Percolation Fractions

Ksat is the saturated permeability in cm/sec.

Percolation Fraction is the estimated fraction of applied water that becomes infiltration.

4.3.9 View/Graphics

When the dose calculations are completed, the results can be displayed by selecting View/Graphics from the main menu. Three plot types are available from this menu selection, as described in 4.3.9.1 through 4.3.9.3.

Plots of individual parameter distributions are also available for each parameter if the user clicks the *Plot* button in the parameter viewing window (i.e., the window that opens when the user clicks *Add Concentrations*, *General Parameters*, or *Element Parameters*; see Section 4.1.2).

See Section 4.1.4 for a description of how to navigate a graphics window.

4.3.9.1 Dose Distribution

The dose distribution graph shown in Figure 4.3.10 shows the complementary cumulative distribution function (CCDF) for peak TEDE. For the possible values of dose, plotted on the x axis, the CCDF shows the fraction of simulations that have larger values. The initial graph depicted following a DandD simulation

shows the PDF for dose from all active pathways due to all radionuclides.

4.3.9.2 Time Distribution

The time distribution graph shown in Figure 4.3.11 shows the CCDF for the time of peak TEDE. For the possible values of time, plotted on the x axis, the CCDF shows the fraction of simulations that have peak doses at later times. If the peak dose occurs at the same time in all simulations (as it always will in the building occupancy scenario), the CCDF is a vertical line at the x location of the common time value.

4.3.9.3 Dose History

A statistical summary of dose histories is available if the *Save Dose History Information* option has been selected by using the *Options* button from the Run Simulation window (see Section 4.2.6). Each set of sampled parameters produces a single dose history. At each timestep, DandD calculates the average value of dose, as well as the standard deviation of dose. The graph shown in Figure 4.3.12 shows the time variation of the average dose and the average plus and minus one standard deviation. The initial graph (following DandD execution) shows the history plots for dose from all active pathways due to all radionuclides.

History plots for selected pathways, due to all radionuclides, can be included in the graph by selecting the pathway (or *All*) from the *Pathways* list box and clicking the *Add to Plot* button. Plots for selected radionuclides, via all pathways, can be included by selecting a radionuclide (or *All*) from the radionuclides list box and clicking the *Add to Plot* button. History information for the combinations of individual pathways and individual radionuclides is not saved because of the large amount of storage space that would be required.

For each selected pathway or radionuclide, three curves are added to the graph, showing the average dose and the average dose plus and minus one standard deviation. In some cases, the average dose minus the standard deviation may be negative. This does not mean that the dose can be negative. This result is caused by a standard deviation of dose that is large relative to the average dose.

4.3.10 Advanced/Report Template Editor

The *Report Template Editor* form allows the user to create, modify, or delete a custom report template. Reports are not created in the Report Template Editor

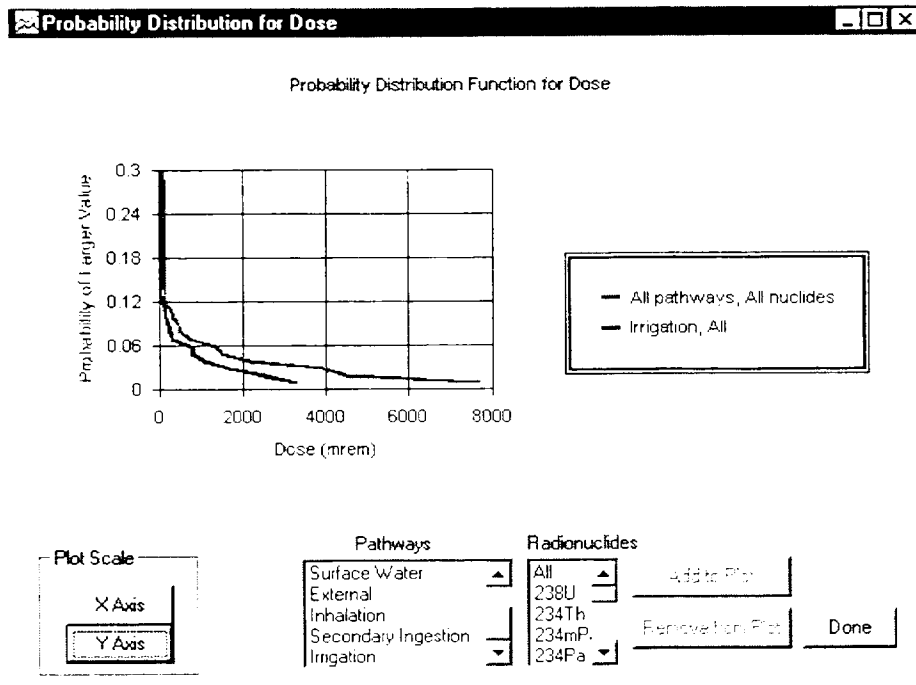


Figure 4.3.10 Dose distribution

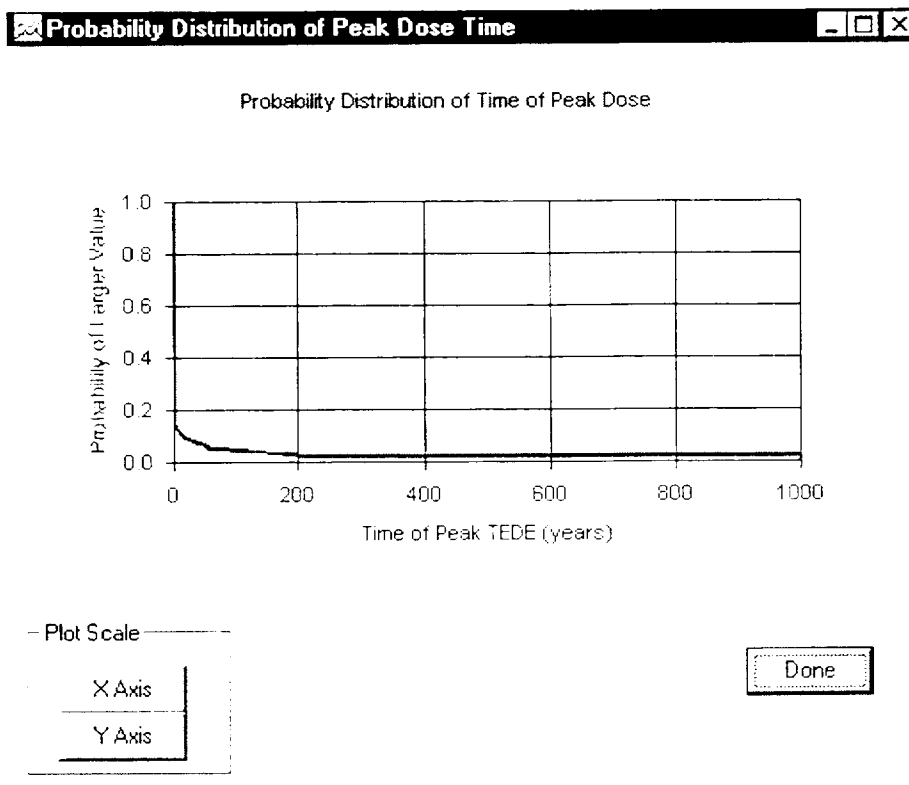


Figure 4.3.11 Time distribution

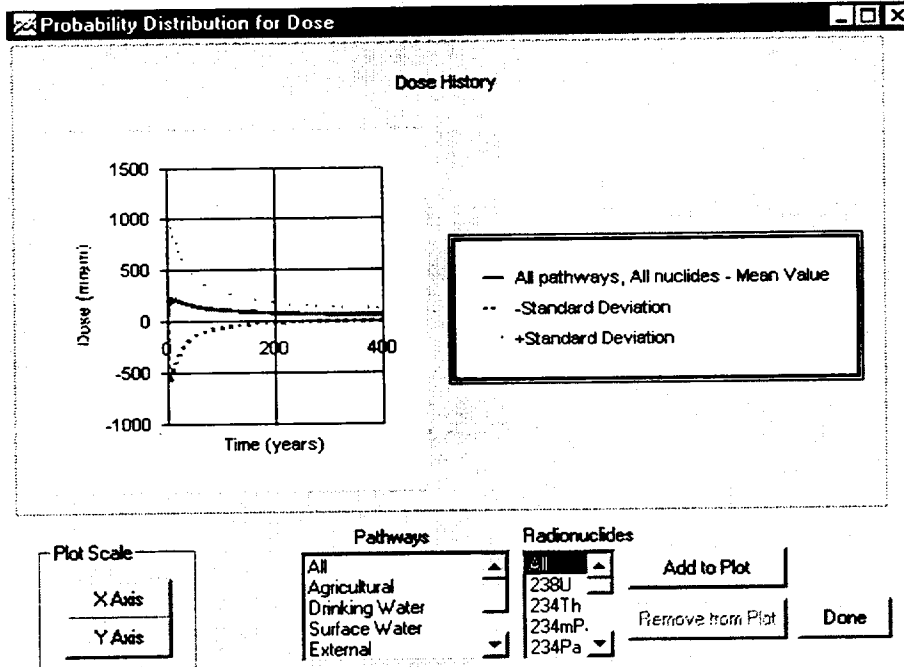


Figure 4.3.12 Dose history

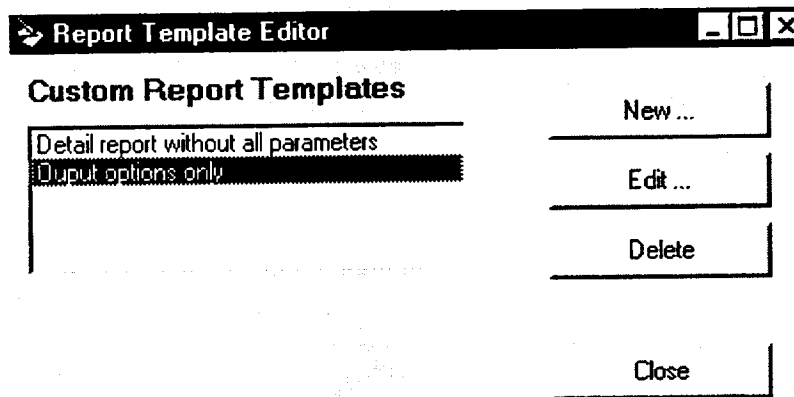


Figure 4.3.13 Selecting a custom report to edit or delete

window. To actually create reports from templates after a DandD simulation, use the *View/Reports* option from the main menu (see Section 4.3.7).

Select *Advanced/Report Template Editor* from the main application menu to open the Report Template Editor window, as shown in Figure 4.3.13. The *Edit Report Template* form will allow the user to change or specify a new custom report template. This form can be accessed by clicking the *New* or *Edit* button on the *Report Template Editor* form.

To create a new report template, click the *New* button. To edit an existing report template, select the template in the *Custom Report Templates* list. Click the *Edit* button. In either case, the *Edit Report Template* form will appear, as shown in Figure 4.3.14.

To delete an existing report template, select the template in the *Custom Report Templates* list. Click the *Delete* button.

To close this window, click the *Close* button.

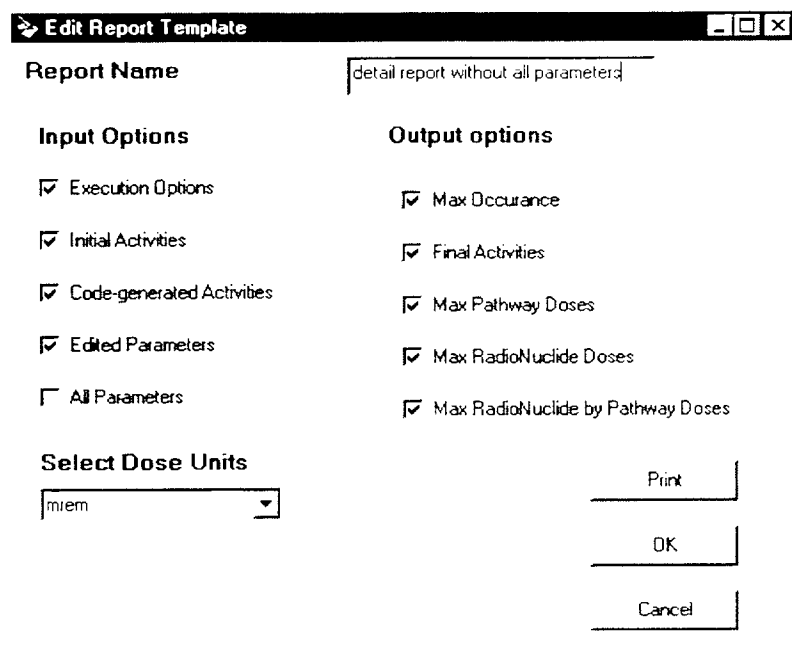


Figure 4.3.14 Report template editor

If creating a new report template (i.e., if the user clicked *New* in the Report Template Editor window), enter a name for the template in the *Report Name* field. Alternatively, if editing an old report template (i.e., the user clicked *Edit* in the Report Template Editor window), the text in the *Report Name* field will already be filled in. This text can be modified.

If an old browser such as Internet Explorer 2.0 is being used to view reports, the template name should have no embedded blanks.

Select (or deselect) the sections wanted on the report by clicking the listed checkboxes. Select the units to report the dose from the *Select Dose Units* pull down menu. Click the *Print* button if a copy of this form is desired.

Click the *OK* button to save the template modifications. Otherwise, click the *Cancel* button.

4.3.11 Advanced/Sensitivity Analysis

Once a simulation is completed by executing the model, the sensitivity analysis portion of DandD can be run to find the relationships between uncertain model parameters and calculated doses. To do this, select

Advanced/Sensitivity Analysis from the application menu. The Data Influence Evaluation window will open, as shown in Figure 4.3.15.

4.3.11.1 Selecting Parameters for Sensitivity Analysis

The upper grid labeled *Available for Analysis* lists the uncertain model parameters defined by probability distributions. This table includes a symbol of each parameter as used by DandD, a description of each parameter, a checkbox indicating if a default or site-specific value was used, the sensitivity ranking, and whether the parameter is in the *Selected for Analysis* grid. The parameters are sorted by decreasing sensitivity.

Sensitivities are not calculated for model parameters with constant values. Parameters with constant values are not available for selection because the sensitivity analysis module in DandD identifies how uncertainty in the parameter value influences uncertainty in dose.

The program calculates a sensitivity ranking for each of the uncertain parameters. A measure of the sensitivity of the dose to the parameter value, which ranges from 0 to 1, is listed for each parameter, where 1 indi-

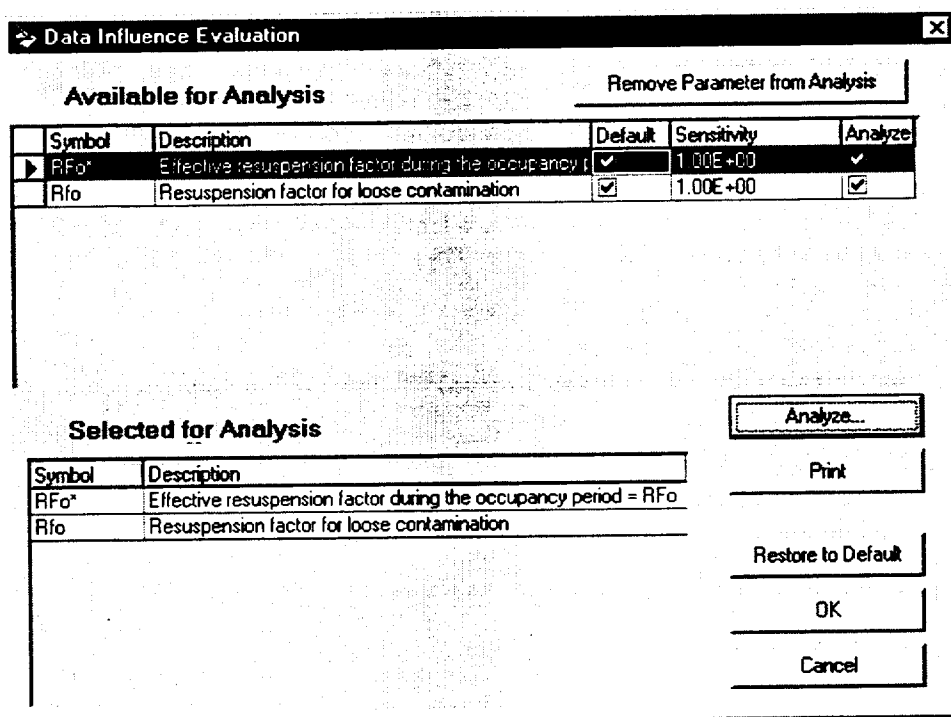


Figure 4.3.15 Data Influence Evaluation window

cates highest sensitivity. This sensitivity measure reflects the dependence of calculated dose on the parameter value. This measure is based on the significance level of the Kolmogorov-Smirnov (K-S) statistic for the parameter (see Section 4.3.11.4 for a description).

The first time the Data Influence Evaluation window is opened after a simulation, the lower table labeled *Selected for Analysis* contains parameters with a sensitivity of 0.95 or greater. This is the default setting.

The upper table indicates that a parameter is currently selected by displaying a checkmark in the column labeled *Analyze*. The user can select new parameters by selecting the appropriate row in the upper table and clicking the *Select Parameter for Analysis* button. An entry for the parameter will be added to the lower table labeled *Selected for Analysis*.

Parameters that are already selected can be removed by selecting the parameter's row in the upper table and clicking the *Remove Parameter from Analysis* button (note that this button toggles between *Select* or *Remove* depending on the current *Analyze* checkbox setting for the parameter). The user can also remove or add parameters from the *Selected for Analysis* grid by double-clicking on the parameter in the *Available for*

Analysis grid.

Click the *Restore to Default* button to restore the *Selected for Analysis* grid to include only parameters with a sensitivity of 0.95 or greater.

After one or more parameters have been selected for analysis, clicking the *Analyze* button will invoke the sensitivity analysis application. A description of this application is provided below. The sensitivity analysis module is an independent application that shares data with DandD.

The *Print* button prints the entire list of parameters, along with their sensitivity indicator values. Click the *OK* button to close this window and save the current state of selected parameters. If this is done, the next time this window is opened the parameters shown in the *Selected for Analysis* grid will reflect this saved state.

Click the *Cancel* button to close this window and disregard the current state of selected parameters as shown in the *Selected for Analysis* grid. If this is done, the next time this window is opened the parameters shown in the *Selected for Analysis* grid will be identical to the initial state the last time the *Data Influence Evaluation* window was opened.

If the simulation is run again, the saved states will be disregarded. The variables selected for analysis in the *Data Influence Evaluation* window will only contain parameters with a sensitivity of .95 or greater.

4.3.11.2 Using the Sensitivity Analysis Application

The objective of the sensitivity analysis is to understand the relationship between the model parameter values and the calculated dose values. This information will help to identify parameter modifications that might lead to significant changes in the calculated dose distribution.

Sensitivity analysis is a separate custom Microsoft[®] Windows[®] application. DandD will launch this application when the user clicks the *Analyze* button from the Data Influence Evaluation window. The sensitivity analysis application loads data from the session file. Each parameter in the *Selected for Analysis* list in the Data Influence Evaluation window will be loaded into the sensitivity analysis application.

This application can be closed using its File:Exit command or the "X" button on the Sensitivity Analysis window. Because this is a separate application that shares data with DandD, this window should be closed before returning to DandD.

The Sensitivity Analysis window is divided into top, middle, and bottom sections that are separated visually by thin horizontal black lines, as shown in Figure 4.3.16.

The top section is relatively small and only contains the number of realizations (or simulations) analyzed and a color legend. The middle section is where the user can modify settings specific to a parameter to study the sensitivity of that parameter. This section contains two graphs. The graph on the left, entitled "Total Dose," is the plot of the probability distribution for dose. This plot is identical to the plot displayed when *View/ Graphics/Dose Distribution* is selected from the main menu, except that the user may change the displayed performance objective (P.O.) dose value.

The graph on the right, labeled with the name of a selected parameter, is a histogram constructed of the selected parameter values sampled by DandD for each simulation. It consists of the sampled parameter value along the x axis versus the number of occurrences on the y axis.

The bottom section is the largest of the three sections and contains histograms for all of the input parameters specified in the Selected for Analysis list in the Data Influence Evaluation window in DandD. The window may need to be scrolled to see the histograms for all selected parameters. To select an input parameter, the user will need to double-click (or right-click) on the small plot to copy the graph from the bottom to the middle section.

4.3.11.3 Description of Controls

Users can explore the relationship between dose and parameter values by adjusting the P.O. value in the dose graph and observing the tendency of high dose values to cluster near the extreme values of certain parameters.

If a parameter has a strong correlation with dose, then the simulations leading to large dose values, colored red, will tend to cluster near one end of the parameter distribution. If a parameter is only weakly correlated to dose, the red and blue values will tend to be evenly distributed over the range of the parameter values.

If a parameter has a strong correlation with dose, then collecting data about that parameter, which will reduce uncertainty about the parameter value, will tend to change the dose distribution and may therefore change the compliance status.

The potential influence of site-specific parameter information can be approximated by "clipping" or truncating parameter values from the high and low ends of the current parameter distribution. For the currently selected parameter (shown in the upper-right hand graph), the largest or smallest values (or both) can be truncated from the distribution by dragging the vertical limit lines in this graph to the right or left. Parameter samples that fall outside the limit lines are colored green on the parameter graph and are excluded from the main dose distribution graph. In this way, the potential effect of narrowing the distribution for a parameter on the resulting dose distribution can be readily estimated and visualized (see Figure 4.3.17).

The legend in the top section shows the following entries:

- **Passes P.O. Value:** Realizations with dose values less than the P.O. value are shown in blue on the total dose graph and on the parameter graphs.

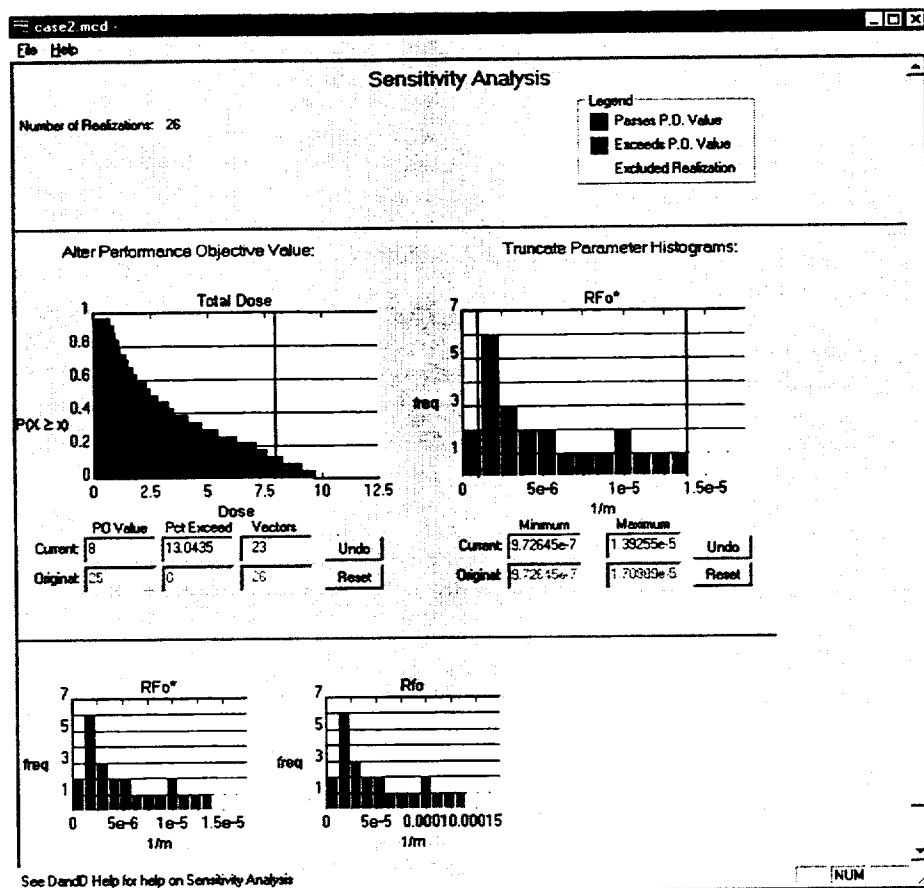


Figure 4.3.16 Three parts of the sensitivity analysis window

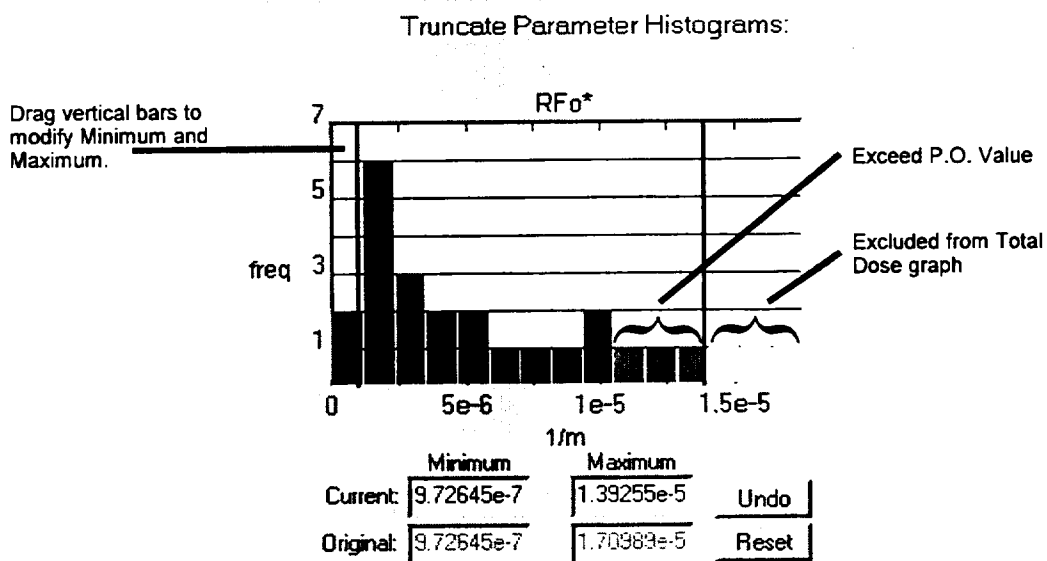


Figure 4.3.17 Histogram of parameter selected for sensitivity analysis

- **Exceeds P.O. Value:** Realizations with dose values larger than the P.O. value are shown in red on the total dose graph and on the parameter graphs.
- **Excluded Realization:** Parameter samples that fall outside the limit lines (maximum and minimum values in the row labeled *Current*) are colored green on the parameter graph and are excluded from the total dose graph.

A given parameter value may have some red and some blue for the same value on the histogram. This indicates that some of the realizations passed and some exceeded for the same value (or close to the same value) of the parameter in question. This happens because other uncertain parameters within that histogram bar may be controlling the total dose.

If all calculated dose values are either above or below the regulatory limit, the entire distribution will be shown as red or blue, respectively. In this case, compliance with the dose standard is either achieved already or is very unlikely given the scenario, pathways, and models.

Both plots in the middle section have two rows of informational text boxes located just below them. The top row, labeled *Current*, shows the current settings of the plot. These may be modified by the user. The next row, labeled *Original*, shows the original settings of the plot.

The total dose plot text boxes have the following meanings:

- **P.O. Value:** The user can modify the P.O. by changing the value of this text box from the default of 25 mrem to a larger or smaller number. The user must tab or select another control for the revised P.O. value to take effect.

If the total dose plot shows values both below and above the P.O. value, the P.O. value is indicated by a vertical line on the chart. This line can be selected and moved to the left and right to change the P.O. value.

- **Pct Exceed:** indicates percentage of realizations that have exceeded the P.O. If the NRC-defined P.O. requires the acceptable percentage of passing results to be 90%, this is equivalent to a 10% exceedance. Lower exceedance rates are better than higher. Excluded vectors are not considered in this calculation. Modifying this number manually will have no effect; it changes automatically

when the P.O. value is modified, or when a parameter histogram is truncated.

- **Vectors:** indicates the number of realizations that were used to graph the total dose plot. The user indirectly modifies the number of realizations used by dragging the vertical bars on the parameter plot. Modifying this number manually will have no effect on the plots.

The *Undo* button will cancel the last modification made to the related row labeled *Current*. For example, if some of the simulations were removed from the total dose graph by changing the value of *Minimum*, clicking the *Undo* button will set the value of *Minimum* to the value it had before it was modified.

The *Reset* button located to the right of these rows will reset the row labeled *Current* to the values in the row labeled *Original*. In other words, the current values in the row will be reset to the default values.

The allowed values for the *Minimum* and *Maximum* are restricted to fall within the actual parameter values calculated by LHS. For this reason, the software will restrict the minimum or maximum that is entered for the parameter bounds. These bounds can be modified by:

- moving the vertical lines on the parameter graph by using a click-and-drag motion;
- manually entering a new value in the text boxes labeled *Minimum* and *Maximum*;
- clicking the *Reset* button to reset the *Minimum* and *Maximum* values to the default (original) values; or
- clicking the *Undo* button to reset the last value entered to its previous value.

If there is difficulty in moving the vertical lines on the graph, clicking the *Reset* button under the parameter histogram will reset the *Minimum* and *Maximum* values to their original values. All simulations, other than those removed by modifying other parameter bounds, will be reset in the total dose plot.

Distributions for more than one parameter can be truncated as described. After the upper and lower limit lines are set for the first parameter, any other parameter can be selected by double-clicking on the small distribution graph for that parameter. The distribution for the second parameter will then be moved to the main

parameter graph, where its upper and lower limits can be set. Any limits set for the first parameter are preserved and can be recalled by selecting that parameter from the field of small parameter graphs.

The eliminated simulations are preserved and cumulative when multiple parameter histograms are modified. For example, if ten realizations have been eliminated by restricting the bounds on parameter one, and the user double-clicks on the histogram representing parameter two, then those realizations previously eliminated will still be eliminated. More simulations can be eliminated by restricting the bounds on parameter two. All of the other plots will be updated to show these additional eliminated simulations.

When eliminating bounds or modifying the P.O., some of the parameter graphs may become greyed out. This means that by calculation of the K-S test, these parameters do not significantly determine whether dose is above or below the P.O. (see Section 4.3.11.4). If a parameter has a sensitivity ranking less than 0.95, the histogram will have a grey background.

Some dose and parameter distributions are more easily viewed using a logarithmic scale. The scales for both the total dose graph and main parameter graph can be changed by right-clicking on the x axis title or the y axis title. A pop-up menu allows the axis scaling to be changed between linear and logarithmic.

Referring to Figure 4.3.17, there were a total of 26 simulations. This can be directly read from the graph by counting the number of squares on the histogram. Each square represents one simulation. The total number of squares in the histogram is the same as the *Number of Realizations* indicated on the upper left corner of the *Sensitivity Analysis* window, as shown in Figure 4.3.16.

The user eliminated three of the 26 simulations from consideration in the total dose graph by changing the value of *Maximum* to 1.39255E-5, indicated by the color green, as shown in Figure 4.3.17. Out of the 23 simulations remaining, three had a total dose that exceeded the performance objective, indicated by the color red, as shown in Figure 4.3.17. The vertical bars in Figure 4.3.17 indicate the *Minimum* and *Maximum* values graphically. The value for *Current Vectors* will be 23 in the total dose graph, indicating that 23 of the 26 vectors are plotted in the total dose graph, as shown in Figure 4.3.16.

4.3.11.4 Kolmogorov-Smirnov Statistical Test for Sensitivity

The sensitivity measure that indicates the dependence of the calculated dose on the value of each uncertain parameter is based on the K-S test for differences between the distributions underlying two sets of sample values.

The calculated dose values are first divided into two groups: one group with "high" doses and the second with "low" doses. Second, the parameter values used in the calculations leading to high doses are grouped together, while the parameter values for the low dose calculations are placed into a separate group. Third, the empirical probability distributions defined by these two groups of samples are compared using the K-S test. Parameters having a strong influence on dose will show large differences between the two distributions, leading to a large value for the K-S test statistic. Parameters with little or no influence on dose will have approximately the same distribution in the high-dose and low-dose groups, leading to a small value for the K-S statistic.

The sensitivity measure reported by DandD is $1 - Q$, where Q is the significance level of the observed value of the K-S statistic. Low values of Q mean that the observed difference between the distributions is unlikely to be the consequence of random error and is therefore likely to reflect a real difference between the high-dose and low-dose parameter sets.

The sensitivity in the Data Influence Evaluation window is based on partitioning the samples by the median dose. In the Sensitivity Analysis window, instead of grouping the simulations based on the median dose, the simulations are grouped based on the *P.O. Value*. This means that it is possible for the Sensitivity Analysis window to indicate that parameters are not sensitive when the same parameter may have had a sensitivity ranking greater than or equal to 0.95 in the Data Influence Evaluation window. This also means that some parameters may be sensitive only for certain *P.O. Values* in the Sensitivity Analysis window.

4.3.12 Window Menu Options

The *Window* menu contains standard windowing operations to help manage the window placement within the application.

The *Window/Cascade* option is very helpful if a window is hidden because one window is directly on top

of another window. Selecting *Window/Cascade* will cause the windows to be stacked. Windows may have to be resized in order to access all of the buttons on each window.

The *Window/Tile Horizontal* and *Window/Tile Vertical* options are useful to compare the contents of two windows. For example, to compare two graphs, minimize the main session window by clicking the *iconize* (or minimize) button on the upper right hand part of the window, as shown in Figure 4.3.18. Open the two graphics windows using the *View/Graphics* selection and select *Window/Tile Horizontal*.

The *Window/Arrange Icons* button may be useful if some of the icons have been moved, and need to be seen. This selection is only relevant if windows have been iconized.

4.3.13 Help Options

The *Help* menu gives access to the online help files (see also Section 4.1.1). Help for using the graphical user interface can be accessed by selecting the *Help/Contents* and *Help/Search On* options.

The *Help/NRC References* addresses the more technical issues of modeling. This will work only if a frame-enabled browser such as Internet Explorer 3.0 or Netscape Navigator 3.0 has been installed.

The *Help/About* option will give information regarding the version of DandD that is currently running.

Additionally, context-sensitive help with the user interface is available by pressing the F1 key.

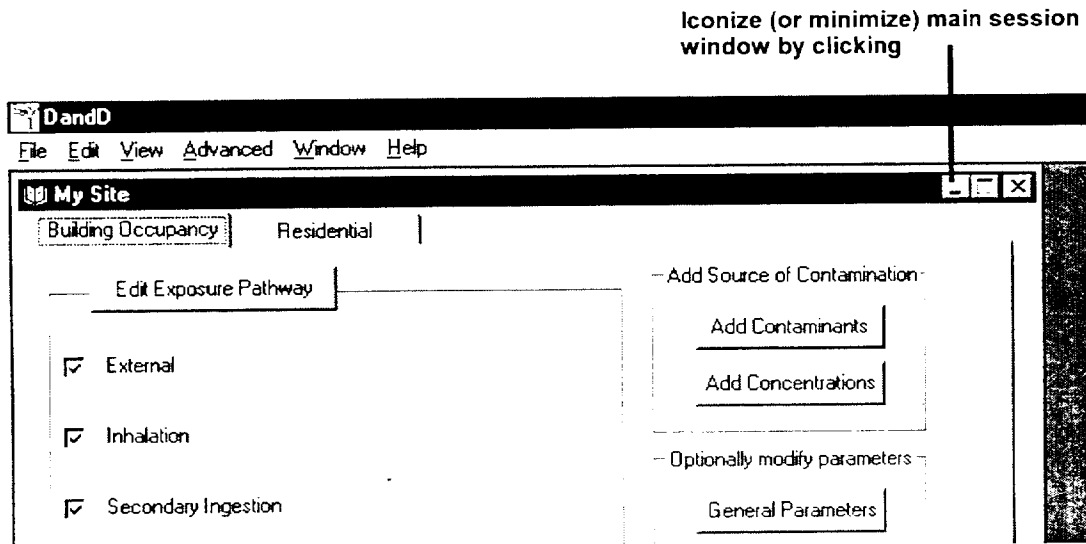


Figure 4.3.18 Iconizing main session window

5 FREQUENTLY ASKED QUESTIONS

Do I need Microsoft® Access® installed in order to run DandD? No.

Do I need Microsoft® Access® installed to look at the raw session file data? Yes.

Can DandD be installed on my new Windows ME or Windows 2000 machines? The DandD Version 2.1 installation procedure was not tested against these platforms. The difficulties that may be encountered are unknown. However, this feature may be supported in future versions.

I am unable to successfully install DandD Version 2.1. Now what do I do? If all of the hints within the "Installation of DandD" section of this document fail, send an e-mail to DandD@nrc.gov including: the version of the Windows® operating system on the computer, the amount of free hard-disk space available, the amount of random access memory (RAM) available, and, if available, the DandD installation log. If the installation has proceeded far enough, an installation log will have been created in a file named "INSTALL.LOG" in the directory where DandD is being installed (usually "C:\Program Files\DandD2").

How do I know what version of DandD I have? Click on "About" or "About DandD" in the "Help" menu. A dialog box will appear giving a multiple digit version number. For example, 2.1.0 is the specific DandD version number available at the time this documentation was published.

How do I know which session file I have open? The bottom left side of the main session window will contain the path name of the file currently opened. Select *File/Properties* for more information.

How do I change the site name and description for a session? Once the session is opened, click on "Properties" in the "File" menu, then edit either the site name or description.

How do I open up a session file using Microsoft® Access®? From the Microsoft® Windows® start menu, start Microsoft® Access®. Select the Open database option. Change the "Files of type:" drop down menu from "Microsoft® Access® Databases" to "All files." Specify the mcd (Monte Carlo DandD session) file in the Open dialog box. Click OK. Enter "2x" for the password.

How do I do a deterministic analysis like I did with DandD Version 1.0? Go through every parameter and change it to a constant along with support justification.

Why do the numbers in the *Summary of Model Parameter Values* disagree with the input values I specified? Because the input units differ from those used by the model. See 4.1.2 for a further discussion.

Why is the *Add Concentration* button dimmed on the scenario tab? This happens if the *Concentration History* toggle from the *Add Contaminants* dialog box is set. To correct this, click on *Add Contaminants*. Set the *Contaminant Input Mode* toggle to *Initial Concentration Values*. Add desired site contaminants. Click OK.

I haven't run a simulation yet, but I need to know what parameter I have modified and their values. How do I do this? The user can see which parameters are modified in the Parameter Viewing windows by looking to see which parameters have their *Default* checkbox unchecked in the main grid. However, it will be easier to create a report called *Model Input Summary* accessed by selecting *View/Reports* from the main menu. All site-specific parameters and contaminations will be reported.

I want to see the Dose History. I ran a simulation, but the dose history is greyed out on the *View/Graphics* menu. What should I do? Click on *Execute*, and click on *Options* in the Run Simulation window. Check the *Save Dose History Information* checkbox in the Advanced Execution Parameters window. Rerun the simulation.

I am getting unclear error messages. My simulation should run but it won't now. What should I do? You may have stumbled onto a bug. Exit DandD, restart DandD, and reopen the session file. Try to run the simulation again. Reproduce the problem and please submit the bug to NRC technical support to repair.

The program was unable to complete the LHS sampling. I received a sequence of error messages from the LHS processor. Why? The system may be low in memory or disk space. The specified parameter distributions or correlations may be invalid. It is also possible that a bug from within LHS may have been found. Try changing the probability distribution and

resampling. If this corrects the problem, the problem is most likely a bug in LHS. If this does not work, exit DandD, restart DandD, and reopen the session file. Try to run the simulation again. If this works, there may be a bug in DandD. Reproduce the problem and please submit the bug to NRC technical support to repair.

I ran the simulation twice. Each time I got different results, even though the random seed and the parameters haven't changed. Is this program broken? In some cases, the random sample values of the parameters depend on the order in which the user defined and modified the parameters. This will result in a slightly different value of the TEDE and 95% confidence interval bounds. The program results are still valid. The user can increase the number of simulations to increase the accuracy of the results. This dependence on the order of input is a bug and may be fixed in a future version.

In the Report, why is the reported all-pathways dose not always equal to the sum of the dose reported for the individual pathways? There are a number of reasons for this apparent inconsistency. First, the numbers reported represent peak values over 1000 simulated years and the pathway peak may occur at different times than the all-pathways peak; thus the all-pathways peak would be less than the sum of the individual pathway peaks. Second, remember that the reported numbers represent a specific quantile of the distributions. There may be an overall relationship between pathway doses such that high values along one pathway coincide with low values on another pathway. The resulting all-pathways quantile would be expected to differ from the sum of the pathway-specific quantile values.

How do I insert a graphic into my Microsoft* Word* or Corel* WordPerfect* Document? Use the Edit/Copy function to copy the graphics to the clipboard from DandD. Use the Paste Special option in the word processing program.

How do I extract the raw data used in the graph? Use the Edit/Copy function to copy the graphics to the clipboard from DandD. Use the Paste option in the word processing or spreadsheet program.

When I try to copy a plot from DandD Version 2.1 and insert it into a word-processor document, all I get are a bunch of numbers. How do I get the plot? When it is desired to "paste" the plot into the document, select "paste special" rather than "paste" to insert the plot.

I used the Edit/Copy function, but when I paste my graphic into the word processing program, the legend is missing. Did I do something wrong? No. This is a missing feature of the Edit/Copy function. Add the legend to the graph within the target word processor application.

How can results be transmitted to the NRC? The session file (the file with the "mcd" filename extension) contains the session data, results, and explanations. Sometimes these files are larger than will fit on a standard floppy diskette. DandD Version 2.1 contains an option to compress these files so they may fit on a diskette or will be smaller to ship electronically. In Section 4, User Interface Reference Guide, read Section 4.3.3 File/Export Session File as Zip.

I entered a probability distribution for some parameters, but a constant value was used instead. Is this a bug in DandD? No. All behavioral parameters use an average of the sampled parameters for every simulation. LHS is used to create a set of values for probabilistic behavioral parameters. However, these values are averaged for use in the model. Parameter help accessed via the Parameter Viewing window (see section 4.1.2) and the online help accessed by selecting *Help/NRC References* from the main menu will tell the user which parameters are behavioral.

6 REFERENCES

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APPENDIX A DIFFERENCES BETWEEN VOLUME 1 AND RELEASE 1.0 OF DandD

A.1 Introduction

NUREG/CR-5512, Volume 1, "Residual Radioactive Contamination From Decommissioning: Technical Basis for Translating Contamination Levels to Annual Effective Dose," (Kennedy and Streng, 1992), provides the technical basis, associated equations, and data tables for translating residual contamination levels to annual dose for decommissioned sites. The NUREG/CR-5512 modeling is intended to be a screening tool for assessing potential doses from decommissioned sites based on a philosophy of moving from simple, prudently conservative, calculations toward more realistic simulations, as necessary.

In 1993, Sandia National Laboratories (SNL) developed codes to perform calculations using the NUREG/CR-5512 methodology to support the NRC's draft regulatory guide on release criteria for decommissioning, NUREG-1500 (Daily et al., 1994). Subsequent to performing these calculations, SNL has developed DandD, a user-friendly software application that implements the NUREG/CR-5512 methodology. DandD incorporates the codes developed for the NUREG-1500 calculations within a graphical user interface. In the process of supporting the NUREG-1500 calculations and implementing and testing the DandD software, several problems and issues related to the original methodology in NUREG/CR-5512 have been identified. Consequently, several changes or corrections were made for implementation of the NUREG/CR-5512 methodology in DandD. Generally, these changes address the following problems or issues:

1. Revisions to the equations published in NUREG/CR-5512, Volume 1;
2. errors found in the data tables published in NUREG/CR-5512, Volume 1; and
3. assumptions and default parameters used in the original NUREG/CR-5512 methodology that have been found to be inconsistent with the iterative screening philosophy of the methodology.

This appendix documents these problems and the corrections/solutions to these problems that have been implemented for Release 1.0 of DandD. Section A.2

describes equation nomenclature. Section A.3 of this report describes (1) the changes made to the equations originally published in NUREG/CR-5512, Volume 1, and (2) changes made as a result of the implementation and testing of DandD to address assumptions that resulted in inconsistencies between the intent of the NUREG/CR-5512 methodology and the originally published equations. Section A.4 identifies the corrections made to the data tables published in NUREG/CR-5512, Volume 1, to develop the data files for the Release 1.0 of the DandD code. Changes in the default parameter values were documented in Beyeler et al., 1999.

A.2 Nomenclature

The mathematical models originally described in Volume 1 of this report involve many equations with numerous parameters. Because of the complexity of the equations, a system of nomenclature was developed to represent symbols used for the parameters. This system of nomenclature is summarized in Section 2 of Volume 1. For ease of reference to understand the changes to the mathematical formulations that are presented in this appendix, the system of nomenclature is presented here in Table A.1. The system of nomenclature includes a definition of units used to permit a full dimensional analysis.

In general, terms beginning with "D" are dose or dose rate factors; "TEDE" are annual total effective dose equivalents; "AF" are ingestion-pathway committed effective dose equivalent factors; "C" are concentrations (per unit mass, volume, or area), or total activity of a radionuclide, as appropriate; and " λ " are radioactive decay rate constants. General subscripts encountered include "i" or "j" for parent or decay-chain-member radionuclides; "s" for soil; "w" for water; and "v" for food crops (agricultural pathways).

In addition to the parameters listed in tables, a special notation is used for radioactive decay calculations. Decay operators are represented by $A\{\}$, $S\{\}$, $R\{\}$, and $G\{\}$, as defined in Appendix B of Volume 1.

$A\{\}$ = Changes in parent and progeny activities or concentrations over time (i.e. radioactive decay and ingrowth).

Table A.1 Parameter Summary

Parameter	Description
A_{sj}	Concentration factor of radionuclide progeny j in soil for the current year per initial unit concentration of chain parent radionuclide in soil.
A_{wj}	Average concentration factor of radionuclide progeny j in water for the current year per initial unit concentration of chain parent radionuclide in soil.
Af_{dj}	Committed effective dose equivalent per unit average concentration of chain member j (as a parent) in water from drinking water contaminated by radionuclide chain member.
AF_{fj}	Committed effective dose equivalent per unit average concentration of chain member j (as a parent) in water from aquatic food products contaminated by radionuclide chain member j.
AF_{sj}	Committed effective dose equivalent per unit concentration of chain member j (as a parent) in soil at the start of the growing season from agricultural products contaminated by radionuclide chain member j in soil.
AF_{wj}	Committed effective dose equivalent per unit average concentration of chain member j (as a parent) in water from agricultural products contaminated by irrigation water for radionuclide j.
C_{1j}	Total activity in box 1 of the three box groundwater model for radionuclide chain member j.
C_{2j}	Total activity in box 2 of either the three box or the multiple-layer-unsaturated-zone box groundwater model for radionuclide chain member j.
C_{3j}	Total activity in box 3 of the three box groundwater model for radionuclide chain member j.
$C_{1,n}$	Total activity in box 1 of the three box groundwater model for radionuclide chain member n.
$C_{2,n}$	Total activity in box 2 of either the three box or the multiple-layer-unsaturated-zone box groundwater model for radionuclide chain member n.
$C_{3,n}$	Total activity in box 3 of the three box groundwater model for radionuclide chain member n.
C_{kj}	Total activity in box k of the three box groundwater model for radionuclide chain member j.
C_{lj}	Total activity in box l of the multiple-layer-unsaturated-zone groundwater box model for radionuclide chain member j.
$C_{l-1,j}$	Total activity in box l-1 of the multiple-layer-unsaturated-zone groundwater box model for radionuclide chain member j.
$C_{l,n}$	Total activity in box l of the multiple-layer-unsaturated-zone groundwater box model for radionuclide chain member n.
$C_{m+1,j}$	Total activity in box m+1 (box immediately above the aquifer box) of the multiple-layer-unsaturated-zone groundwater box model for radionuclide chain member j.
$C_{m+2,j}$	Total activity in box m+2 (aquifer box) of the multiple-layer-unsaturated-zone groundwater box model for radionuclide chain member j.
$C_{m+2,n}$	Total activity in box m+2 (aquifer box) of the multiple-layer-unsaturated-zone groundwater box model for radionuclide chain member n.
$C_{\pi Cc}$	Carbon-14 average concentration factor in forage crop at time of forage feeding resulting from resuspension and root uptake from soil for an average unit concentration of carbon-14 in ground water.

Table A.1 Parameter Summary

Parameter	Description
C_{rgCc}	Carbon-14 average concentration factor in stored grain at time of grain feeding resulting from resuspension and root uptake from soil for an average unit concentration of carbon-14 in ground water.
C_{rhCc}	Carbon-14 average concentration factor in stored hay at time of stored hay feeding resulting from resuspension and root uptake from soil for an average unit concentration of carbon-14 in ground water.
C_s	Initial activity in soil for a chain parent radionuclide.
C_{si}	Initial activity in soil for chain i parent radionuclide.
$C_{s_i}(0)$	Initial activity in soil for chain i parent radionuclide.
C_{swjt}	Activity concentration factor for transfer from soil to water for radionuclide chain member j at time t.
C_{ti}	Total activity in soil for chain i parent radionuclide.
C_{wfcC}	Carbon-14 concentration factor in fresh forage at time of animal consumption for unit initial concentration of carbon-14 in ground water.
C_{wfcD}	Carbon-14 concentration factor in soil at time of animal consumption for unit initial concentration of carbon-14 in ground water.
C_{wgcC}	Carbon-14 concentration factor in stored grain at time of animal consumption for unit initial concentration of carbon-14 in ground water.
C_{whcD}	Carbon-14 concentration factor in stored hay at time of animal consumption for unit initial concentration of carbon-14 in ground water.
C_{wwC}	Carbon-14 concentration factor in water at time of animal consumption for unit initial concentration of carbon-14 in ground water.
CDG	Dust loading factor for gardening activities.
CDI	Dust loading factor for indoor exposure periods.
CDO	Dust loading factor for outdoor exposure periods.
DAR_i	Committed effective dose equivalent from ingestion of aquatic foods for radionuclide chain i.
$DEXR_i$	External dose for radionuclide chain i.
$DFER_j$	External dose rate factor for radionuclide chain member j from contamination uniformly distributed in the top 15 cm of residential soil.
DFG_j	Committed effective dose equivalent from ingestion of radionuclide chain member j.
DFH_j	Committed effective dose equivalent from inhalation of radionuclide chain member j from contaminated air.
DFO_o	Committed effective dose equivalent to organ o from ingestion of radionuclide chain member j.
DGR	Committed effective dose equivalent from ingestion of home-grown food and animal products for a radionuclide chain.
DGR_i	Committed effective dose equivalent from ingestion of home-grown food and animal products for radionuclide chain i.

Table A.1 Parameter Summary

Parameter	Description
DHR _i	Committed effective dose equivalent from inhalation of airborne soil and house dust for radionuclide chain i.
DIET	Fraction of annual diet derived from home-grown foods.
DIRR	Committed effective dose equivalent from ingestion of home-grown foods and animal products produced with irrigation water for a radionuclide chain.
DIRR _i	Committed effective dose equivalent from ingestion of home-grown foods and animal products produced with irrigation water for radionuclide chain i.
DSR _i	Committed effective dose equivalent from secondary ingestion of soil for radionuclide chain i.
DWR _i	Committed effective dose equivalent from ingestion of drinking water and irrigated food for radionuclide chain i (also used for committed effective dose equivalent from ingestion of drinking water for radionuclide chain member j after modification of Eqn. 5.74).
F _i	Fraction of water removed from the aquifer box that is deposited on the surface layer by irrigation.
GR	Effective transfer rate for ingestion of soil and dust transferred to the mouth during the residential scenario.
HOCDE _i	Highest annual organ committed dose equivalent for radionuclide chain i from ingestion of drinking water.
HOCDE _m	Highest annual organ committed dose equivalent for a mixture of radionuclides from ingestion of drinking water.
J _i	Number of radionuclides in decay chain for radionuclide chain i.
L _{12j}	Rate constant for movement of radionuclide j between boxes 1 and 2 in the groundwater box model.
L _{23j}	Rate constant for movement of radionuclide j between boxes 2 and 3 in the groundwater three box model.
L̂ _{23j}	Rate constant for movement of radionuclide j between boxes 2 and 3 in the multiple-layer-unsaturated-zone groundwater box model.
L̂ _{l-1,j}	Rate constant for movement of radionuclide j between boxes l-1 and l in the multiple-layer-unsaturated-zone groundwater box model.
L̂ _{l+1,j}	Rate constant for movement of radionuclide j between boxes l and l+1 in the multiple-layer-unsaturated-zone groundwater box model.
L̂ _{m+1,m+2,j}	Rate constant for movement of radionuclide j between the box immediately above the aquifer and the aquifer box in the multiple-layer-unsaturated-zone groundwater box model.
M	Number of radionuclide chains.
P _c	Floor dust loading factor for residential scenario.
PF _{soil} _j	Pathway transfer factor providing uptake by humans per unit concentration in soil for chain member j caused by unit activity of radionuclide chain member i.
PF _{water} _j	Pathway transfer factor providing uptake by humans per unit concentration in water for chain member j caused by unit activity of radionuclide chain member i.

Table A.1 Parameter Summary

Parameter	Description
PPTF _{awc}	Partial pathway transfer factor of animal product for carbon-14 due to irrigation.
RF _r	Resuspension factor for indoor activity in the residential scenario.
Q _d	Soil dry weight consumption rate as a fraction of the fresh forage consumption rate.
Q _f	Consumption rate of wet weight fresh forage by animal.
Q _g	Consumption rate of wet weight stored grain by animal.
Q _h	Consumption rate of wet weight stored hay by animal.
Q _w	Consumption rate of water by animal.
S{A _{sj} ,t _{ig} }	Time integral of total soil activity for radionuclide chain member j over the gardening period from time t to time t+t _{ig} .
S{A _{sj} ,t _r }	Time integral of soil total activity for radionuclide chain member j over the residential period from time t to time t+t _r .
S _{ab} {C _{kj} ,t _y }	Time integral of drinking water scenario aquifer total activity for radionuclide chain member j over the time period t _y (one year).
SA _{TaC}	Specific activity equivalence of animal product and the specific activity of the total feed intake.
SFI	Shielding factor by which external dose rate is reduced during periods of indoor residence.
SFO	Optional shielding factor by which external dose rate is reduced during periods of outdoor residence.
TEDED _i	Annual total effective dose equivalent for the drinking water scenario for radionuclide chain i.
U _w	Ingestion rate of drinking water by humans.
V _{aq}	Aquifer volume.
V _g	Volumetric breathing rate for gardening activities for residential scenario.
V _{lr}	Volume of water infiltrating through contaminated area in a year for the residential scenario water-use model.
V _{dd}	Volume of water used for domestic purposes during a year of the drinking water scenario.
V _{dr}	Volume of water used for domestic purposes during a year of the residential scenario.
V _{irr}	Volume of water used for irrigation during a year of the residential scenario.
V _{Td}	Total aquifer volume for the drinking water scenario.
V _{Tr}	Total aquifer volume for the residential scenario.
V _r	Volumetric breathing rate for indoor activities for the residential scenario.
V _{sw}	Volume of water in the surface-water pond used in production of aquatic foods.
V _x	Volumetric breathing rate for outdoor activities for the residential scenario.
W _f	Factor to convert mass of fresh forage from a wet-weight to a dry-weight basis.
C _{aq}	Concentration of radionuclides in the aquifer.

Table A.1 Parameter Summary

Parameter	Description
c_{sw}	Concentration of radionuclides in the surface-water pond.
$d_{n,j}$	Fraction of radionuclide n that decays to radionuclide j.
dgr_j	Partial committed effective dose equivalent fro ingestion of home-grown food and animal products for radionuclide chain member j.
$dirr_j$	Partial committed effective dose equivalent from ingestion of home-grown food and animal products produced with irrigated water for radionuclide chain member j.
f_{ca}	Fraction of animal product that is carbon.
f_{cf}	Fraction of wet fresh forage that is carbon.
f_{cd}	Fraction of dry soil that is carbon.
f_{cg}	Fraction of wet stored grain that is carbon.
f_{ch}	Fraction of wet stored hay that is carbon.
m	Number of boxes in the unsaturated zone in the multiple-layer-unsaturated-zone groundwater box model.
t	Time.
t_{ca}	Time period over which animal product is consumed by humans.
t_{ff}	Time period over which animal is fed fresh forage.
t_{fg}	Time period over which animal is fed stored grain.
t_{fh}	Time period over which animal is fed stored hay.
t_{fw}	Time period over which animal consumes water.
t_d	Water intake period for drinking water scenario.
t_g	Time (in 24 hour days) spent gardening for residential scenario.
t_i	Time (in 24 hour days) spent indoors for residential scenario.
t_g	Length of gardening period for residential scenario.
t_r	Length of time in an exposure period for the residential scenario.
t_o	Time (in 24 hour days) spent outdoors for residential scenario.
t_y	Time representing one year.
x_f	Fraction of fresh forage consumed by animals that is contaminated.
x_g	Fraction of stored grain consumed by animals that is contaminated.
x_h	Fraction of stored hay consumed by animals that is contaminated.
x_w	Fraction of water consumed by animals that is contaminated.
w_d	Groundwater removal rate constant for the drinking water scenario.
w_r	Groundwater removal rate constant for the residential scenario.

Table A.1 Parameter Summary

Parameter	Description
λ_j	Decay constant for radionuclide chain member j.

S{} = time integrals of activity or concentration.

R{} = accumulation of deposited activity over a time period.

G{} = deposition, accumulation, and time-integration of a constant deposition rate (used for deposition from irrigation water onto plants).

The operations are performed on an initial array of chain member activities or concentrations for a specific time period. For example, the decay calculation is represented as follows:

$$A\{C_o, t_o\}$$

where A{} = the operation of decay calculation (in appropriate units)

C_o = the array of chain members, activities, or concentrations (in appropriate units).

t_o = time period over which the decay occurs (in time units)

For additional information on nomenclature, the reader is referred to Volume 1 of this report.

A.3 Corrections and Changes to Equations

To address several concerns about the equations originally published in NUREG/CR-5512, Volume 1, and to address inconsistent assumptions in the original methodology, several model equations originally published in Volume 1 have been changed for the implementation of the methodology in DandD. The modifications are presented in the following sections. Equation numbers refer to the equation number in Volume 1. The modified version of an equation includes an "m" in the equation number. Equations from Volume 1 modified by more than one equation also have a,b,c, notation.

A.3.1 Ingestion Dose from Food Grown in Contaminated Soil

Equations 5.71 and 5.72 were modified slightly in order to perform the calculations to obtain information requested by the NRC. The NRC requested that dose be specified for each radionuclide in a chain. With the method described in NUREG/CR-5512, Volume 1, calculations are performed for an entire chain. In order to obtain dose by radionuclide, the order for double summation which would occur by combining Equations 5.71 and 5.72 had to be reversed. A matrix can be set up to perform the calculations. The matrix of calculations would look like:

$PF_{s11} * DFG_1 * A_{s11}$	0	0	--	0	$dgr_j / (C_s * DIET)$
$PF_{s21} * DFG_2 * A_{s11}$	$PF_{s22} * DFG_2 * A_{s12}$	0	--	0	$dgr_j / (C_s * DIET)$
$PF_{s31} * DFG_3 * A_{s11}$	$PF_{s32} * DFG_3 * A_{s12}$	$PF_{s33} * DFG_3 * A_{s13}$	--	0	$dgr_j / (C_s * DIET)$
--	--	--	--	0	--
$PF_{sm1} * DFG_m * A_{s11}$	$PF_{sm2} * DFG_m * A_{s12}$	$PF_{sm3} * DFG_m * A_{s13}$	--	$PF_{smm} * DFG_m * A_{sm}$	$dgr_j / (C_s * DIET)$
AF_{s1}	AF_{s2}	AF_{s3}	--	AF_{sm}	$DGR / (C_s * DIET)$

In NUREG/CR-5512, Volume 1, Equation 5.72 sums down each column to obtain the AF_{sj} 's. Equation 5.71 then sums the AF_{sj} terms across the bottom row to obtain DGR. In order to obtain doses by radionuclide, DandD sums along each row to obtain the dgr_j terms.

The dgr_j terms are stored for use in calculating doses by radionuclide. The column containing the dgr_j terms are then summed to obtain the DGR for the entire chain. This change was made prior to the calculations done in support of NUREG-1500.

A.3.2 Dose Due to Food Grown with Contaminated Irrigation Water

Equations 5.74 and 5.76 model the dose due to food grown with contaminated irrigation water in much the same manner as food grown in contaminated soil. (See Section A.3.8 for separation of Equation 5.74 into drinking water and irrigation components). In Volume 1, the above matrix (with PF_w substituted for PF_s , AF_w substituted for AF_s , A_{wt} substituted for A_{st} , dwr substituted for dgr , and $DIRR$ substituted for DGR) is first summed down each column to obtain the AF_{wt} terms and then summed along the bottom row to obtain the dose due to ingestion of food grown with contaminated irrigation water, DWR , for the chain. Since the NRC wanted doses for each radionuclide in the chain, the sum was first taken along each row to obtain "dirr_j" for each radionuclide in the chain. The $dirr_j$ terms are stored for use in calculating doses by radionuclide. The column containing the $dirr_j$ terms is then summed to obtain the $DIRR$ for the entire chain. This change was made prior to the calculations done in support of NUREG-1500.

A.3.3 Secondary Ingestion of Soil

Equation 5.73, which models the secondary ingestion of soil by humans, was modified to account for the time a person was actually on the contaminated site.

The original equation was:

$$DSR_i = GR C_{st} \sum_{j=1}^{J_i} DFG_j S\{A_{st}, t_{tr}\} \quad (5.73)$$

which was based on the assumption of a person being on the contaminated site for the entire year.

The modified equation, as implemented in DandD, is now:

$$DSR_i = GR C_{st}(0) \sum_{j=1}^{J_i} [DFG_j \left(\frac{t_i + t_x + t_g}{t_{tr}} \right) S\{A_{st}, t_{tr}\}] \quad (5.73m)$$

The $\left(\frac{t_i + t_x + t_g}{t_{tr}} \right)$ term represents the portion of the year that a person was on the site. This change was made

prior to the calculations done in support of NUREG-1500.

A.3.4 Surface Water Pond Decoupling

Following the calculations for NUREG-1500 and during the development and testing of DandD, SNL staff noted that if the surface water pond was not included in a model run, doses due to ground water, most notably the drinking water portion, would increase dramatically. By removing the surface water pond, the aquifer volume decreased causing a concentrating effect on the radionuclide concentrations in the aquifer. Because the dilutive effects of the surface water pond volume were removed, higher groundwater radionuclide concentrations would result than if the surface water pond were present. In addition, removing the surface water pond also removed the aquatic food pathway. However, it was found that if the aquatic pathway was removed as a result of removing the surface water pond, total dose would increase. This did not make intuitive sense because, if pathways are removed, total dose should decrease.

To overcome this problem the surface water pond was decoupled from the aquifer. In Volume 1 the aquifer volume is based on either the amount of water withdrawn from the aquifer plus the surface water pond volume or the amount of recharge to the aquifer, whichever is greater. In addition, Volume 1 essentially sets the surface water radionuclide concentration to the same value as the aquifer radionuclide concentration. To decouple the pond from the aquifer, two modifications to the drinking water methodology were made. First, the aquifer volume depended only on amounts withdrawn from the aquifer and the amount of recharge to the aquifer and not on the surface water pond volume. Thus, Equation 5.88 was modified from:

$$= \max(V_{ir}, V_{irr} + V_{dr}) \quad (5.88)$$

to:

$$V_{ir} = \max(V_{ir}, V_{irr} + V_{dr}) \quad (5.88m)$$

In a second modification, a model to estimate radionuclide concentration in the surface water pond was developed. The methodology presented in Volume 1 assumed an equivalent radionuclide concentration between the aquifer and the surface water pond. However, in this type of modification an equivalent concentration between the aquifer and the surface pond, while conservative, would be unreasonable. For a surface water pond larger than the aquifer, equivalent radionuclide concentrations between the aquifer and the sur-

face water pond would create additional radionuclide mass. In essence, mass would not be conserved. Another approach would be to transfer the entire radionuclide mass in the aquifer into the surface water pond. However, if the entire radionuclide mass in the aquifer were transferred to the surface pond, then the radionuclide concentration in the pond would become extremely high for small surface water ponds. It would be unreasonable for the radionuclide concentration in the surface water pond to exceed the concentration in the aquifer. A model that allowed the intermingling of water and radionuclides between the aquifer and surface water pond was developed. In this model, the radionuclide mass in the aquifer was allowed to mix instantaneously with that in the surface water pond so that radionuclide mass is conserved:

$$A_{wq} V_{Tr} = C_{sw} (V_{Tr} + V_{sw})$$

where A_{wq} is the concentration in the aquifer, C_{sw} is the concentration in the surface water pond, V_{Tr} is the volume of the aquifer, and V_{sw} is the volume of the surface water pond. Upon rearranging, this equation becomes:

$$C_{sw} = \frac{A_{wq}}{(1 + V_{sw}/V_{Tr})}$$

which is the equation used by DandD to calculate the surface water pond concentration. This model not only conserves radionuclide mass, but also limits radionuclide concentration in the surface water pond so that it does not exceed the radionuclide concentration in the aquifer.

A.3.5 Water Balance Model - Drinking Water Scenario

Aquifer concentrations for the drinking water scenario (as well as for the residential scenario) are generally calculated with a three-box ground-water model. To a lesser extent the concentrations are calculated with a multiple layer unsaturated zone box ground-water model. The top box represents a soil layer generally consisting of 15 cm of soil. The middle box (or boxes in the multiple layer unsaturated zone box model) represents the unsaturated zone and models radionuclide transport through that zone. The bottom box represents the aquifer and models the radionuclide concentration in the aquifer. Infiltration enters the box model through the top of the soil layer box and transports radionuclides from the soil layer through the unsaturated zone and into the aquifer. Contaminated water is only removed from the aquifer by pumping.

Following the calculations for NUREG-1500 and during the development and testing of DandD, SNL staff observed that in cases where recharge to the aquifer box exceeds pumpage from the box, radionuclides can build up in the aquifer box. This build-up occurs because there is no mechanism for excess radionuclides to leave the box other than through pumpage. Since recharge is greater than pumpage, excess water in the aquifer box must leave the box by natural discharge. This natural discharge would carry radionuclides with it. However, the ground-water contamination models described in Volume 1 do not account for the natural discharge.

An analogy of what happens is in order. There are two cases to consider. First, let a filled bucket of water represent a box aquifer with no contamination. In the bottom of the bucket is a small hole through which water slowly drips out. The hole represents pumpage from the aquifer. At the top of the bucket is a rapidly flowing hose which is used to fill the bucket with salt water. As the salt water flows out the hose and into the bucket, two events happen: (1) the concentration of salt in the bucket increases and (2) the bucket overflows as long as water flows from the hose faster than it leaves through the hole. Logic dictates that the concentration of salt in the water in the bucket never increases above the concentration of salt in water flowing out the hose. However, the aquifer model defined in Volume 1 does not allow the bucket to overflow. The model indicates that the bucket will always remain full (i.e., the hose only flows at the rate water drips out the bottom of the bucket) but that salt is added at a rate consistent with the rapidly flowing hose. (In an extreme case, if the hole in the bottom of the bucket is sealed, the model in Volume 1 indicates that pure salt would be continuously added to the bucket. It is easy to see that the concentration of salt in the water will always increase with time). The model in Volume 1 essentially results in a rapid buildup of salt in the bucket. The concentration of salt in the bucket may then actually exceed that of salt in the rapidly flowing hose.

The second case represents the opposite of the first. The hose slowly drips salt water into the bucket and a large hole in the bottom lets water leave the bucket rapidly. In this case, the concentration of salt in the bucket increases somewhat and the bucket empties. After time there is no water in the bucket, which is analogous to the aquifer drying up. However, the model in Volume 1 keeps the bucket full but without an additional source of water to do so.

To overcome this, a ground-water water balance model has been included in the box equation governing con-

tamination in the aquifer box. The soil layer and unsaturated zone boxes also have an implicit water balance model included in them, i.e. infiltration that enters the top of the box leaves the bottom in a steady-state manner. The ground-water water balance model now includes a natural ground-water underflow recharge and discharge component, which allows radionuclides to leave the aquifer box through natural means other than pumpage and flow downgradient. In the above analogy the ground-water underflow terms account for the overflow of the bucket (first case) or the additional source of water (second case). The result is that radionuclides no longer build up in the aquifer box in an unreasonable manner.

In order to implement the water balance model, Equation 4.16 had to be modified into a simpler form than in the existing model. Equation 4.16 in NUREG/CR-5512, Volume 1, was changed from:

$$\text{Fractional Removal} = \frac{V_{dd}}{V_{Td}} \quad (4.16)$$

to:

$$\text{Fractional Removal} = 1 \quad (4.16m)$$

This modification, in turn, impacts Equation 4.15 in NUREG/CR-5512, Volume 1, which was changed from:

$$w_d = \left[\frac{\text{Fractional Removal}}{y} \right] \left[\frac{y}{365.25 d} \right] \quad (4.15)$$

to:

$$w_d = \frac{1}{365.25 d} \quad (4.15m)$$

A.3.6 Water Balance Model - Residential Scenario

Following the calculations for NUREG-1500 and during the development and testing of DandD, SNL staff observed that, for similar reasons presented under the drinking water scenario, a water balance must also be included in the residential scenario ground-water model. Several equations are impacted by the inclusion of the water balance model. Equation 5.86 in Volume 1 was changed from:

$$\text{Fractional Removal} = \frac{V_{irr} - V_{dr}}{V_{Tr}} \quad (5.86)$$

to:

$$\text{Fractional Removal} = 1 \quad (5.86m)$$

This modification, in turn, impacts Equation 5.85, which was changed from:

$$w_r = \left[\frac{\text{Fractional Removal}}{y} \right] \left[\frac{y}{365.25 d} \right]$$

to:

$$w_r = \frac{1}{365.25 d} \quad (5.85m)$$

In addition, Equation 5.89, which describes the fraction of pumped water that is applied to the surface layer, was changed from:

$$F_r = \frac{V_{irr}}{(V_{irr} + V_{dr})} \quad (5.89)$$

to:

$$F_r = \frac{V_{irr}}{V_{Tr}} \quad (5.89m)$$

Equation 5.89m now describes the fraction of water in the aquifer that is applied to the surface layer in one year.

A.3.7 Including Initial Soil Concentration Twice in Dose Calculations

Drinking Water Scenario. In the drinking water scenario, the initial concentration of the parent radionuclide in the soil is included twice in the dose calculations. It is used once in the calculation of the ground-water concentration and again in the calculation of dose from the ground-water concentration. For the drinking water scenario, the groundwater concentration is given by Equation 4.13 in Volume 1 as:

$$C_{s_{\text{soil}}} = \frac{1}{V_{Td} t_y} \int_0^{t_y} C_{3j}(t) dt = \frac{S_{j3} \{ C_{k,t_y} \}}{V_{Td} t_y} \quad (4.13)$$

The definitions of terms for Equation 4.13 in Volume 1 assigns C_{3j} the units of pCi per pCi in the soil in the above equation. However, in the development of the groundwater equations (Equations 4.1 to 4.6 in Volume 1) C_{3j} has the units of pCi. For implementation of the methodology in DandD, Equation 4.13 is used exactly as shown in Volume 1. However, the concentration terms have to be redefined from pCi per pCi in the soil to pCi; from pCi-d per pCi in the soil to pCi-d; and from pCi/L per pCi in the soil to pCi/L. This is a result of having the units of concentration terms changed in the middle of Section 4 of Volume 1.

As a result, the C_{swjt} term is based on the total concentration in the soil layer and not on a unit activity as the definitions would imply. Therefore, the units on C_{swjt} are pCi/L and not pCi/L per pCi in the soil as in NUREG/CR-5512, Volume 1. This has an impact on the drinking water dose equations (Equations 4.18, 4.21, and 4.22). In NUREG/CR-5512, Volume 1, the dose equations are based on the units of C_{swjt} being pCi/L per pCi in the soil. However, as has been shown, C_{swjt} is actually based on the initial concentration of radionuclides in the soil and not on a unit concentration of parent radionuclides. Therefore, because the dose equations contain an initial soil concentration, C_{si} , and the C_{swjt} based on pCi, the initial concentration is included twice in the dose equations. In order to correct this, Equations 4.18, 4.21, and 4.22 were modified by dropping the C_{si} term from the respective equations. Thus, Equation 4.18 was changed from:

$$TEDED_i = U_w t_d C_{ti} \sum_{j=1}^{J_i} C_{swjt} DFG_j \quad (4.18)$$

to:

$$TEDED_i = U_w t_d \sum_{j=1}^{J_i} C_{swjt} DFG_j \quad (4.18m)$$

Equation 4.21 was changed from:

$$HOCDE_i = U_w t_d C_{ti} \sum_{j=1}^{J_i} C_{swjt} DFO_{jo} \quad (4.21)$$

to:

$$HOCDE_i = U_w t_d \sum_{j=1}^{J_i} C_{swjt} DFO_{jo} \quad (4.21)$$

Equation 4.22 was changed from:

$$HOCDE_m = U_w t_d C_{ti} \sum_{i=1}^M \sum_{j=1}^{J_i} C_{swjt} DFO_{jo} \quad (4.22)$$

to:

$$HOCDE_m = U_w t_d \sum_{i=1}^M \sum_{j=1}^{J_i} C_{swjt} DFO_{jo} \quad (4.22m)$$

Residential Scenario. In a manner similar to that for the drinking water scenario described above, the dose equations for the residential scenario in Volume 1 have the initial soil concentrations included twice. The soil concentration equation, Equation 5.90, and the average ground-water concentration equation, Equation 5.92, as presented in Volume 1 both are based on the initial

concentration of radionuclides in the soil layer. The definitions of terms associated with the equations indicate that the equations are based on a unit initial value concentration. Again, the units on concentration terms have been redefined in the middle of Section 5.0 of Volume 1. Taking the same approach as that for the drinking water scenario, Equations 5.90 and 5.92 are used exactly as presented in Volume 1 for implementation in DandD. This necessitates modifying the dose terms by removing the C_{si} from the dose equations, Equations 5.69, 5.70, 5.71, 5.73, 5.74, and 5.77. Thus, Equation 5.69 was changed from:

$$DEXR_i = \left[24 \left(\frac{t_g}{t_{ig}} \right) SFO C_{si} \sum_{j=1}^{J_i} S \{ A_{stj} t_{ig} \} DFER_j \right] + \left[24 \left(\frac{t_x}{t_{tr}} \right) SFO C_{si} \sum_{j=1}^{J_i} S' \{ A_{stj} t_{tr} \} DEFR_j \right] + \left[24 \left(\frac{t_i}{t_{tr}} \right) SFI C_{si} \sum_{j=1}^{J_i} S' \{ A_{stj} t_{tr} \} DEFR_j \right] \quad (5.69)$$

to:

$$DEXR_i = \left[24 \left(\frac{t_g}{t_{ig}} \right) SFO \sum_{j=1}^{J_i} S \{ A_{stj} t_{ig} \} DFER_j \right] + \left[24 \left(\frac{t_x}{t_{tr}} \right) SFO \sum_{j=1}^{J_i} S' \{ A_{stj} t_{tr} \} DEFR_j \right] + \left[24 \left(\frac{t_i}{t_{tr}} \right) SFI \sum_{j=1}^{J_i} S' \{ A_{stj} t_{tr} \} DEFR_j \right] \quad (5.69m)$$

Equation 5.70, which was:

$$DHR_i = \left[24 V_g \left(\frac{t_g}{t_{ig}} \right) CDG C_{si} \sum_{j=1}^{J_i} S \{ A_{stj} t_{ig} \} DFH_j \right] + \left[24 V_x \left(\frac{t_x}{t_{tr}} \right) CDO C_{si} \sum_{j=1}^{J_i} S \{ A_{stj} t_{tr} \} DFH_j \right] + \left[24 V_r \left(\frac{t_i}{t_{tr}} \right) (CDI + P_d RF_r) C_{si} \sum_{j=1}^{J_i} S \{ A_{stj} t_{tr} \} DFH_j \right] \quad (5.70)$$

becomes:

$$DHR_i = \left[\begin{aligned} &24 V_g \left(\frac{t_g}{t_{ig}} \right) CDG \sum_{j=1}^{J_i} S \{ A_{stj}, t_{ig} \} DFH_j \\ &+ 24 V_x \left(\frac{t_x}{t_{tr}} \right) CDO \sum_{j=1}^{J_i} S \{ A_{stj}, t_{tr} \} DFH_j \\ &+ 24 V_r \left(\frac{t_r}{t_{tr}} \right) (CDI + P_d RF_r) \\ &\quad \sum_{j=1}^{J_i} S \{ A_{stj}, t_{tr} \} DFH_j \end{aligned} \right] \quad (5.70m)$$

Equation 5.71 was changed from:

$$DGR_i = C_{st} DIET \sum_{j=1}^J A_{stj} AF_{sj} \quad (5.71)$$

to:

$$DGR_i = DIET \sum_{j=1}^J A_{stj} AF_{sj} \quad (5.71m)$$

Equation 5.73, including the modification noted in Section 3.3, becomes:

$$DSR_i = GR \sum_{j=1}^{J_i} DFG_j \frac{t_l + t_x + t_g}{t_{tr}} S \{ A_{stj}, t_{tr} \} \quad (5.73m)$$

Equation 5.74, which was:

$$DWR_i = C_{st} \left[\sum_{j=1}^{J_i} A_{wtj} AF_{dj} - DIET \sum_{j=1}^{J_i} A_{wtj} AF_{wj} \right] \quad (5.74)$$

is now:

$$DWR_i = \sum_{j=1}^{J_i} A_{wtj} AF_{dj} + DIET \sum_{j=1}^{J_i} A_{wtj} AF_{wj} \quad (5.74m)$$

(See further modification to this equation in Section A.3.8.)

Equation 5.77 was changed from:

$$DAR_i = C_{st} \sum_{j=1}^{J_i} A_{wtj} AF_{fj} \quad (5.77)$$

to:

$$DAR_i = \sum_{j=1}^{J_i} A_{wtj} AF_{fj} \quad (5.77m)$$

A.3.8 Separation of Irrigation and Drinking Water Dose Equation into Components

At the request of the NRC, the equation for irrigation and drinking water dose for the residential scenario, Equation 5.74, was separated into its two components so that a separate drinking water dose could be calculated. There are now an equation for the drinking water dose and an equation for the irrigation water dose. The drinking water dose equation, including the correction mentioned in Section A.2.7 for Equation 5.74, is:

$$DWR_i = \sum_{j=1}^{J_i} A_{wtj} AF_{dj} \quad (5.74)$$

The equation for the irrigation dose, including the correction mentioned above for Equation 5.74 is:

$$DIRR_i = DIET \sum_{j=1}^{J_i} A_{wtj} AF_{wj} \quad (5.74m)$$

where DIRR_i is the dose due to irrigation for the *i*th chain.

A.3.9 Multiple Layering in the Unsaturated Zone

The capability to model multiple layers in the unsaturated zone has been added to DandD. This capability can increase the response time for radionuclides deposited at land surface to show in the aquifer over the response time for a single layer unsaturated zone. In Volume 1 the original equation for the soil layer box (box 1), Equation 5.80, for the residential scenario ground-water model (adding commas to separate the subscript, in the discussion that follows) was:

$$\frac{DC_{1,j}}{dt} = \lambda_j \sum_{n=1}^{i-1} d_{n,j} C_{1,n} - (L_{12,j} + \lambda_j) C_{1,j} + F_r w_r C_{2,j} \quad (5.80)$$

For the multiple layering case, this equation now becomes:

$$\frac{d C_{1j}}{dt} = \lambda_j \sum_{n=1}^{j-1} [d_{nj} C_{1,n} - (L_{12j} + \lambda_j) C_{1j} + F_r w_r C_{m-2j}] \quad (5.80m)$$

where m is the number of layers in the unsaturated zone.

The original equation for the unsaturated zone, Equation 5.82, was:

$$\frac{d C_{2j}}{dt} = \lambda_j \sum_{n=1}^{j-1} [d_{nj} C_{2,n} + L_{12j} C_{1j} - (L_{23j} + \lambda_j) C_{2j}] \quad (5.82)$$

It is now replaced with two equations. The first one describes the transport from the soil layer to the top layer in the unsaturated zone. It is given by:

$$\frac{d C_{2j}}{dt} = \lambda_j \sum_{n=1}^{j-1} [d_{nj} C_{2,n} + L_{12j} C_{1j} - (L_{23j} + \lambda_j) C_{2j}] \quad (5.82ma)$$

where

$$L_{23} = mL_{23j} \quad (5.82mb)$$

The second equation, which describes transport among the remaining boxes in the unsaturated zone, is given by:

$$\frac{d C_{lj}}{dt} = \lambda_j \sum_{n=1}^{j-1} [d_{nj} C_{1,n} + L_{l-1,lj} C_{e-1j} - (L_{l,l-1j} + \lambda_j) C_{lj}] \quad (5.82mc)$$

where l ranges from 3 to m+1, and

$$L_{l-1,lj} = mL_{23j} \quad (5.82md)$$

The equation describing transport in the aquifer box (box 3), Equation 5.84, has been changed from:

$$\frac{d C_{3j}}{dt} = \lambda_j \sum_{n=1}^{j-1} [d_{nj} C_{3,n} + L_{23j} C_{2j} - (w_r + \lambda_j) C_{3j}] \quad (5.84)$$

to:

$$\frac{d C_{m-2j}}{dt} = \lambda_j \sum_{n=1}^{j-1} [d_{nj} C_{m-2,n} + L_{m-1,m-2j} C_{m-1j} - (w_r + \lambda_j) C_{(3j)m-j}] \quad (5.84m)$$

The above equations are valid for the drinking water scenario by setting F_r to zero and replacing w_r with w_d .

A.3.10 Addition of Root Uptake and Resuspension to the C-14 in Water Special Model

Equation C.3 of NUREG/CR-5512, which calculates the partial pathway transfer factor from water to animals ($PPTF_{aw}$), does not include a root uptake/resuspension term. Equation C.3 was modified to include this term. Thus, Equation C.3 was modified from:

$$PPTF_{awC} = [V_{Ca} (Q_r^x C_{w/Cc} t_{ff} + Q_d W_f Q_r^x C_{w/Cc} t_{ff} + Q_g^x C_{w/Cc} t_{fg} + Q_h^x C_{whCc} t_{fh} + Q_w^x C_{wwCc} t_{fw}) t_{ca} SA_{1ac}] / [(f_{Cf} Q_f t_{ff} + f_{Cd} Q_d W_f Q_f t_{ff} + f_{Cg} Q_g t_{fg} + f_{Ch} Q_h t_{fh}) 365.25] \quad (C.3)$$

to:

$$PPTF_{awC} = [V_{Ca} (Q_r^x (C_{w/Cc} + C_{r/Cc}) t_{ff} + Q_d W_f Q_r^x C_{w/Cc} t_{ff} + Q_g^x (C_{w/Cc} + C_{r/Cc}) t_{fg} + Q_h^x (C_{whCc} + C_{rhCc}) t_{fh} + Q_w^x C_{wwCc} t_{fw}) t_{ca} SA_{1ac}] / [(f_{Cf} Q_f t_{ff} + f_{Cd} Q_d W_f Q_f t_{ff} + f_{Cg} Q_g t_{fg} + f_{Ch} Q_h t_{fh}) 365.25] \quad (C.3m)$$

where $C_{r/Cc}$, C_{rhCc} , and C_{rgCc} are the resuspension/root uptake terms defined by Equations 5.47, 5.52, and 5.57 of NUREG/CR-5512.

A.3.11 Modification of the Irrigation Rate Parameter

The parameter IR is defined in Chapter 5 of NUREG/CR-5512 as the annual average irrigation rate and is used that way in the groundwater model. This same parameter is used to calculate the rate of deposition of radionuclides onto plants and soil. Actually, radionuclide deposition occurs only during the growing period of the particular plant. Because irrigation will only realistically occur during the growing period of the plant, the use of an annual average irrigation rate to the plant underestimates the deposition of groundwater and, hence, radionuclides to the plant surfaces and soils. The amount withdrawn for irrigation during a

year is actually withdrawn over the growing period of the plant. Therefore, the rate of irrigation over the plant growing period is much higher than the average rate over the year. Each plant type considered (food crops, forage, hay, and grain) has the same annual average irrigation rate IR. For each plant type, irrigation occurs only during its growing period. In each case, the rate of deposition of radionuclides due to irrigation should be increased from its current value by a factor of $365.25/t_{\text{growth}}$, where t_{growth} is the plant growing period. This modification entails changes to the way the R_w terms are calculated in Equations 5.22, 5.27, 5.37, 5.43, 5.48, 5.50, 5.53, 5.55, 5.58, and D.8. Thus, the following modifications were made to those equations:

- Edible plant Equations 5.22 and 5.27 were multiplied by the factor $(365.25/t_{\text{gv}})$ for each edible plant type.
- Forage feeding Equations 5.37 and 5.43 were multiplied by the factor $(365.25/t_{\text{ff}})$ for each animal type, assuming that the feeding period of forage was the same as the growing period of forage.
- The hay Equations 5.48 and 5.50 were multiplied by the factor $(365.25/t_{\text{gh}})$ for each animal type.
- The grain Equations 5.53 and 5.55 were multiplied by the factor $(365.25/t_{\text{gg}})$ for each animal type.
- The soil consumption Equation 5.58 was multiplied by the factor $(365.25/t_{\text{ff}})$ for each animal type, assuming that the feeding period of forage and, hence, soil was the same as the growing period of forage.
- The special tritium model for soil consumption Equation D.8 was multiplied by the factor $(365.25/t_{\text{ff}})$ for each animal type, which is actually a special case of Equation 5.58 for long-lived radionuclides.

The parameters t_{ff} , t_{gg} , t_{gh} , and t_{gv} are the times for feeding on forage, time to grow grain, time to grow hay, and the time to grow edible plants, respectively. These changes are also incorporated into the special C-14 model.

A.3.12 Corrections to Equations

In a number of the pathway equations specified in the Volume 1 report, environmental concentration equations are multiplied by $C_i(0)$, the initial activity of the parent radionuclide. This multiplication was intended to correct a normalization to $C_i(0)$. However, in several equations (e.g., Equations 4.13, 5.90, and 5.92) the normalization was omitted in the equations published in Volume 1. The effect of this is that the equations in the Volume 1 document contain a spurious factor of $C_i(0)$. For the methodology implemented in DandD, unnormalized versions of the equations were implemented, so the current equations represent a correct implementation of the methodology.

A.4 Corrections and Changes to Data Tables in Volume 1

Several data files are used by the various scenarios in DandD. These files, a description of the data contained in the files, the scenarios for which the data are used, and table numbers from Volume 1 where the data were originally referenced are presented in Table A.2. After the completion of the NUREG-1500 calculations, the following data files referenced in Table A.2 were modified: BIOACCUM.TXT, CEDE.TXT, CHAIN.TXT, ORGAN1.TXT, ORGAN2.TXT, and ORGAN3.TXT. The primary reason for the modifications were errors and incomplete chain descriptions in Table E.1 of Volume 1. This resulted in extensive revisions, modifications, and additions to the CHAIN.TXT file. As a result of additions to CHAIN.TXT, some new radionuclides were introduced into the modeling process. Some or all of these new radionuclides were not included in the versions of these data files used for the

Table A.2 NUREG/CR-5512 Data Descriptions

Data File Name	Data Description	Scenario	NUREG/CR-5512, Volume 1 Table
BIOACCUM.TXT	Fish bioaccumulation data	Residential	Table 6.19
CARBON.TXT	Carbon data for the C-14 model.	Residential	Table 6.24

Table A.2 NUREG/CR-5512 Data Descriptions

Data File Name	Data Description	Scenario	NUREG/CR-5512, Volume 1 Table
CEDE.TXT	Internal committed effective dose equivalent and external effective dose equivalent factors.	Renovation Occupancy Drinking Water Residential	Table E.2
CHAIN.TXT	Radioactive decay data and decay chain specifications.	Renovation Occupancy Drinking Water Residential	Table E.1
CONCEN.TXT	Soil-to-plant concentration factors	Residential	Table 6.16
DW.TXT	Drinking water scenario parameters	Drinking Water	Table 6.22
TRITIUM.TXT	Hydrogen data used for the tritium model	Residential	Table 6.25
KD.TXT	Partition coefficients for water use model	Residential Drinking Water	Table 6.7
OCC.TXT	Building occupancy and scenario parameters	Occupancy	Table 6.21
ORGAN1.TXT	Ingestion organ dose equivalent factors for organ set 1.	Drinking Water	Table E.3
ORGAN2.TXT	Ingestion organ dose equivalent factors for organ set 2.	Drinking Water	Table E.4
ORGAN3.TXT	Ingestion organ dose equivalent factors for organ set 3.	Drinking Water	Table E.5
REN.TXT	Building renovation scenario parameters	Renovation	Table 6.20
RES.TXT	Residential scenario parameters	Residential	Table 6.23
TRANSFER.TXT	Animal product transfer factors	Residential	Table 6.18

NUREG-1500 calculations. The bioaccumulation factors, internal and external committed effective dose equivalents, and organ dose equivalent factors for the new radionuclides had to be added to the respective data files.

A.4.1 Changes to the CHAIN.TXT File

The CHAIN.TXT file for DandD implements Table E.1 from Volume 1, in the DandD code. Reviews of the chain decay data file, CHAIN.TXT, used for the NUREG-1500 calculations indicated that many decay chains were incomplete. Some chains were missing as many as 12 radionuclides. The decay chains as presented in Table E.1 of Volume 1 were compared to the source document from which they were derived (ICRP, 1983). The review of Table E.1 of Volume 1 consist-

ed of the following items:

- (1) Confirmation that they were listed correctly, if a parent radionuclide has progeny. Note: progeny are implicit, and are to be listed without half life if they meet the following criteria: they have half life less than 9 hours and their half life is less than one-tenth of the parent's.
- (2) Confirmation that the transformation fractions were listed correctly, if a parent radionuclide has progeny.
- (3) Confirmation that the position listed in the chain was correct.
- (4) Confirmation that no implicit progeny were listed

explicitly, and that no explicit progeny were listed as implicit.

To determine the correctness of the decay chains, the full decay chains were redeveloped using ICRP Publication 38 (1983). All decay chains corrections were checked twice independently.

The review did not examine whether a parent belonged in the list, nor did the review look at all possible parents that might have been included. It was assumed that the no parent nuclides needed to be added to those listed in Table E.1 were agreed to by NRC for the original NUREG/CR-5512 methodology of Volume 1. However, note that some very short-lived radionuclides were included as parents (e.g., ^{115m}In is implicit in some chains, but it is also a parent).

A.4.2 Changes to BIOACCUM.TXT

The DandD data file BIOACCUM.TXT was modified to include bioaccumulation data for the element Xe. Since Xe is a gas, it is assigned the same bioaccumulation value (0.0) as other gases in the data file.

A.4.3 Changes to CEDE.TXT

The additions to this file show the inclusion of committed effective dose equivalent factors for ^{103m}Rh , ^{115}In , ^{123}Te , ^{131m}Xe , ^{133}Xe , ^{133m}Xe , ^{135}Xe , ^{152}Gd , and ^{218}At . These were new radionuclides that appeared after the CHAIN.TXT file was corrected. After comparison of the CHAIN.TXT file with the decay chains presented in the ICRP document [1983],

the decay fraction value for ^{214}Pb was changed from 1.0000 to 0.9998.

A.5 References

- Beyeler, W.E., W.A. Hareland, F.A. Duran, T.J. Brown, E. Kalinina, D.P. Gallegos, and P.A. Davis, 1999. "Residual Radioactive Contamination From Decommissioning, Parameter Analysis, Draft Report for Comment," Sandia National Laboratories, NUREG/CR-5512, Volume 3, October 1999.
- Daily, M.C., A. Huffert, F. Cardile, and J.C. Malaro, 1994. Working Draft Regulatory Guide on Release Criteria for Decommissioning: NRC Staff's Draft for Comment, NUREG-1500, U.S. Nuclear Regulatory Commission, Washington, DC.
- ICRP, 1983. Radionuclide Transformations-Energy and Intensity of Emissions. Vol. 11-13, International Commission on Radiological Protection, Publication 38, Pergamon Press, New York, NY.
- Kennedy, Jr., W.E., and D.L. Strenge, 1992. Residual Radioactive Contamination From Decommissioning: Technical Basis for Translating Contamination Levels to Annual Effective Dose Equivalent, Vol. 1, NUREG/CR-5512, PNL-7994, U.S. Nuclear Regulatory Commission, Washington, DC.

APPENDIX B SAMPLE PROBLEMS

B.1 Introduction

Running through a sample problem will help the user become familiar with the program and confirm that DandD is producing the same results as the documented sample problems. For instructions on running a sample problem, see Section 3.2.

The facilities described in the sample problems were taken from the *Draft Generic Environmental Impact Statement in Support of Rulemaking on Radiological Criteria for Decommissioning of NRC-Licensed Nuclear Facilities* (NRC, 1994). The baseline sample problems assume the standard methodology presented in Kennedy and Strenge (1992) as modified by Wernig et al. (1999, Appendix A) and default probability distributions and respective parameters listed in Beyeler et al. (1999). Additional sample problems that go beyond the defaults are also included and contain a brief discussion of how the changes affect the results. All of the sample problems only include the residential scenario because it exercises all exposure pathways and is the most complex. The output option in the "Add Contaminants" window was set so that implicit progeny doses were combined with their respective parent doses. The results for some problems do not show a table for the radionuclide component of the total dose because there are no progeny for the parent radionuclide.

The following sample problems are for illustrative purposes only and may not represent good examples for license termination applications. For example, the user should be aware that deselecting a pathway without modifying any other parameters may be nonconservative. This is because the effect of deselecting a pathway only deactivates the associated dose calculation; it does not eliminate radionuclide transport. The user should keep this in mind when applying DandD 2.1 to license termination analyses.

B.2 Reference Facilities

The sample problems use reference facilities considered to be sufficiently representative of facilities licensed by NRC. They are divided into fuel cycle and non-fuel-cycle groups. A brief description of each type of facility is provided along with the parameters needed to set up the sample problems for the DandD software and the results that were calculated.

Fuel cycle facilities include:

- power reactors
- non-power (research and test) reactors
- uranium fuel fabrication plants
- uranium hexafluoride conversion facilities
- uranium mills
- independent spent fuel storage installations (ISFSI)

Non-fuel-cycle facilities include:

- sealed source manufacturers
- research and development laboratories
- rare metal refineries

B.3 Nuclear Fuel Cycle Facilities

Nuclear fuel cycle facilities are those facilities involved in any of the steps leading to or resulting from the generation of electricity by controlled nuclear fission of uranium. The nuclear fuel cycle process consists of several steps in which uranium ore is processed into fuel elements. The facilities involved in these steps include uranium mills, uranium hexafluoride conversion plants, enrichment plants, and uranium fuel fabrication plants. The next step in the fuel cycle is the generation of electricity by nuclear power plants. The end of the fuel cycle consists of steps in which fuel removed from the reactor is stored and then disposed of in some manner. The facility considered in this step is ISFSI.

B.3.1 Nuclear Power Reactors

There are two major types of nuclear power reactors in the United States; pressurized water reactors (PWRs) and boiling water reactors (BWRs). The analysis described in Appendix C of NRC (1994) indicates that, within the common variations of contamination levels in nuclear power plants, the contaminants and contamination of a PWR approximate the levels for a BWR. Therefore, the reference power reactor in this case is a large PWR (1095 Mwe). The reference power reactor comprises five major structures: the reactor containment, the auxiliary building, the fuel handling building, the turbine building, and the control building. For the reference facility, it is assumed that there are areas of contaminated soil resulting from on-site spills.

The sample problem file names for this group are preceded by "NPP" and the contaminants consist of ⁶⁰Co, ⁹⁰Sr, and ¹³⁷Cs with initial activities of 1 pCi/gram. The results shown are for the residential scenario only.

B.3.1.1 NPP Baseline Sample Problem

This sample problem is set up by selecting the three radionuclides shown below and using all default probability distributions and parameters.

Selected Radionuclides	Initial Activity
⁶⁰ Co	1 pCi/gram
⁹⁰ Sr	1 pCi/gram
¹³⁷ Cs	1 pCi/gram

Results (see Tables B.1 and B.2):

There is a 90% chance that a total effective dose equivalent (TEDE) of 2.22E+01 mrem with a 95% confidence interval from 2.02E+01 mrem to 2.88E+01 mrem will not be exceeded within 1000 years after license termination.

Table B.1. Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the NPP Sample Problem

Pathway	TEDE (mrem)
External	7.67E+00
Inhalation	4.29E-04
Agricultural	2.05E+01
Secondary Ingestion	3.20E-03
Drinking Water	2.14E-13
Irrigation	6.84E-13
Surface Water	218E-13
All	2.88+01

Table B.2 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the NPP Sample Problem

Radionuclide	TEDE (mrem)
⁶⁰ Co	6.69E+00
⁹⁰ Sr	1.96E-01
⁹⁰ Y	9.75E-01
¹³⁷ Cs	2.34E-00
All	2.88E-001

B.3.1.2 NPP1 Contamination Under a House

This sample problem assumes that all the contamination lies directly under a 2000 ft² house and turns off

all pathways except for external exposure inside the house, soil ingestion inside the house, and inhalation inside the house.

This sample problem is set up by deselecting the Agricultural, Drinking Water, Irrigation, and Surface Water pathway doses from the "Edit Exposure Pathway" button under the "Residential" tab.

The selected radionuclides are the same as in the NPP baseline sample problem and are shown below.

Selected Radionuclides	Initial Activity
⁶⁰ Co	1 pCi/gram
⁹⁰ Sr	1 pCi/gram
¹³⁷ Cs	1 pCi/gram

The following parameters were changed to constants:

Time Outdoors	0.0000	days/year
Time Gardening	0.0000	days/year
Cultivated Area	186.000	m ²

These parameters are changed by clicking on the "General Parameters" button under the "Residential" tab.

The bases for the changes in the above default parameters are as follows:

- The Time Outdoors is set to zero on the assumption that when a person is outdoors, they are not exposed to contamination because the contaminated area is under the house.
- The Time Gardening is set to zero because there is no contamination present in the garden.
- The area is based upon a 2000 ft² (186 m²) house.

Results (see Tables B.3 and B.4):

There is a 90% chance that a TEDE of 5.79E-00 mrem with a 95% confidence interval from 5.79E-00 mrem to 5.79E-00 mrem will not be exceeded within 1000 years after license termination.

B.3.1.3 NPP2 Contamination in the Garden

This sample problem assumes that the contamination is only in the garden. Therefore:

- The Time Indoors is set to zero to turn off exposure from inside the house.
- The Time Outdoors assumes that a person has the same behavior as in the default case and spends 104.44 days spread over 3800 m² of ground, but

only 4.89% of that time is spent on contaminated ground: $40.2 * 186/3800 = 1.97$.

Table B.3 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the NPP1 Sample Problem

Pathway	TEDE (mrem)
External	5.78E+00
Inhalation	2.34E-04
Agricultural	0.00E+00
Secondary Ingestion	2.71E-03
Drinking Water	0.00E+00
Irrigation	0.00E+00
Surface Water	0.00E+00
All	5.79E+00

Table B.4 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the NPP1 Sample Problem

Radionuclide	TEDE (mrem)
⁶⁰ Co	4.67E+00
⁹⁰ Sr	2.14E-03
⁹⁰ Y	8.15E-03
¹³⁷ Cs	1.10E+00
All	5.79E+00

- The area is based upon a 2000 ft² (186m²) garden.
- The diet parameters are proportionately scaled against the default site area of 3800 m² as follows:

Diet-Leafy	$21.4 * 186/3800 = 1.05$
Diet-Roots	$44.6 * 186/3800 = 2.18$
Diet-Fruit	$52.8 * 186/3800 = 2.58$
Diet-Grain	$14.4 * 186/3800 = 0.705$
Diet-Beef	$39.8 * 186/3800 = 1.95$
Diet-Poultry	$25.3 * 186/3800 = 1.24$
Diet-Leafy	$233. * 186/3800 = 11.4$
Diet-Leafy	$19.1 * 186/3800 = 0.935$

Selected Radionuclides	Initial Activity
⁶⁰ Co	1 pCi/gram
⁹⁰ Sr	1 pCi/gram
¹³⁷ Cs	1 pCi/gram

This sample problem is set up by selecting the three radionuclides specified above and changing the following parameters:

Time Indoors	0.0000	days/year
Time Outdoors	5.1121	days/year
Cultivated Area	186.000	m ²

Diet-Leafy	1.05	kg/y
Diet-Roots	2.18	kg/y
Diet-Fruit	2.58	kg/y
Diet-Grain	0.705	kg/y
Diet-Beef	1.95	kg/y
Diet-Poultry	1.24	kg/y
Diet-Milk	11.4	L/y
Diet-Egg	0.935	kg/y

Results (see Tables B.5 and B.6):

There is a 90% chance that a TEDE of 9.94E-01 mrem with a 95% confidence interval from 8.93E-01 mrem to 1.25E+00 mrem will not be exceeded within 1000 years after license termination.

Table B.5 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the NPP2 Sample Problem

Pathway	TEDE (mrem)
External	2.19E-01
Inhalation	1.24E-04
Agricultural	1.00E+00
Secondary Ingestion	5.52E-05
Drinking Water	1.41E-10
Irrigation	2.70E-11
Surface Water	2.73E-10
All	1.25E+00

Table B.6 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the NPP2 Sample Problem

Radionuclide	TEDE (mrem)
⁶⁰ Co	2.02E-001
⁹⁰ Sr	9.58E-001
⁹⁰ Y	5.34E-002
¹³⁷ Cs	8.52E-02
All	1.25E+00

B.3.2 Non-Power Reactors

Non-power reactors are generally divided into two classes; research reactors and test reactors. The reference research reactor is considered to be a 1 mW nuclear training and research facility. The facility is made up of a reactor tank, a core structure, and a TRIGA-type control system.

The reference research reactor comprises these major structures:

- reactor building—housing the reactor and support area
- annex—housing a hot laboratory and hot cell
- heat exchanger building—housing a water purification system, water pumping systems, and an air compressor system
- pump house—housing a liquid waste retention tank
- cooling tower

Test reactors are larger facilities than research reactors and the reference test reactor considered is a 60-mW test reactor, light-water moderated and cooled, used in testing materials for certain applications. The system is made up principally of the test reactor vessel (containing the nuclear core and experimental beam tubes) and the reactor water recirculation system.

The reference test reactor comprises these major structures:

- reactor building—housing the test reactor
- hot laboratory building
- primary pump house
- office and laboratory building—housing radio-chemistry laboratories
- fan house—housing ventilation systems and waste ion exchangers and filters
- hot retention area—holding waste tanks
- waste handling building

B.3.2.1 Research Reactor

The sample problem file names for this group are preceded by "RR" and the contaminants consist of ⁶⁰Co, ⁹⁰Sr, and ¹³⁷Cs with initial activities of 1 pCi/gram. The baseline sample problem for the research reactor is the same as the one used for the power reactor in Section B.3.1.1 and will not be included here. The results shown are for the residential scenario only.

B.3.2.1.1 RR1 Contamination Under a House

This sample problem is comparable to the sample problem in Section B.3.1.2, except the area of contamination is smaller ($.25 * 186 \text{ m}^2 = 46.5 \text{ m}^2$) and the time spent indoors is therefore reduced to 60.0 ($240 * .25$) days per year. The change in the time indoors assumes that a person spends 240 days spread over the 2000 ft² house but that only 25% of the time is on contaminated ground because of the smaller contaminated area.

Selected Radionuclides	Initial Activity
⁶⁰ Co	1 pCi/gram
⁹⁰ Sr	1 pCi/gram

¹³⁷Cs 1 pCi/gram

This sample problem is set up by selecting the three radionuclides specified above and changing the following parameters:

Time Indoors	60.0	days/year
Time Outdoors	0.0	days/year
Time Gardening	0.0	days/year
Cultivated Area	46.5	m ²

Doses from human consumption of food and water are eliminated by deselecting the Agricultural, Drinking Water, Irrigation, and Surface Water pathway doses.

Results (see Tables B.7 and B.8):

There is a 90% chance that a TEDE of 1.45E-00 mrem with a 95% confidence interval from 1.45E+00 mrem to 1.45E+00 mrem will not be exceeded within 1000 years after license termination.

Table B.7 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the RR1 Sample Problem

Pathway	TEDE (mrem)
External	1.45E+00
Inhalation	5.84E-05
Agricultural	0.00E-00
Secondary Ingestion	6.78E-04
Drinking Water	0.00E-00
Irrigation	0.00E-00
Surface Water	0.00E+00
All	1.45E+00

Table B.8 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the RR1 Sample Problem

Radionuclide	TEDE (mrem)
⁶⁰ Co	1.17E+00
⁹⁰ Sr	5.35E-004
⁹⁰ Y	2.04E-003
¹³⁷ Cs	2.76E-001
Total	1.45E+000

B.3.2.1.2 RR2 Contamination in the Garden

This sample problem assumes that the contamination is only in the garden and is comparable to the sample problem in B.3.1.3 except the area of contamination is smaller (46.5 m²), which was used to scale the time outdoors and the diet parameters.

This sample problem is set up by selecting the three radionuclides specified below:

Selected Radionuclides	Initial Activity
⁶⁰ Co	1 pCi/gram
⁹⁰ Sr	1 pCi/gram
¹³⁷ Cs	1 pCi/gram

The following parameters were changed:

Time Indoors	0.0000	days/year
Time Outdoors	0.492	days/year
Cultivated Area	46.5	m ²
Diet-Leafy	0.262	kg/y
Diet-Roots	0.546	kg/y
Diet-Fruit	0.646	kg/y
Diet-Grain	0.176	kg/y
Diet-Beef	0.487	kg/y
Diet-Poultry	0.310	kg/y
Diet-Milk	2.85	L/y
Diet-Egg	0.234	kg/y

Results (see Tables B.9 and B.10):

There is a 90% chance that a TEDE of 3.57E-01 mrem with a 95% confidence interval from 3.11E-01 mrem to 4.54E-01 mrem will not be exceeded within 1000 years after license termination.

Table B.9 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the RR2 Sample Problem

Pathway	TEDE (mrem)
External	1.54E-01
Inhalation	1.23E-04
Agricultural	2.13E-01
Secondary Ingestion	3.85E-05
Drinking Water	2.12E-01
Irrigation	6.74E-03
Surface Water	5.84E-01
All	4.54E-01

B.3.2.2 Test Reactor

The sample problem file names for this group are preceded by "TR" and the contaminants consist of ⁶⁰Co, ⁹⁰Sr, and ¹³⁷Cs with initial activities of 1 pCi/gram. The baseline sample problem for the test reactor is the same as the one used for the power reactor in Section B.3.1.1 and will not be included here. The results shown are for the residential scenario only and have the Combine Progeny switch turned on.

Table B.10 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the RR2 Sample Problem

Radionuclide	TEDE (mrem)
⁶⁰ Co	1.33E-01
⁹⁰ Sr	3.37E-01
⁹⁰ Y	2.01E-02
¹³⁷ Cs	3.92E-02
All	4.54E-01

B.3.2.2.1 TR1 Contamination Under a House

This sample problem is comparable to the sample problem in Section B.3.1.2 except that the area of contamination is larger (465 m² or 5000 ft²). This is larger than the default house but smaller than the default area, which assumes that there is contamination under the entire house with 3000 ft² (279m²) left over to contaminate the garden. The default parameters are changed as shown below based on a 279 m² contaminated area and a 3800 m² default area:

Selected Radionuclides	Initial Activity
⁶⁰ Co	1 pCi/gram
⁹⁰ Sr	1 pCi/gram
¹³⁷ Cs	1 pCi/gram

The following parameters were changed:

Time Outdoors	2.95	days/year
Cultivated Area	465.0	m ²
Diet-Leafy	1.57	kg/y
Diet-Roots	3.27	kg/y
Diet-Fruit	3.88	kg/y
Diet-Grain	1.06	kg/y
Diet-Beef	2.92	kg/y
Diet-Poultry	1.86	kg/y
Diet-Milk	17.1	L/y
Diet-Egg	1.40	kg/y

Results (see Tables B.11 and B.12):

There is a 90% chance that a TEDE of 7.12E+00 mrem with a 95% confidence interval from 6.97E+00 mrem to 7.60E+00 mrem will not be exceeded within 1000 years after license termination.

B.3.2.2.2 TR2 Garden Contamination

This sample problem assumes that the contamination is only in the garden and is comparable to the sample problem in Section B.3.1.3 except that the area of

Table B.11 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the TR1 Sample Problem

Pathway	TEDE (mrem)
External	6.05E-00
Inhalation	3.17E-04
Agricultural	1.50E+00
Secondary Ingestion	2.78E-03
Drinking Water	1.54E-13
Irrigation	3.61E-14
Surface Water	6.62E-14
All	7.60E+00

Table B.12 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the TR1 Sample Problem

Radionuclide	TEDE (mrem)
⁶⁰ Co	4.92E+00
⁹⁰ Sr	1.44E+00
⁹⁰ Y	7.93E-02
¹³⁷ Cs	1.22E+00
All	7.60E+00

contamination is larger (465 m²). The default parameters are changed based on a default area of 3800 m² as shown below:

Selected Radionuclides	Initial Activity
⁶⁰ Co	1 pCi/gram
⁹⁰ Sr	1 pCi/gram
¹³⁷ Cs	1 pCi/gram

The following parameters were changed:

Time Indoors	0.0	days/year
Time Outdoors	4.92	days/year
Cultivated Area	465.0	m ²
Diet-Leafy	2.62	kg/y
Diet-Roots	5.46	kg/y
Diet-Fruit	6.46	kg/y
Diet-Grain	1.76	kg/y
Diet-Beef	4.87	kg/y
Diet-Poultry	3.10	kg/y
Diet-Milk	28.5	L/y
Diet-Egg	2.34	kg/y

Results (see Tables B.13 and B.14):

There is a 90% chance that a TEDE of 2.29E+00 mrem with a 95% confidence interval from 1.95E-00 mrem to 2.93E+00 mrem will not be exceeded within 1000 years after license termination.

Table B.13 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the TR2 Sample Problem

Pathway	TEDE (mrem)
External	3.48E-01
Inhalation	1.26E-04
Agricultural	2.51E+00
Secondary Ingestion	8.86E-05
Drinking Water	2.15E-10
Irrigation	1.03E-10
Surface Water	6.28E-10
All	2.93E+00

Table B.14 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the TR2 Sample Problem

Radionuclide	TEDE (mrem)
⁶⁰ Co	3.42E-01
⁹⁰ Sr	2.39E+00
⁹⁰ Y	1.18E-01
¹³⁷ Cs	1.76E-01
All	9.07E+00

B.3.3 Uranium Fuel Fabrication Plants

A uranium fuel fabrication plant (U-fab plant) is a facility in which enriched uranium, received as uranium hexafluoride (UF₆), is converted to UO₂ and formed into fuel pellets that are inserted into fuel rods. These fuel rods are, in turn, assembled into fuel bundles. The reference fuel manufacturing plant consists of five potentially contaminated buildings, including the fuel manufacturing building, the chemical manufacturing laboratory, the uranium scrap recovery room, the contaminated waste incinerator, and the fluoride and nitrate waste treatment plant. Operation of the reference facility is assumed to result in areas of contaminated soil on the site. The principal contaminant in the buildings and soils is uranium. The files for this sample problem have the prefix UFFP.

B.3.3.1 U_Nat Baseline Sample Problem

This sample problem is set up by selecting the U_Nat (natural uranium) radionuclide and using all default probability distributions and parameters. The results shown are for the residential scenario only.

Selected Radionuclides	Initial Activity
U_Nat	1 pCi/gram

Results (see Tables B.15 and B.16):

There is a 90% chance that a TEDE of 2.17E+00 mrem with a 95% confidence interval from 1.26E+00 mrem to 3.83E+00 mrem will not be exceeded within 1000 years after license termination.

Table B.15 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the UFFP Sample Problem

Pathway	TEDE (mrem)
External	3.74E-02
Inhalation	3.51E-02
Agricultural	1.16E+00
Secondary Ingestion	3.90E-03
Drinking Water	7.62E-01
Irrigation	1.82E+00
Surface Water	8.66E-01
All	3.83E+00

Table B.16 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the UFFP Sample Problem

Radionuclide	TEDE (mrem)
²³⁴ U	1.89E+00
²³⁰ Th	4.51E-04
²²⁶ Ra	5.87E-05
²²² Rn	7.81E-05
²¹⁰ Pb	1.61E-03
²¹⁰ Bi	1.24E-06
²¹⁰ Po	1.04E-03
²³⁵ U	8.33E-02
²³¹ Th	5.75E-04
²³¹ Pa	7.91E-03
²²⁷ Ac	2.21E-03
²²⁷ Th	8.87E-06
²²³ Ra	1.20E-04
²³⁸ U	1.70E+00
²³⁴ Th	1.08E-01
All	3.83E+00

B.3.4 Uranium Hexafluoride Plants

The function of a uranium hexafluoride (UF₆) conversion plant is to convert uranium concentrates, received from various uranium mills, to the purified uranium hexafluoride that is used as the feed material for the enrichment of ²³⁵U. Buildings or site areas associated with the reference UF₆ plant include processing buildings, including warehouse and storage areas of normal

industrial construction with heavy concrete floors to support equipment, a series of on-site retention ponds for storage of process raffinates and sanitary wastes, and a burial area for disposal of defunct equipment.

Operation of the reference facility is assumed to result in areas of contaminated soil on the site. The principal contaminant in the buildings and in soils is uranium. The U_{Nat} baseline sample problem for this facility is the same as the Uranium Fuel Fabrication Plant in Section B.3.3.1. Additional baseline sample problems for the ²³⁰Th and ²²⁶Ra radionuclides are included below. The files for these sample problems are preceded with UHP.

B.3.4.1 ²³⁰Th Baseline Sample Problem

This sample problem is set up by selecting the ²³⁰Th radionuclide and using all default probability distributions and parameters.

Selected Radionuclides	Initial Activity
²³⁰ Th	1 pCi/gram

Results (see Tables B.17 and B.18):

There is a 90% chance that a TEDE of 1.40E+01 mrem with a 95% confidence interval from 1.28E+01 mrem to 1.55E+01 mrem will not be exceeded within 1000 years after license termination.

Table B.17 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the UHP1 Sample Problem

Pathway	TEDE (mrem)
External	1.61E+00
Inhalation	8.21E-02
Agricultural	1.29E+01
Secondary Ingestion	4.86E-02
Drinking Water	5.29E-01
Irrigation	8.23E-01
Surface Water	1.47E+00
All	1.55E+01

Table B.18 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the UHP1 Sample Problem

Radionuclide	TEDE (mrem)
²³⁰ Th	1.93E+00
²²⁶ Ra	1.50E+00
²²² Rn	1.60E+00
²¹⁰ Pb	7.32E+00
²¹⁰ Bi	9.16E-03
²¹⁰ Po	2.90E+00
All	1.55E+01

B.3.4.2 ²²⁶Ra Baseline Sample Problem

This sample problem is set up by selecting the ²²⁶Ra radionuclide and using all default probability distributions and parameters.

Selected Radionuclides	Initial Activity
²²⁶ Ra	1 pCi/gram

Results (see Tables B.19 and B.20):

There is a 90% chance that a TEDE of 3.53E+01 mrem with a 95% confidence interval from 3.36E+01 mrem to 3.71E+01 mrem will not be exceeded within 1000 years after license termination.

Table B.19 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the UHP2 Sample Problem

Pathway	TEDE (mrem)
External	4.63E+00
Inhalation	9.61E-03
Agricultural	3.22E+01
Secondary Ingestion	1.13E-01
Drinking Water	1.63E-05
Irrigation	2.25E-05
Surface Water	1.36E-04
All	3.71E+01

B.3.5 Uranium Mill Facilities

The two most common methods of mining and uranium milling operations are conventional removal and processing and in situ leach mining. The reference case is for conventional mining and the scope is limited to the uranium mill buildings and the immediate lands surrounding the mill buildings.

Table B.20 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the UHP2 Sample Problem

Radionuclide	TEDE (mrem)
²²⁶ Ra	4.45E+00
²²² Rn	4.35E+00
²¹⁰ Pb	2.03E+01
²¹⁰ Bi	2.55E-02
²¹⁰ Po	8.52E+00
Total	3.71E+01

A model (or reference) uranium mill is described in Section 5 of NUREG-0706, *Final GEIS on Uranium Milling* (NRC, 1980c). At that model mill, ore is brought to the mill in trucks and is stored on ore pads, usually occupying an area of about 1.3 acres. Yellowcake produced in the mill is shipped by truck in 55-gallon drums. The product purity is 90% U₃O₈.

The baseline sample problem for this facility is the same as the Uranium Fuel Fabrication Plant in Section B.3.3.1 (U_{Nat} Baseline Sample problem).

B.3.6 Independent Spent Fuel Storage Installations

An ISFSI is a facility for handling and storing irradiated spent fuel assemblies from nuclear power reactors until they can be permanently disposed of as high-level waste. The two basic design categories of ISFSIs are wet storage and dry storage. The design of the wet storage ISFSI is similar to that of reactor spent fuel storage pools, except that the storage capacity is significantly greater. Dry storage ISFSIs take several different forms; the four basic types considered here are drywell storage, silo storage, vault storage, and cask storage. These dry storage designs depend on air currents, heat dissipation in the soil, and metal heat transfer fins for cooling the fuel.

A dry ISFSI is used as the reference facility because it represents the current designs in use. Although the major structures and areas of a dry ISFSI vary with the type of design, the reference dry ISFSI consists of three reinforced open air concrete pads on which the vertical sealed metal casks are placed. The contaminants, ⁶⁰Co and ¹³⁷Cs, are similar to those used for the research reactor in Section B.3.2.1 but they are not combined for this sample problem. The files for these sample problems are preceded by ISFSI.

B.3.6.1 ⁶⁰Co Baseline Sample problem

This sample problem is set up by selecting the ⁶⁰Co radionuclide and using all default probability distributions and parameters.

Selected Radionuclides	Initial Activity
⁶⁰ Co	1 pCi/gram

Results (see Table B.21):

There is a 90% chance that a TEDE of 6.60E+00 mrem with a 95% confidence interval from 6.55E+00 mrem to 6.68E+00 mrem will not be exceeded within 1000 years after license termination.

Table B.21 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the ISFSI1 Sample Problem

Pathway	TEDE (mrem)
External	6.20E+00
Inhalation	7.42E-05
Agricultural	4.84E-01
Secondary Ingestion	3.57E-04
Drinking Water	1.60E-18
Irrigation	7.54E-18
Surface Water	1.10E-17
All	6.68E+00

B.3.6.2 ¹³⁷Cs Baseline Sample Problem

This sample problem is set up by selecting the ¹³⁷Cs radionuclide and using all default parameters.

Selected Radionuclides	Initial Activity
¹³⁷ Cs	1 pCi/gram

Results (see Table B.22):

There is a 90% chance that a TEDE of 2.20E+00 mrem with a 95% confidence interval from 2.14E+00 mrem to 2.30E+00 mrem will not be exceeded within 1000 years after license termination.

B.4 Non-Fuel-Cycle Nuclear Facilities

Non-fuel-cycle facilities handle byproduct, source, and/or special nuclear materials that are not involved in the production of electric power. These non-fuel-cycle

Table B.22 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the ISFSI2 Sample Problem

Pathway	TEDE (mrem)
External	1.46E+00
Inhalation	9.31E-06
Agricultural	8.24E-01
Secondary Ingestion	6.99E-04
Drinking Water	5.17E-21
Irrigation	2.67E-20
Surface Water	2.25E-19
All	2.30E+00

facilities must be licensed by the NRC or the Agreement States.

Non-fuel-cycle facilities comprise a variety of different facilities with widely varying levels of contamination. These materials licensees include universities, medical institutions, radioactive source manufacturers, and companies that use radioisotopes for industrial or analytical purposes. Certain types, such as radioactive source manufacturers, radiopharmaceutical producers, and radioactive ore processors conduct operations that could result in substantial radioactive contamination in portions of the facility. Broad Research and Development (R&D) facilities also use isotopes in a way that could potentially produce contamination requiring decommissioning activities. About 75% of NRC's 7,000 materials licensees use either sealed radioactive sources or small amounts of short-lived radioactive materials in their business operations.

B.4.1 Sealed Sources

B.4.1.1 Sealed Source Users

A sealed source is defined in 10 CFR Part 30 as any byproduct material that is encased in a capsule designed to prevent leakage or escape of the byproduct material. Sealed source users are licensed under 10 CFR Parts 30, 33, and 35 and include medical users of sealed sources (teletherapy, brachytherapy), users of industrial gauges, well loggers, radiographers, and irradiators. Nuclides contained in the capsules and used by sealed source users include ⁶⁰Co, ¹³⁷Cs, ¹²⁵I, ¹⁹²Ir, ⁹⁰Sr, and ²⁴¹Am. The sealed sources are designed and tested according to the requirements of industrial standards and radiation safety criteria set out in the regulations to prevent leakage.

B.4.1.2 Sealed Source Manufacturers

Sealed sources are manufactured for such uses as reference standards, moisture probes, quality control instruments, therapy units, and smoke detectors. The sealed source manufacturing process is carried out in buildings that contain a number of small laboratories, each of which is devoted to a specific process and/or isotope. Each laboratory contains one or more hoods, glove boxes, and/or hot cells. Alpha and beta emitters are plated on platinum, stainless steel, or aluminized mylar film and mounted in aluminum rings to form standard disc sources. Liquid gamma sources are sealed in plastic or glass vials, and solid gamma sources are mounted in rods or plastic discs. Depending on the exposure potential of the isotope being handled, the materials are handled in hoods, glove boxes, or hot cells, which have controlled ventilation systems.

The major radionuclides considered for this facility include ^{60}Co , ^{137}Cs , ^{125}I , ^{192}Ir , ^{90}Sr , and ^{241}Am . The baseline sample problems for ^{60}Co and ^{137}Cs are the same ones used for the ISFSI facility in Section B.3.6 and will not be included here.

B.4.1.3 ^{125}I Baseline Sample problem

This sample problem is set up by selecting the ^{125}I radionuclide and using all default probability distributions and parameters.

Selected Radionuclides	Initial Activity
^{125}I	1 pCi/gram

Results (see Table B.23):

There is a 90% chance that a TEDE of $2.30\text{E}-01$ mrem with a 95% confidence interval from $1.70\text{E}-01$ mrem to $3.25\text{E}-01$ mrem will not be exceeded within 1000 years after license termination.

B.4.1.4 ^{192}Ir Baseline Sample Problem

This sample problem is set up by selecting the ^{192}Ir radionuclide and using all default probability distributions and parameters.

Selected Radionuclides	Initial Activity
^{192}Ir	1 pCi/gram

Table B.23 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the SSU1 Sample Problem

Pathway	TEDE (mrem)
External	1.94E-03
Inhalation	2.36E-06
Agricultural	2.63E-01
Secondary Ingestion	1.27E-04
Drinking Water	4.96E-10
Irrigation	1.48E-09
Surface Water	5.46E-09
Total	3.25E-01

Results (see Table B.24):

There is a 90% chance that a TEDE of $6.05\text{E}-01$ mrem with a 95% confidence interval from $6.06\text{E}-01$ mrem to $6.05\text{E}-01$ mrem will not be exceeded within 1000 years after license termination.

Table B.24 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the SSU2 Sample Problem

Pathway	TEDE (mrem)
External	6.02E-01
Inhalation	3.27E-06
Agricultural	3.29E-03
Secondary Ingestion	2.30E-05
Drinking Water	1.91E-18
Irrigation	1.01E-18
Surface Water	8.17E-19
All	6.05E-01

B.4.1.5 ^{90}Sr Baseline Sample Problem

This sample problem is set up by selecting the ^{90}Sr radionuclide and using all default probability distributions and parameters.

Selected Radionuclides	Initial Activity
^{90}Sr	1 pCi/gram

Results (see Tables B.25 and B.26):

There is a 90% chance that a TEDE of $1.40\text{E}+01$ mrem with a 95% confidence interval from $1.19\text{E}+01$ mrem to $2.08\text{E}+01$ mrem will not be exceeded within 1000 years after license termination.

Table B.25 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the SSU3 Sample Problem

Pathway	TEDE (mrem)
External	1.10E-02
Inhalation	3.81E-04
Agricultural.	1.67E+01
Secondary Ingestion	2.14E-03
Drinking Water	2.34E-12
Irrigation	4.72E-12
Surface Water	2.71E-12
All	2.08E+01

Table B.26 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the SSU3 Sample Problem

Radionuclide	TEDE (mrem)
⁹⁰ Sr	1.96E+01
⁹⁰ Y	1.21E+00
All	2.08E+01

B.4.1.6 ²⁴¹Am Baseline Sample Problem

This sample problem is set up by selecting the ²⁴¹Am radionuclide and using all default probability distributions and parameters.

Selected Radionuclides	Initial Activity
²⁴¹ Am	1 pCi/gram

Results (see Tables B.27 and B.28):

There is a 90% chance that a TEDE of 1.18E+00 mrem with a 95% confidence interval from 1.10E+00 mrem to 1.39E+00 mrem will not be exceeded within 1000 years after license termination.

B.4.2 Short-Lived Radionuclides

Licenses using short-lived byproduct radionuclides are licensed under 10 CFR Parts 30, 33, and 35 and use short-lived nuclides for specific reasons, primarily in the area of medical diagnostics. Short-lived nuclides licensed for such use include ^{99m}Tc, ¹³¹I, and ¹²³I.

Table B.27 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the SSU4 Sample Problem

Pathway	TEDE (mrem)
External	2.13E-02
Inhalation	1.35E-01
Agricultural.	1.17E+01
Secondary Ingestion	5.15E-02
Drinking Water	1.64E+00
Irrigation	2.70E+00
Surface Water	8.58E+00
All	1.39E+01

Table B.28 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the SSU4 Sample Problem

Radionuclide	TEDE (mrem)
²⁴¹ Am	1.39E+01
²³⁷ Np	1.63E-03
²³³ Pa	7.60E-07
²³³ U	5.65E-10
²²⁹ Th	5.32E-12
²²⁵ Ra	5.69E-13
²²⁵ Ac	3.28E-13
Total	1.39E+01

B.4.2.1 Generic R&D Facilities

R&D facilities using radioactive materials cover an extremely broad range of activities, including laboratories or health treatment facilities that use radioisotopes. University or industrial chemistry and physics laboratories use radioisotopes in basic experiments, and biological laboratories use them to investigate absorption and metabolic phenomena. These laboratories, in general, present no decommissioning problems because the isotopes used are short-lived and of low activity. Medical facilities, such as hospitals and clinics, also use radioisotopes for various medical purposes. These uses include both radiation exposure from sealed sources and injections of short-lived isotopes.

Contaminated areas associated with the reference R&D facility include laboratory floor and wall areas and storage areas. It is assumed that operation of the facility results in some soil contamination on the site.

The baseline sample problems include the ^{99m}Tc and ¹³¹I radionuclides. File associated with these sample problems are preceded with "SLN."

B.4.2.2 ^{99m}Tc Baseline Sample Problem

This sample problem is set up by selecting the ^{99m}Tc radionuclide and using all default probability distributions and parameters.

Selected Radionuclides	Initial Activity
^{99m} Tc	1 pCi/gram

Results (see Tables B.29 and B.30):

There is a 90% chance that a TEDE of 2.79E-04 mrem with a 95% confidence interval from 2.78E-04 mrem to 2.79E-04 mrem will not be exceeded within 1000 years after license termination.

Table B.29 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the SLN1 Sample Problem

Pathway	TEDE (mrem)
External	2.76E-004
Inhalation	1.52E-11
Agricultural	3.10E-06
Secondary Ingestion	8.72E-10
Drinking Water	1.75E-17
Irrigation	1.81E-16
Surface Water	5.72E-18
All	2.79E-04

Table B.30 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the SLN1 Sample Problem

Radionuclide	TEDE (mrem)
^{99m} Tc	2.79E-04
⁹⁹ Tc	5.22E-09
All	2.79E-04

B.4.2.3 ¹³¹I Baseline Sample Problem

This sample problem is set up by selecting the ¹³¹I radionuclide and using all default probability distributions and parameters.

Selected Radionuclides	Initial Activity
¹³¹ I	1 pCi/gram

Results (see Tables B.31 and B.32):

There is a 90% chance that a TEDE of 6.28E-02 mrem with a 95% confidence interval from 5.51E-02 mrem

to 7.14E-02 mrem will not be exceeded within 1000 years after license termination.

Table B.31 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the SLN2 Sample Problem

Pathway	TEDE (mrem)
External	3.25E-02
Inhalation	4.92E-07
Agricultural	3.89E-02
Secondary Ingestion	2.40E-05
Drinking Water	2.92E-17
Irrigation	2.87E-17
Surface Water	3.15E-16
All	7.14E-02

Table B.32 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the SLN2 Sample Problem

Radionuclide	TEDE (mrem)
¹³¹ I	7.14E-02
^{131m} Xe	4.02E-06
All	7.14E-02

B.4.3 Rare-Metal Ore Processors

A rare-metals ore processor is a facility, not part of the fuel cycle, that refines raw ore materials to recover rare metals such as tantalum and niobium. These ores can contain appreciable concentrations of radionuclides, such as uranium and thorium, which are found in the waste tailings of the refining process. The NRC licenses such facilities principally to regulate the handling of these waste tailings. While relatively few such facilities operate in the United States, the volumes of tailings are sufficient to require a significant decommissioning effort.

The raw material can be a slag produced by smelters. The slag can consist of glassy flakes or tin pellets containing 0.1 to 0.5 wt% U₃O₈ and ThO₂. In one building, the slag is ground, roasted, and digested with hydrofluoric acid. The hydrofluoric acid is passed to a facility for the chemical extraction of the rare metals, such as niobium and tantalum.

The reference rare metal ore processor is a plant that refines raw ore materials for the recovery of rare metals such as tantalum and niobium. The raw ores can contain appreciable quantities of uranium and thorium, which are waste tailings of the refining process.

Contaminated facilities and areas associated with the reference rare metal ore processor include:

- buildings in which slag is processed and the rare metals are extracted,
- settling ponds on site that contain the tailings from the metal extraction process, and that contain essentially all of the radioactivity (the pond is assumed to be unlined at the reference rare metal ore processor, although it may be lined at newer facilities),
- a slag pile containing solid wastes from the extraction process.

It is assumed that operation of the facility results in soil contamination on the site. The U_Nat baseline sample problem for this facility is the same as for the Uranium Fuel Fabrication Plant in Section B.3.3.1. An additional baseline sample problem for the ²³²Th radionuclide in equilibrium is shown here. The files associated with this sample problem is preceded with "RMOP."

B.4.3.1 ²³²Th+C Baseline Sample Problem

This sample problem is set up by selecting the ²³²Th+C radionuclide and using all default probability distributions and parameters. The "Calculation option for +C radionuclides" option on the "Add Contaminants" screen is set to "Do not distribute."

Selected Radionuclides	Initial Activity
²³² Th+C	1 pCi/gram

Results (see Tables B.33 and B.34):

There is a 90% chance that a TEDE of 2.30E+01 mrem with a 95% confidence interval from 2.24E+01 mrem to 2.59E+01 mrem will not be exceeded within 1000 years after license termination.

Table B.33 Upper Limit of the 95% Confidence Interval of the Pathway Component of All Maximum Annual Doses for the RMOP Sample Problem

Pathway	TEDE (mrem)
External	6.53E+00
Inhalation	6.65E-01
Agricultural	1.67E+01
Secondary Ingestion	7.05E-02
Drinking Water	8.63E-09
Irrigation	1.39E-08
Surface Water	1.28E-08
All	2.59E+01

Table B.34 Upper Limit of the 95% Confidence Interval of the Radionuclide Component of All Maximum Annual Doses for the RMOP Sample Problem The "Calculation option for +C radionuclides" option on the "Add Contaminants" screen is set to "Do not distribute."

Radionuclide	TEDE (mrem)
²³² Th	1.04E+01
²²⁸ Ra	7.76E+00
²²⁸ Th	1.53E+00
²²⁴ Ra	1.44E+00
²¹² Pb	4.15E+00
All	2.59E+01

B.5 References

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APPENDIX C FORMAT OF IMPORT CONCENTRATION FILE

The residential scenario includes the ability to import concentrations calculated by other modeling codes to compute doses. To use this capability, an import concentration data file is required for inputting soil and groundwater radioactivity concentrations. This appendix (Table C.1) describes the format for the concentration input files. Table C.2 provides an example import concentration file.

The first record in the file tells how many chains will be in the input file and is followed by two more groups of records. The second group gives the number and description of the radionuclides for each chain. The third group contains the time step values and the concentration data associated with each time step.

Table C.1 Residential Scenario Import Concentration File Format

Record	Description
Group 1:	Number of Chains
Record:	Number of radionuclide chains that will be imported.
Format:	Free-format integer: Valid values are 1 - 50.
Description:	The number of chains in the scenario. A description of each individual chain must be provided in the Radionuclide Description group of records following this record (one group per chain).
Comment:	The number of chains must be less than or equal to 50. If not, the results may be undefined. For the purpose of importing concentrations, the natural uranium (U-Nat) chain must be broken into its components and, therefore, counts as three chains.
Error Messages:	<ul style="list-style-type: none"> • <u>Premature end of file reached reading number of chain records in import concentration file</u>: The file has no data in it. • <u>Error reading number of chain records in import concentration file</u>: Input/Output system error. An error number will be shown that allows support personnel to determine the cause of the problem. If an error code of 6101 is encountered, an invalid integer (such as text) was entered. • <u>Number of chains in import concentration file exceeds maximum allowable (50)</u>: This number must be less than or equal to 50.
Group 2:	Radionuclide Descriptions
Record 1:	Number of explicit radionuclides in this chain.
Format:	Free-form integer; valid values are 1 - 50.
Description:	The number of explicit radionuclides in this chain including the parent radionuclide. This number determines the number of explicit Radionuclide Name records immediately following this record.
Comment:	The number of explicit radionuclides must be less than or equal to 50. Do not include any implicit radionuclides associated with this chain.
Record 2:	Name of the explicit radionuclide.
Format:	Six characters, alphanumeric, in columns 1 through 6.

Table C.1 Residential Scenario Import Concentration File Format

Record	Description
Description:	Explicit radionuclide name. There must be one record for each explicit radionuclide in the chain. For example, if there are seven explicit radionuclides in the chain, there must be seven records of this type.
Comment:	The order and number of explicit radionuclides in this description must comply exactly with the chain descriptions in the Radioactive Decay Data tables (see Section 4.3.8). The code compares this description with the one presented in the table and, if there are any discrepancies, the code will abort the run and issue an error message.
Error Messages:	<ul style="list-style-type: none"> • <u>Premature end of file reached reading names of explicit radionuclides in chain</u>: The file is truncated too soon. • <u>Error reading names of explicit radionuclides in chain</u>: Input/Output system error. An error number will be shown that allows support personnel to determine the cause of the problem. • <u>Radionuclide name is not a valid radionuclide name</u>: The code was unsuccessful in comparing the radionuclide name entered with.
Group 2 is repeated until all chain descriptions have been entered.	
Group 3:	Concentration Description.
Record 1:	Time of Interest
Description:	The Time of Interest is the time at which the imported concentrations were calculated and at which time the subsequent dose results will be calculated. The input must be in days.
Record 2:	Residential soil and groundwater concentrations.
Format:	Free-format, floating point, one pair of variables per record, separated by a space.
Description:	The first variable is the soil concentration in pCi/g for the radionuclides described in Group 2, above, at the beginning of the Time of Interest. The second variable is the average groundwater concentration in pCi/L of the same radionuclide over a one-year time frame beginning with the Time of Interest.
Comment:	This record is repeated for each radionuclide described in Group 2, above. In Table C.2, there are three chains with 7, 6, and 9 radionuclides in each chain respectively. Therefore, there must be 22 (7 + 6 + 9) records of this type for each time step. The order of presentation of the concentrations must comply with the order presented in Group 2. The code has no way to check if the concentrations are in the correct order. Therefore, caution must be used in the order and number of these concentration records.
Group 3 is repeated as many times as necessary. The code will read Group 3 records until the scenario end time given in the Residential Basic Parameters is reached or an end-of-file condition is reached. A sample file is shown that includes four time steps for the natural uranium chain. Do not include the description shown in parentheses in an actual input file.	

Table C.2 Example File for Importing Concentrations for the U_Nat Chain (U234, U235, U238)

Value	Value	Comments
3		(Number of Chains)
7		(Number of Radionuclides in chain 1)
234U		(Radionuclide Names for chain 1)
230Th		
226Ra		
222Rn		
210Pb		
210Bi		
210Po		
6		(Number of Radionuclides in chain 2)
235U		(Radionuclide Names for chain 2)
231Th		
231Pa		
227Ac		
227Th		
223Ra		
9		(Number of Radionuclides in chain 3)
238U		(Radionuclide Names for chain 3)
234Th		
234U		
230Th		
226Ra		
222Rn		
210Pb		
210Bi		
210Po		
0.0000000000000000		(Time of Interest)
0.0000000000000000	0.247522757808938D-009	(Concentrations)
0.0000000000000000	0.484858183517552D-015	
0.0000000000000000	0.396815555468826D-019	
0.0000000000000000	0.189522392289388D-017	
0.0000000000000000	0.114417255157419D-019	
0.0000000000000000	0.103885438401388D-019	
0.0000000000000000	0.247829211431455D-020	
0.0000000000000000	0.113891077868471D-010	
0.0000000000000000	0.112124311179322D-010	
0.0000000000000000	0.528562229862447D-016	
0.0000000000000000	0.317236495338320D-018	
0.0000000000000000	0.218981181517277D-018	
0.0000000000000000	0.177312704861995D-018	
0.0000000000000000	0.247523276052333D-009	
0.0000000000000000	0.179475815505557D-009	
0.0000000000000000	0.366644216333686D-015	
0.0000000000000000	0.554102623933457D-021	
0.0000000000000000	0.330316344522203D-025	
0.0000000000000000	0.118831796675130D-023	
0.0000000000000000	0.0000000000000000	
0.0000000000000000	0.0000000000000000	
0.0000000000000000	0.387340435476567D-024	
365.250000000000		(Time of Interest)
0.685469165302906D-009	0.134741024908478D-008	(Concentrations)

Table C.2 Example File for Importing Concentrations for the U_Nat Chain (U234, U235, U238)

Value	Value	Comments
0.175871147027935D-014	0.495362899770729D-014	
0.180111318876507D-018	0.776131599674565D-018	
0.630573744828938D-017	0.174234077170609D-016	
0.477334332848322D-019	0.188000175498888D-018	
0.441835648737467D-019	0.178169650961613D-018	
0.123247502921888D-019	0.664865553040717D-019	
0.315400817560165D-010	0.619976830856126D-010	
0.311885356501322D-010	0.614777022667660D-010	
0.192885440984453D-015	0.548391965969810D-015	
0.144706730419307D-017	0.629031681703798D-017	
0.106100397269115D-017	0.507338766497242D-017	
0.894389208483707D-018	0.456388539794910D-017	
0.685471110732884D-009	0.134741631416726D-008	
0.539059448934161D-009	0.112433606659562D-008	
0.148840725562149D-014	0.511011675415349D-014	
0.276333981176464D-020	0.146035126829713D-019	
0.000000000000000	0.177935345835221D-023	
0.464827012918598D-023	0.253708387955905D-022	
0.000000000000000	0.274573361685459D-024	
0.000000000000000	0.421344011293412D-024	
0.000000000000000	0.172359583696953D-024	
730.500000000000		(Time of Interest)
0.206879336191261D-008	0.285187089665718D-008	(Concentrations)
0.903777804491166D-014	0.145081994022596D-013	
0.169366852946708D-017	0.331261541522632D-017	
0.326728487233615D-016	0.575680706015900D-016	
0.407145837169490D-018	0.835776321078462D-018	
0.388745850894128D-018	0.803567262443758D-018	
0.159893738089962D-018	0.367820596468893D-018	
0.951904187751751D-010	0.131222001499207D-009	
0.945051445996075D-010	0.130377562981958D-009	
0.100528461620271D-014	0.162396085407654D-014	
0.137743262380402D-016	0.270814455674890D-016	
0.114419666828799D-016	0.231249634432062D-016	
0.104923428582542D-016	0.215971076532749D-016	
0.206880510481380D-008	0.285189150527488D-008	
0.177048526051827D-008	0.248112032955631D-008	
0.102389493906991D-013	0.185035180403758D-013	
0.344371423650410D-019	0.749019946800425D-019	
0.496419537842190D-023	0.135319565732186D-022	
0.619363558574050D-022	0.150151780226801D-021	
0.625908757379270D-024	0.175685216656883D-023	
0.573455698477810D-024	0.164872343100813D-023	
0.245519978623145D-024	0.682968925414381D-024	
1095.75000000000		(Time of Interest)
0.364671423177404D-008	0.444454267854206D-008	(Concentrations)
0.204720606482233D-013	0.270903875440447D-01	
0.527880440156510D-017	0.787895755091530D-017	
0.879295903899320D-016	0.130412336018944D-015	
0.139407830043134D-017	0.225891066434437D-017	
0.134514657550422D-017	0.218692384046246D-017	

Table C.2 Example File for Importing Concentrations for the U_Nat Chain (U234, U235, U238)

Value	Value	Comments
0.650941479418464D-018	0.111951764593952D-017	
0.167795027852860D-009	0.204505545609364D-009	
0.166794414137780D-009	0.203354588605064D-009	
0.230237188616761D-014	0.306465073296225D-014	
0.433096232478005D-016	0.649656442895449D-016	
0.375113673072341D-016	0.569570227737363D-016	
0.353629674552019D-016	0.541436534350816D-016	
0.364674528108021D-008	0.444458720426173D-008	
0.320488262938123D-008	0.393428619996491D-008	
0.283336250978395D-013	0.411984665622026D-013	
0.127318200099534D-018	0.205208884640300D-018	
0.258386353915024D-022	0.474492466919941D-022	
0.275567255043353D-021	0.501436105729973D-021	
0.356620193728023D-023	0.721972314186154D-023	
0.340581445167568D-023	0.695579766118310D-023	
0.145960036701288D-023	0.319243681886171D-023	

APPENDIX D DandD DATABASE TABLE DESCRIPTIONS

D.1 Introduction

The input and output of DandD are saved in a Microsoft® Access® database. This appendix describes the tables and fields in this database.

When a new session is created, a copy of the database InitVBASession.mdb is created. This database will have an extension of mcd (Monte Carlo DandD); for example, "session.mcd."

The tables in the database are identified by a three-character prefix. These are as follows.

Prefix	Meaning
app	Tables used by application. These tables are only modified by the programming staff. They contain initialization constants and default values.
bld	Tables containing data for the building scenario. These tables can be modified by the user indirectly through the DandD interface.
dat	Tables created as a result of the model runs.
err	Tables generated by Latin Hypercube Sampling (LHS) or scenario models containing error details.
par	Tables output from LHS.
res	Tables containing data for the residential scenario. These tables can be modified by the user indirectly through the DandD interface.
sen	Tables related to sensitivity analysis.
usr	General session settings.

Input to the dose model program takes on many characteristics. In most cases, the user can specify the input as probability distributions or constants.

General parameter data will always be fed to the modeling code. The user will have the option to modify this data from within the graphical interface. Within the residential model, this data is also grouped in categories such as Basic, Growing Period, etc. (15 categories total).

Data associated with contaminants will also be input to the modeling code. The user will be able to add contaminants, modify the area associated with a contaminant, and input the concentration of the contaminant.

Each nuclide additionally has decay or daughter products. Each daughter product has parameters associated with it in the residential model. The user will be able to modify these parameters also.

All of the user-modifiable data has been stored in the database in tables, as discussed in Section D.2.

D.2 Table Descriptions

D.2.1 Application Tables (app tables)

appAuxCHAIN, appCHAIN

This is a list of decay or daughter nuclide data that is used by the dose model program. This data will be accessible to the user for viewing as a table. This table contains constants that cannot be changed by the user.

Most of the information on the nuclides is in the *appChain* table. However, some extra decay data that is used only by the user interface is stored in the *appAuxChain* table. These tables have an identical structure. The user interface unites these tables to define the element parameters for any contaminant. The underlying modeling software only uses table *appChain*.

The table *appAuxChain* was initially designed because of the special case introduced for U_Nat and Th_Nat. These two elements have many associated element parameters, but the interface requires that this information is not present in the *appChain* table. It is required that all entries in table *appAuxChain* not have values equal for [Parent] and [Radionuclide]. Since each [Parent] will have an entry where [Parent] and [Radionuclide] fields are equal, this particular record will be in the *appChain* table.

From this table, all daughter nuclides in the decay chain can be accessed. The decay products, or daughters, are found by looking up records based on the value of the field [Parent]. The source contaminants are found in the *appCandC_Decode* table.

The user will input the contaminants. The DandD software will then find the decay products in the *appChain* table and offer the user the ability to modify data related to these daughter product contaminants.

[RecordID]	is an index used to order the table records.
[Parent]	refers to the original contaminant, not the immediate parent in the decay chain.
[Radionuclide]	is a by-product in the decay chain of [Parent].
[HalfLife]	is the half-life of [Radionuclide].
[PositionInChain]	is the number of decay generations from [Parent]. A radionuclide directly descended from [Parent] will have a value of 2 for [PositionInChain]. If [Parent] and [Radionuclide] are equal, then [PositionInChain] will be equal to one.
[FirstParentIndex]	indicates which radionuclide in the chain is the immediate parent of this nuclide.
[FirstParentFraction]	is the fraction of decays of the first parent that produce [Radionuclide].
[SecondParentIndex]	indicates alternate radionuclide that can decay to [Radionuclide].
[SecondParentFraction]	is the fraction of decays of the second parent that produces [Radionuclide].
[AtomicNumber]	is the number of protons in the [Radionuclide].

Example:

RecordID	Parent	Radionuclide	HalfLife	PositionInChain
303	228Ra	228Ra	2.10E+03	1
304	228Ra	228Ac		
305	228Ra	228Th	6.99E+02	2
306	228Ra	224Ra	3.66E+00	3
307	228Ra	220Rn		
308	228Ra	216Po		
309	228Ra	212Pb	4.43E-01	4
310	228Ra	212Bi		
311	228Ra	212Po		

FirstParentIndex	FirstParentFraction	SecondParentIndex	SecondParentFraction
1	1.00		
1	1.00	0	0.00
2	1.00	0	0.00
3	1.00		
3	1.00		
3	1.00	0	0.00
4	1.00		
4	0.64		

AtomicNumber
88
89
90
88
82

appBldCorrelations, appResCorrelations

These tables define the default Spearman (rank) correlation coefficients between pairs of parameters. Table *appResCorrelations* and *appBldCorrelations* contain the default correlation coefficients for the residential and building occupancy scenarios, respectively. If two parameters do not have an entry in the *appResCorrelations* or *appBldCorrelations* tables, then the default correlation coefficient is assumed to be zero for the appropriate scenario. This means that the parameters are statistically independent.

- [ParameterID1] identifies one of the pair of correlated parameters.
- [ParameterID2] identifies the other correlated parameter.
- [Correlation] is the correlation coefficient between the ranks of the parameter values, between -1 and 1 inclusive.

The following integrity rules should be followed for this table:

- [ParameterID1] must be strictly less than [ParameterID2].
- [ParameterID1, ParameterID2] are also a key for each of these tables. In other words, the ordered pair [ParameterID1, ParameterID2] is unique for the given table.

Example:

ParameterID1	ParameterID2	Correlation
84	85	-0.49
85	86	-0.49
84	86	-0.49

appCandC_Decode

This is a list of possible nuclide contaminants and corresponding keys used to identify them in the dose model program. This table contains constants that cannot be changed by the user.

[SourceNumber] is used to identify contaminants. This number is passed to the dose model program to communicate the presence of a contaminant.

[Source] identifies the contaminant. It is prefixed by the atomic weight.

[ElementID] identifies the chemical element for the nuclide.

[HasElement] indicates that element-dependent parameters are associated with the nuclide.

Example:

SourceNumber	Source	ElementID	HasElement
62	101Tc	Tc	Yes

appCEDE

This is a list of nuclide data that is used by the dose model program. This table contains constants that cannot be changed by the user.

[Parent]	is the name of the parent radionuclide.
[Radionuclide]	is the name of the radionuclide.
[ImplicitProgenyFraction]	is the fraction of parent transitions that produce this radionuclide.
[Ingestion]	is the unit committed effective dose equivalent (CEDE) conversion factor for ingestion.
[Inhalation]	is the unit CEDE conversion factor for inhalation.
[ExternalSurface]	is the unit CEDE conversion factor for external surface exposure.
[External15cm]	is the unit CEDE conversion factor for external exposure at 15 cm.

Example:

Parent	Radionuclide	ImplicitProgenyFraction	Ingestion	Inhalation	ExternalSurface
240U	240U		1.20E-09	6.13E-10	3.65E-13
240U	240mNp	1.00	0.00E+00	0.00E+00	2.82E-11

External15cm
6.58E-16
8.20E-13

appCHAIN: see *appAuxChain*

appDependencies

This is a description of the potential dependencies among parameters. Only parameters in the *appParameter* table that have 'Derived' as a default distribution are present in this table. These should also be the parameters that have the field [Derived] set to Yes in the table *appParameter*. Neither element nor nuclide parameters can be derived.

Only if the user has the distribution type set to 'Derived' for a parameter will its values be calculated from the independent parameters listed in this table.

These dependencies are implemented in the LHS preprocessor, and are used to obtain the values for parameters having the special distribution type 'Derived.' In other words, a parameter identified by the field [ParameterID] is derived functionally in code, using the value of [IndependentParameterID].

The user cannot modify this table.

The graph of dependencies defined by this table must be acyclic.

[ParameterID] identifies the parameter whose value can be provided by the dependency. Only parameters that have a default value of 'Derived' and whose field [Derived] is set to Yes in the *bld/resParameterDetail* table are listed in this table. All such parameters must have one or more entries in the table.

[DependencyNumber] indexes the independent parameters that are used in the dependency, beginning with one.

[IndependentParameterID] identifies a parameter used to derive the value of the dependent parameter. These are only parameters from table *appParameter*.

Example:

If the parameter INFIL has its distribution set to 'Derived,' then its value will be calculated in the code using the parameters Ksat1, IR, and AP

ParameterID	DependencyNumber	IndependentParameterID
INFIL	1	Ksat1
INFIL	2	IR
INFIL	3	AP

appDerivationMethod

This table lists the methods used to derive the values for 'Derived' parameters. The named methods are implemented by the LHS preprocessor. This table contains constants that cannot be changed by the user.

[ParameterID] identifies the parameter whose value can be provided by the dependency. Only parameters that can be "Derived," or whose unit conversion factors are also model parameters, are listed in this table. All such parameters must have one entry in the table.

[MethodName] identifies the procedure used to derive the parameter value from the value(s) of other model parameters. The specific parameters used in the derivation are listed in the *appDependencies* table.

Example:

ParameterID	MethodName
INFIL	InfiltrationModel

appDistributions

Contains data related to distributions. This table contains constants that cannot be changed by the user.

[DistributionID] is an index that identifies the distribution.

[DistributionName] is the name (or description) of the distribution.

[Empirical] indicates whether the distribution requires a set of ordered pairs or a fixed sized set of parameters for definition. For example, the Normal distribution is not empirical because it has exactly two parameters. The Continuous Linear distribution is empirical because it is defined by a set of ordered pairs.

[DistributionDesc] contains a description of integrity rules for the distribution.

Example:

DistributionID	DistributionName	Empirical	DistributionDesc
17	CONTINUOUS FREQUENCY	Yes	Y >= 0
20	EXPONENTIAL	No	
21	MAXIMUM ENTROPY	No	

appDistributionSymbols

This table identifies the number of parameters and their associated parameter names for each non-empirical distribution. This table contains constants that cannot be changed by the user.

[DistributionID] matches with field [DistributionID] in table *appDistributions*.

[ParameterNumber] identifies the parameter number the [ParameterLabel] is associated with (this is a sequence number starting at 1 for the first label, 2 for the second label, etc.).

[ParameterLabel] is the label as it will appear on the graphical user interface (GUI).

For example: assume the following in the *appDistributions* table:

DistributionID	DistributionName	Empirical
2	NORMAL	No

Then, the following entries are in the *appDistributionSymbols* table.

DistributionID	ParameterNumber	ParameterLabel
2	1	Mean
2	2	Standard Deviation

The entry {15, "Continuous Linear," Yes} in the *appDistributions* table has no corresponding entries in the *appDistributionSymbols* table because the distribution is empirical.

appElementParameterNames, appElementParameters

These tables contain information related to parameters whose values depend on the chemical composition of the contamination. Each daughter product within the decay chain for a source contaminant will have additional parameters that the user can modify. These parameters are only used in the residential scenario model. The default values for these additional parameters, referred to as element parameters, are defined in these tables.

The labels associated with the element parameters and the units required by the dose model are stored in the *appElementParameterNames* table. The element parameters have corresponding default values and limits for each of the variables in each of the categories.

The table *appElementParameterNames* contains the following data.

NuclideParameterNameID	Name	ModelUnitsID
0	Coefficient	mL/g
1	Leafy	pCi/kg dry-wt leafy per pCi/kg soil
2	Root	pCi/kg dry-wt roots per pCi/kg soil
3	Fruit	pCi/kg dry-wt fruit per pCi/kg soil
4	Grain	pCi/kg dry-wt grain per pCi/kg soil
5	Beef	d/kg
6	Poultry	d/kg
7	Milk	d/L
8	Eggs	d/kg
9	Factor	pCi/kg wet-wt fish per pCi/L water

Note: the field [ModelUnitsID] is a long integer that joins with table *appUOM* to obtain the string shown describing the units.

Finally, each of the 73 elements will have ten entries in the *appElementParameters* table that describe default values for each parameter listed in the above table. The fields in this table are described as follows.

[ParameterID]: by convention, all element parameters will have ParameterIDs between 2001 and 9999. Parameter IDs for element-dependent parameters will be assigned as follows.

$$ID = 2000 + NuclideParameterNameID * 100 + SourceNumber$$

In this expression, SourceNumber is the identifying number of the element used in the *appKd Decode* table.

[Source] corresponds to symbol identifying element in the periodic table of elements. This entry should match on field [Source] with a record in table *appKd Decode*.

[NuclideParameterNameID] identifies in which of the ten categories this element parameter belongs.

[Description] is used as a label in the user interface.

[DistributionID] is the default distribution used for this parameter.

[NoEdit] is not used at this time.

[Derived] is not used at this time.

[LowerBound] [UpperBound]: if the user has specified parameter values outside of these bounds, the user will be warned that the value may be inappropriate and may require additional justification. However, the user will be permitted to use the value.

[HardLowerBound] [HardUpperBound]: if the user has selected a constant distribution and enters a value outside these bounds, the user will not be permitted to run a simulation. If the user has entered a distribution other than constant, and any of the values from LHS fall outside these bounds, the user will not be permitted to run any Monte Carlo simulations, even if the values for a given simulation are within bounds.

[DefaultUnitsID] are the units that correspond to default values in the tables *appEmpirical*, etc.

[HelpLink] is a hyperlink to documentation related to this parameter from Beyeler et al. (1999) as saved in HTML format. This is expected to be a relative link. However, the software will use the path of the application for the bases of this relative link.

Example from table *appElementParameters*:

ParameterID	Source	NuclideParameterNameID	Description
2073	Cf	Partition Coefficients : Coefficient	Partition coefficient for Cf
2101	H	Soil to Plant Concentration : Leafy	Leafy plant concentration factor for H

DistributionID	NoEdit	Derived	LowerBound	UpperBound	HardLowerBound	HardUpperBound
NORMAL	No	No	0		0	
CONSTANT	No	No	0		0	

DefaultUnitsID	HelpLink
Log10(mL/g)	
pCi/kg dry-wt leafy	nrcvol3\SessionGenBuildSummary.htm

Note: the field [NuclideParameterNameID] is actually a long integer that joins to field [NuclideParameterNameID] in the *appElementParameterNames* table. Similarly, the field [DistributionID] and [DefaultUnitsID] are actually long integers that join to tables *appDistributions* and *appUOM*, respectively.

The data associated with these parameters will be placed in the same tables as the data for the parameter values, namely *appEmpirDefValues*, *resEmpirValues*, *bldEmpirValues*, *appNonEmpirDefValues*, *resNonEmpirValues*, and *bldNonEmpirValues*. However, the data will only be in the *res** and *bld** tables if the associated elements are present in the source decay chain. All default data for the element-dependent parameters will be in the *appEmpirDefValues* and *appNonEmpirDefValues* tables.

appElementParameters: see *appElementParameterNames*

appEmpirDefValues, resEmpirValues, bldEmpirValues

Each of these tables contains values for parameters with empirical (tabulated) default distributions. These distributions are defined by tables of varying lengths containing numbers representing the parameter value and the probability of that value.

If the default distribution type in the relevant parameter table (*appParameter* or *appElementParameters*) is set to a distribution that is flagged as empirical in the *appDistributions* table, the default data will be found in table *appEmpirDefValues*. This table contains constants that cannot be changed by the user.

When a new session is created, tables *resEmpirValues* and *bldEmpirValues* are initialized to the default parameter values. These tables will not be the same because not all parameter numbers used for the different scenarios are the same. These tables, *resEmpirValues* and *bldEmpirValues*, will be modified when the user changes parameter values in the residential and building scenarios, respectively.

Example:

The default value for parameter one has been set to an empirical distribution in the *bldParameterDetail* table as follows:

ParameterID	Name	DistributionID
1	Time In Building	CONTINUOUS LINEAR

Because the distribution Continuous Linear is an empirical distribution, the data corresponding to this will be stored in the *appEmpirDefValues* table. The meaning of fields [Value1] and [Value2] are dependent on the empirical distribution. The data are stored as follows.

ParameterID	Value1	Value2
1	35	0
1	39	0.1
1	40	0.1001
1	40.01	0.581
1	41	0.5811
1	48	0.739
1	49	0.7391
1	59	0.892
1	60	0.8921
1	65	1

appKd_Decode

This is a list of element names that are passed to the dose model program.

[SourceNumber] contains a key used by the dose model program to identify the chemical element.

[Source] contains the text identifying the nuclide. The atomic weight has been stripped from the chemical name.

Example:

SourceNumber	Source
10	Ca

appNonEmpirDefValues, resNonEmpirValues, bldNonEmpirValues

If the default distribution type in the relevant parameter table (*appParameter* or *appElementParameters*) is set to a distribution that is flagged as nonempirical in the *appDistributions* table, the default data will be found in table *appNonEmpirDefValues*. This table contains constants that cannot be changed by the user.

The default data for the nuclide parameters are not stored in *appNonEmpirDefValues* because the default is the same for all nuclides; namely, the concentration is zero and the distribution is Constant.

Each entry in this table contains nonempirical values for parameters. These tables are handled by the application similar to the empirical tables (*appEmpirDefValues*, *resEmpirValues*, and *bldEmpirValues*).

Example:

The default values for parameter 5 has been set to the non-empirical Lognormal distribution in the *bldParameterDetail* table as follows:

ParameterID	Name	DistributionID
5	Ingestion Rate	LOGNORMAL

The data corresponding to the default values used can be found in the *appNonEmpirDefValues* table as follows:

ParameterID	ParameterNumber	Value
5	1	0.0112
5	2	1.4268

DandD determines the meaning of the [ParameterNumber] and [Value] fields by looking up the Lognormal distribution in the *appDistributionSymbols* table as follows:

DistributionID	ParameterNumber	ParameterLabel
LOGNORMAL	1	Mean
LOGNORMAL	2	Error Factor

In this example, the distribution is LOGNORMAL with a mean of .0112 and an error factor of 1.4268 for the Ingestion Rate.

Note: the actual value stored in these tables for the Distribution ID is a long integer, not the character string "LOGNORMAL." The field [DistributionID] is joined with the field [DistributionID] in table *appDistributions* in order to find the [DistributionName]. In the above example, the [DistributionID] is 6. The entry in the *appDistribution* table is as follows:

DistributionID	DistributionName	Empirical
6	LOGNORMAL	No

appNuclides

The *appNuclides* table contains the list of all possible nuclides.

The default value for the nuclide parameters (namely, the concentrations of the nuclides) is set to zero. The nuclide concentration default values cannot be changed by modifying the database, but are initialized in the software. These values are not stored in the *appNonEmpirDefValues* table, but are inserted by the software into the *resNonEmpirValues* and *bldNonEmpirValues* tables when contaminants are added.

The fields have the following meaning:

[ParameterID] is used to find the associated data in the tables *resNonEmpirValues*, *bldNonEmpirValues*, *resEmpirValues*, and *bldEmpirValues* when contaminants are added. By convention, all values of [ParameterID] will be between 1001 and 2000 for the nuclide parameters.

[NukeID] is the ID to pass to the dose model program.

[NuclideSymbol] is the symbol used by the GUI to identify the nuclide.

[IsSource] flags nuclides that can be explicitly included in the source term. This includes most nuclides except a few that have very short half-lives.

[HelpLink] is a hyperlink to documentation related to this parameter from Beyeler et al. (1999) as saved in HTML format. This is expected to be a relative link. However, the software will use the path of the application for the bases of this relative link.

The data associated with the nuclides will be placed in the same tables as the data for the other parameters, namely *resEmpirValues*, *resNonEmpirValues*, etc.

Example:

ParameterID	NukeID	NuclideSymbol	IsSource	HelpLink
1001	1	3H	Yes	
1002	2	10Be	Yes	nrcvol3\SessionGenBuildSummary.htm
1003	3	14C	Yes	

appParameter

Each parameter listed in this table is used as input to the dose model program. There are no parameters associated with nuclides or elements in this table. By convention, all values for the [ParameterID] will be between 1 and 1000 for the parameters in *appParameter* table.

The fields [DistributionID], [Scenario], [Residential Category], [DefaultUnitsID], [ParameterCategoryID], and [ModelUnitsID] are joined to tables *appDistribution*, *appSenario*, *appResidentialCategories*, *appUOM*, *appParameterCategories*, and *appUOM*, respectively.

The fields have the following meaning:

[ParameterID] identifies associated data in one of the data tables *bldEmpirValues*, *resEmpirValues*, *bldNonEmpirValues*, or *resNonEmpirValues*. The default data associated with this parameter will be in tables *appNonEmpirDefValues* or *appEmpirDefValues*.

[Name] is the concise description of the parameter.

[Description] is the detailed description of the parameter.

[DistributionID] is the default distribution used for this parameter.

[Input] indicates parameters that are directly required by the dose model. Not all parameters are input to the dose model. The parameters that have [Input] set to No are used to calculate other parameters that are input to the model.

[InputSequence]: for input parameters, this gives a sequence number that is unique for each scenario. This sequence number defines the order that the parameters are required by the dose model. If the parameter is not an input parameter, then the input sequence number should be Null. If the [Input] field is set to Yes, then [InputSequence] value must be a number.

[NoEdit]: if set, the user cannot modify this value from the default value.

[Derived]: if set, the user is allowed to set the distribution type to 'Derived.' If this is Yes, the [DistributionID] in this table must also be set to 'Derived.'

[LowerBound] [UpperBound]: if the user has specified a value outside of these bounds, the user will be warned that the value may be inappropriate and will require additional justification. However, the user will be permitted to use the value.

[HardLowerBound] [HardUpperBound]: if the user has selected a constant distribution and enters a value outside these bounds, the user will not be permitted to run a simulation. If the user has entered a distribution other than constant, and any of the values from LHS fall outside these bounds, the user will not be permitted to run any Monte Carlo simulations, even if the values for a given simulation are within bounds.

[DefaultUnitsID] are the units that correspond to default values associated with this parameter.

[Symbol] is used to identify this parameter in the dose model program.

[Scenario] identifies if parameter is used for the building occupancy or residential scenario. Because there are different default values associated with parameters in this table depending on the scenario, this table can be partitioned into parameters used for the residential and parameters used for the building occupancy scenarios.

[ResidentialCategory]: if the scenario is residential, this field identifies the parameter category for grouping within the GUI. Otherwise, this entry is Null.

[ParameterCategoryID] assigns the parameter to one of the categories given in the *appParameterCategories* table.

[ModelUnitsID] indicates the units of measure required by the dose model. This may differ from the values used to specify the default. These fields are joined with table *appUOM* to obtain a full description and label.

[HelpLink] is a hyperlink to documentation related to this parameter from Beyeler et al. (1999) as saved in HTML format. This is expected to be a relative link. However, the software will use the path of the application for the bases of this relative link.

[ExternalCode], [InhalationCode], [SecIngestionCode], [FarmCode], [DrinkingCode], [IrrigationCode], and [PondCode] are not used at this time. The intention was to use these fields as binary flags to indicate to which pathways the parameter is applicable.

Example:

ParameterID	Name	Description	DistributionID
1	Time In Building	The time in the building (converted to effective 24-hr days) during the occupancy period	CONTINUOUS LINEAR
2	Occupancy Period	The duration of the occupancy exposure period	CONSTANT
3	Breathing Rate	The average volumetric breathing rate during building occupancy for an eight-hour work day	CONTINUOUS LINEAR

Input	InputSequence	NoEdit	Derived	LowerBound	UpperBound
Yes	1	No	No	0	250
Yes	2	No	No	1	365.25
Yes	3	No	No	0	3.63

HardLower Bound	HardUpper Bound	DefaultUnitsID	Symbol	Scenario
0	250	days/year	To	Building Occupancy
1	365.25	days	Tto	Building Occupancy
0	3.63	m**3/hr	Vo	Building Occupancy

ResidentialCategory	ParameterCategoryID	ModelUnitsID	HelpLink
	Behavioral	days/year	nrcvol3\SessionGenBuildSummary.htm
	Behavioral	days	
	Metabolic	m**3/hr	

ExternalCode	InhalationCode	SecIngestionCode	FarmCode	DrinkingCode

IrrigationCode	PondCode

appParameterCategories

This table names the four categories of the parameters required by the scenario models. The LHS sampling used depends on the categories for these parameters. If a parameter is in the Metabolic or Program Control category, then only the Constant distribution is allowed. If the parameter is Behavioral, then the average value of the LHS sampling is used when the field [AverageBehavior] is set to True in the *resSettings* or *bldSettings* table.

[ParameterCategoryID] is the category index, referenced in table *appParameter*.

[ParameterCategory] is the name of the category.

ParameterCategoryID	ParameterCategory
0	Metabolic
1	Behavioral
2	Physical
3	ProgramControl

appResCorrelations: see *appBldCorrelations*

appResidentialCategories

This table lists the categories used to classify residential parameters. It contains the following information:

ResidentialCatID	ResidentialCatName
1	Basic
2	Human Diet
3	Food Consumption Period
4	Holdup Period
5	Growing Period
6	Animal Feeding Periods
7	Interception Fraction
8	Translocation Factor
9	Contaminated Fraction
10	Crop Yields
11	Wet-To-Dry Conversion
12	Animal Intake Rates
13	Plant Mass-Loading
14	Carbon Model
15	Hydrogen Model

appResSoilCharacteristics

This table holds the parameters that describe the hydrologic characteristics of 12 soil types defined by the U.S. Bureau of Reclamation (USBR) (see Appendix E). These characteristics can be used to derive interrelated values for the soil parameters of the residential scenario model.

- [SoilClass] is the name of the soil classification.
- [SoilID] is the index of the soil classification.
- [KdistType] is an index for the probability distribution type for Ksat, the saturated conductivity. If zero, the lognormal distribution is used. If one, the beta distribution is used.
- [MeanLnKsat] is the mean value of the natural log of saturated conductivity, in cm/sec, for soils with a lognormal distribution for Ksat.
- [SLnKsat] is the standard deviation of the natural log of Ksat for soils with a lognormal distribution for Ksat.
- [KMinimum] is the minimum value of Ksat for soils with a beta distribution of Ksat.
- [KMaximum] is the maximum value of Ksat for soils with a beta distribution of Ksat.
- [KP] is the P parameter of the beta distribution of Ksat for beta-distributed soils.
- [KQ] is the Q parameter of the beta distribution of Ksat for beta-distributed soils.
- [BdistType] is an index for the probability distribution type for the "b" parameter of the saturation/permeability model. If zero, the lognormal distribution is used. If one, the beta distribution is used.
- [MeanLnBeta] is the mean value of the natural log of parameter "b" for soils with a lognormal distribution for "b."
- [SLnBeta] is the standard deviation of the natural log of "b" for soils with a lognormal distribution for "b."
- [BMinimum] is the minimum value of "b" for soils with a beta distribution of "b."
- [BMaximum] is the maximum value of "b" for soils with a beta distribution of "b."
- [BP] is the P parameter of the beta distribution of parameter "b" for beta-distributed soils.
- [BQ] is the Q parameter of the beta distribution of parameter "b" for beta-distributed soils.
- [MeanN1] is the expected value of porosity.
- [SN1] is the standard deviation of porosity.

Example:

SoilClass	SoilID	KDistType	MeanLnKsat	SLnKsat	KMinimum	KMaximum
silty clay	4	0	-13.78	1.224		
loamy sand	5	1			0.000039	0.0134
clay	6	0	-11.36	1.509		

KP	KQ	BDistType	MeanLnBeta	SLnBeta	BMinimum	BMaximum
		0	2.282	0.2844		
0.79836133	1.90143765	0	0.2978	0.2781		
		1			4.93	75

BP	BQ	MeanN1	SN1
		0.36	0.07
		0.41	0.09
1.74608936	11.5961659	0.38	0.09

appResUSBRPercolationFraction

This table holds the estimated fraction of applied water that becomes infiltration as a tabulated function of saturated permeability.

- [ID] is an index used to order the tabulated values.
- [Ksat] is the saturated permeability in cm/sec.
- [PercFraction] is the estimated fraction of applied water that becomes infiltration.

Example:

ID	KSat	PercFraction
2	0.0000353	0.03
3	0.0000706	0.05
4	0.000141	0.08

appScenario

This table names the available scenarios. It currently contains the following information:

SenarioID	SenarioName
1	Building Occupancy
2	Residential

appSettings

This single record table contains the default application settings for each run. These settings are not modifiable by the user.

The following fields have the same basic meaning as the same fields in the *bld/resSettings* tables: [CombineProgeny], [DistActivity], [NumberSim], [Seed], [Tracking], [AverageBehavior], [SaveHistory], and [DoseQuantile].

[NuRegThree] is a hyperlink to the home page of Beyeler et al. (1999) as saved in HTML format. This is expected to be a relative link. However, the software will use the path of the application for the bases of this relative link.

Example:

CombineProgeny	DistActivity	NumberSim	Seed	Tracking	AverageBehavior
Yes	Yes	100	8718721	1	Yes

SaveHistory	DoseQuantile	NuRegThree
No	0.9	Nrcvol3\vol3Home.html

appStatNames

This table names the various dose statistics reported in the dose statistics tables *datBldDoseStats* and *datResDoseStats*.

[StatID] is a unique integer identifier for the statistic.

[StatName] is a descriptive name for the statistic.

[StatDesc] is an optional extended description of the statistic.

Example:

StatID	StatName	StatDesc
1	Minimum	Smallest value in the set of simulations
2	Maximum	Largest value in the set of simulations
3	Average	Average value in the set of simulations
4	StdDev	Sample standard deviation from the set of simulations
5	Xcrit	Maximum likelihood estimate of the Pcrit quantile value
6	XcritLCL	Lower bound of the symmetric 95% confidence interval for the Pcrit quantile value
7	XcritUCL	Upper bound of the symmetric 95% confidence interval for the Pcrit quantile value

appUOM

This table defines the units of measure used in specifying the values of model parameters.

Example:

UnitsID	Units	Description
1	pCi	Picocuries
2	nCi	Nanocuries

appUOMConversionFactors

The following table indicates how units listed in table *appUOM* can be interchanged.

The fields are as follows:

[UnitFrom] and [UnitTo] are long integers that match with field [UnitsID] in table *appUOM*. [UnitTo] identifies the conversion family.

[Factor] is optional. If the field [Factor] is not Null, then [UnitFrom] can be converted to [UnitTo] by multiplying [UnitFrom] by [Factor].

[Functional] is a boolean field. If it is set to Yes, a conversion between the units exists. However, this conversion is not done using multiplication by [Factor], but via a special function identified in field [FunctionID].

[FunctionID] identifies the function used for functional conversions. This field matches the [FunctionID] field in the *appUOMConversionFunctions* table.

[ConversionParameter] names an optional model parameter that may be required by the conversion function. This field matches with the [Symbol] field in the *appParameter* table.

The following integrity rules should hold for this table:

If [Functional] is No, then [Factor] is not Null.

If [Factor] is Null, then [Functional] should be Yes.

If [Functional] is Yes, then [Factor] is Null and [FunctionID] is not Null.

For each record in this table, there should exist exactly one method to convert from [UnitFrom] to [UnitTo].

By grouping these records into (disjoint) subsets where the [UnitTo] field is equal, the result is a conversion family that allows conversion between any units within this subset. For example, perhaps there is a need to convert between lengths, and a need to support centimeters, meters, inches, and miles. There will be exactly four entries in this table. A family must be selected, say, "meters," for this example. The user sets the [UnitTo] field to meters for each of the four new records. The values for the [UnitFrom] field will be set to centimeters, meters, inches, and

miles for the four records. The DandD software has sufficient information to convert between any of these four units. It will not be allowed to have an entry in this table to convert, for example, from inches to miles. This type of entry would not support the DandD algorithm used for unit conversion. The way the DandD software uses this table, the value of UnitFrom must be unique to this table. To enforce this, the [UnitFrom] field is a key to this table.

Note: there must be an entry for the base unit within the conversion family. In the above example, this means that DandD software requires that there be an entry for the field where [UnitFrom] is set to meters, [UnitTo] is set to meters, and the conversion factor is set to one.

Example:

UnitFrom	UnitTo	Factor	Functional
grams	kg	0.001	No
kg	kg	1	No
mg	kg	0.000001	No
pCi/kg wet-wt leafy per pCi/kg soil	pCi/kg dry-wt leafy per pCi/kg soil		Yes

FunctionID	ConversionParameter
Divide	WV(1)

appUOMConversionFunctions

This table lists the functions used to convert units.

FunctionID	FunctionName
0	Exponentiate
1	Multiply
2	Divide
3	Power10

D.2.2 Scenario Specific Tables (bld/res tables)

bldCorrelations, resCorrelations

Tables *resCorrelations* and *bldCorrelations* contain parameter correlation coefficients specific to the user scenario. If a parameter is constant or from a derived distribution, DandD will not permit the parameter to be correlated to any other parameter. With the exception of two additional fields described below, the fields in these tables are identical to the fields used in tables *appResCorrelations* and *appBldCorrelations*.

[DefaultVal] indicates if this record is a member of the default table *appBldCorrelations* or *appResCorrelations* for the scenario (e.g., this record agrees with a record in *appBld/ResCorrelations* with respect to [ParameterID1], [ParameterID2], and [Correlation]).

[Justification] contains text that the user has entered justifying the correlation coefficient and the dependence of the parameters [ParameterID1] and [ParameterID2]. This description is only relevant if the [DefaultVal] field is set to False.

Example:

ParameterID1	ParameterID2	Correlation	DefaultVal	Justification
109	111	-0.35	Yes	
110	111	-0.35	Yes	
2465	2565	0.2	No	Ac Beef and grain are dependant variables

bldElementParameters table is unused.

bldEmpirValues: see *appEmpirDefValues*.

bldNonEmpirValues: see *appNonEmpirDefValues*.

bldNuclides, resNuclides

The *resNuclides* and *bldNuclides* tables contain the contaminants for the current session, residential and building scenarios, respectively.

The fields have the following meaning:

[ParameterID] identifies associated data in the data tables *resEmpirValues*, etc., and matches with a [ParameterID] in table *appNuclides*.

[NuclideSymbol] is identical to [NuclideSymbol] in table *appNuclides*.

[Area] is a constant representing the area of contamination. This is a variable that cannot be associated with a probability distribution. By default, it is set to zero. A zero value implies that the contaminant is spread over the total area of concern.

[DistributionID] is the probability distribution associated with the concentration of this contaminant. By default, this is initialized to the Constant distribution.

[Justification] is a memo field that is defined by the user when the user enters the concentration for the nuclide. This justification should contain evidence to support the concentration value or probability distribution.

[UnitsID] identifies the units of concentration. The default values used can be found in field [SourceUnits] within tables *bldSettings* and *resSettings*. At this time, the default units are set to 'dpm/100cm**2' for the building scenario and 'pCi/g' for the residential scenario.

Example:

ParameterID	NuclideSymbol	Area	DistributionID
1002	10Be	0	CONSTANT
1003	3H	0.2	TRUNCATED NORMAL

Justification	UnitsID
	dpm/100cm**2
	dpm/100cm**2

bldParameterDetail, resParameterDetail

These tables contain data related to the parameters listed in the *appParameter* table for a session. This table is created from the *appParameter* table fields [ParameterID] and [DistributionID]. When the table is first created, [DefaultVal] is set to Yes. As the user modifies the parameter values, the data tables (*resEmpirValues*, etc.) will be modified. The values of these fields represent user input to the GUI.

The fields have the following meaning:

[ParameterID] identifies the parameter data in tables *resNonEmpirValues*, etc.

[DefaultVal] indicates if the current value of this parameter is set to the default value. Initially, this value is set to True.

[DistributionID] indicates the associated distribution for this parameter. Initially, this value is set to the default distribution, [DistributionID], from table *appParameter*.

[Justification] is user-supplied documentation of any non-default value or distribution.

[UnitsID] indicates the current units corresponding to the data associated with this parameter. Initially, this value is set to the default units, [DefaultUnitsID], from table *appParameter*.

Example:

ParameterID	DefaultVal	DistributionID	Justification	UnitsID
1	Yes	CONTINUOUS LINEAR		hr/week
2	Yes	CONSTANT		days
3	Yes	CONTINUOUS LINEAR		m**3/hr

bldReports, resReports

These tables are used to store information about custom reporting capabilities.

[ReportID] is an index used to order the table records.

[Name] is the name of report template.

[Units] are the units used in the simulation results portion of the report for the total dose.

The following Yes/No fields determine the contents of the custom report:

[Execution] Set to True if execution settings will be reported.

[InitialAct] Set to True if initial activities will be reported.

[CodeAct] Set to True if calculated activities will be reported.

[ChangedParam] Set to True if all changed parameters will be reported.

[AllParam] Set to True if all parameters will be reported, including those set to default values.

[MaxOcc] Set to True if the total effective dose equivalent (TEDE) value will be reported.

[MaxPath] Set to True if the dose due to each pathway is reported.

[MaxRadioDose] Set to True if the dose due to each nuclide through all active pathways is reported.

[MaxPathRadioDose] Set to True if the dose due to each nuclide and each pathway is reported.

[FinalAct] Set to True if Concentration of time at peak dose for each nuclide is reported.

ReportID	Name	Units	Execution	InitialAct
4	Summary	mrem	Yes	Yes
5	Final Activity	mrem	No	No
6	Detailed results	mrem	No	No

CodeAct	ChangedParam	AllParam	MaxOcc	MaxPath
No	Yes	No	Yes	No
No	No	No	No	No
No	No	No	Yes	Yes

MaxRadioDose	MaxPathRadioDose	FinalAct
No	No	No
No	No	Yes
Yes	Yes	Yes

bldSettings, resSettings

These single record tables contain the actual settings for the building occupancy and the residential scenarios, respectively. The user can modify these values via advanced execute options. These tables should initially agree with the values in table *appSettings*.

The fields are as follows:

[CombineProgeny] is set to Yes or No. This indicates if the daughter product results are included with the parent dose results when the model is run.

[DistActivity] is set to Yes or No. This is a calculation option that applies only to equilibrium (+C) nuclides. If set to Yes, then the initial activity for the +C nuclide is shared with all of its daughter nuclides.

[NumberSim] is set to the number of times the model will be run with different values from LHS.

[Seed] is set to Random Seed used to generate parameter values that have associated distributions for the Monte Carlo simulation.

[Tracking] is the time delay for tracking the peak dose.

The following settings indicate allowable nuclide pathways and initial default settings:

[ExternalPathway] is set to Yes.

[InhalationPathway] is set to Yes.

[SecIngestionPathway] is set to Yes.

[FarmPathway] is set to Yes (always No for the building occupancy scenario).

[DrinkingWaterPathway] is set to Yes (always No for the building occupancy scenario).

[IrrigationPathway] is set to Yes (always No for the building occupancy scenario).

[PondPathway] is set to Yes (always No for the building occupancy scenario).

[SourceUnits] indicates the units of measure used to specify source concentration. Different units are used for the *resSettings* and *bldSettings* tables. The user cannot change this value. These are the units used by the model.

[AverageBehavior] is set to Yes or No to indicate whether the behavioral parameters should be averaged to represent the average member of the critical group, or sampled to represent individual members of the critical group.

[SaveHistory]: if this is True, then the average dose and the standard deviation of the dose at every time step broken down for every pathway, every individual nuclide, and for the combined nuclides will be saved. This information will be saved in tables *datBld/ResHistNucMean*, *datBld/ResHistNucStdDev*, *datBld/ResHistPathMean*, and *datBld/ResHistPathStdDev*.

[DoseQuantile] indicates the order of the quantile of the estimated TEDE distribution reported for comparison against the dose standard.

[Justification] is a memo field that is defined by the user when the user changes the pathway behavior.

[FarmCat], [WellCat], and [WaterCat] are not used at this time. However, the intention was that the user could turn on or off categories that allow access to certain pathways. This may become a feature in the future, hence, it was not removed from the code nor the database.

[ImportConcen] is a software mode that is only relevant for the residential scenario, but is in both *bldSettings* and *resSettings* tables for convenience only. By default, the user will enter the source contaminants and their respective concentrations. In this case, [ImportConcen] will be set to False. However, on occasion, the user will want to specify this in a file instead. This file, known as the *Import Concentration File* (*.con file), is of a specialized format that was defined for DandD Version 1.0. This is included for backward compatibility. If [ImportConcen] is set to True, then table *resImportCon* will be populated with the file contents.

[JustImportConc] is the justification for importing the concentration. This is only relevant if [ImportConcen] is set to True.

[Stamp] is the date and time corresponding to the dat tables in the database. This value is Null if there is no current execution data present.

Example:

CombineProgeny	DistActivity	NumberSim	Seed	Tracking	ExternalPathway	InhalationPathway
No	Yes	100	8718721	1	Yes	Yes

SecIngestionPathway	FarmPathway	DrinkingWaterPathway	IrrigationPathway	PondPathway	SourceUnits
Yes	Yes	Yes	Yes	Yes	pCi/g

AverageBehavior	SaveHistory	DoseQuantile	Justification	FarmCat	WellCat	WaterCat	ImportConcen
Yes	No	0.9		Yes	Yes	Yes	No

JustImportConc	Stamp
	10/25/00 1:21:59 AM

resCorrelations: *see bldCorrelations*

resElementParameters

This table contains the parameters associated with the nuclide elements. For the residential scenario, each element will have a total of ten entries in this table. An element will be in this table only if the element was entered as a source of contamination or if the element is in the decay chain of a nuclide that the user added as a source of contamination. These parameters have default settings that the user can edit through the GUI. These default settings are read from the *appElementParameters* table and the associated data tables (*appEmpirDefValues*, *appNonEmpirDefValues*). The actual values used in the model calculations are stored in tables *resNonEmpirValues* and *resEmpirValues*.

The meaning of the fields is identical to the meanings in tables *bldParameterDetail* and *resParameterDetail*.

Example:

ParamaterID	DefaultVal	DistributionID	Justification	UnitsID
2005 Na:Coefficient	No	NORMAL	Reason this was modified from default	Log10(mL/g)
2105 Na:Leafy	Yes	LOGNORMAL-N		pCi/kg dry-wt leafy per pCi/kg soil

resEmpirValues: see *appEmpirDefValues*.

resImportCon

This table contains the import concentration data if *resSettings*.[ImportConcen] is set to True. This is specially formatted data that is used as an alternative to data in the bld/res data tables with respect to nuclide concentrations. A description of the meaning of this data is not contained in this document (see Appendix C). The data in this table is read from an ASCII file. Fields are separated by blanks. There are at most two fields per record, which corresponds to one line in the ASCII file.

[Index] is an automatically generated key field corresponding to the line number of the file.

[Col1] corresponds to field 1.

[Col2] corresponds to field 2.

Example: The first three lines of an import concentration file are stored as follows

Index	Col1	Col2
1	3	
2	7	
3	234U	

resNonEmpirValues: see *appNonEmpirDefValues*.

resNuclides: see *bldNuclides*.

resParameterDetail: see *bldParameterDetail*.

resReports: see *bldReports*.

resSettings: see *bldSettings*.

D.2.3 Model Result Tables (dat tables)

datBldConcStats, datResConcStats

These tables contain statistics related to the estimated concentration distributions for individual nuclides and locations.

- [NuclideID] is the nuclide identifier from *appNuclides*.
- [StatID] is the identifier of the statistic from *appStatNames*.
- [medium] is the value for the given statistic for the initial concentration in the given medium.

Example:

NuclideID	StatID	Soil	Water
196	1	4.16084457563249E-02	0
196	2	14.964099652933	1239.70825282387
196	3	8.66493478048292	31.462158203012
196	4	3.624682408305	140.484521900805
196	5	12.1437	43.0735269616935
196	6	11.6443851913763	6.34659042206096E-11
196	7	12.5712	108.611964210352

datBldDoseStats, datResDoseStats

These tables contain statistics related to the estimated dose distributions for individual nuclides and pathways, and for total dose.

- [NuclideID] is the nuclide identifier from *appNuclides*, or zero to denote total dose.
- [StatID] is the identifier of the statistic from *appStatNames*.
- [Total] is the value for the given statistic for the current values of dose through all pathways.
- [pathway] is the value for the given statistic for the current values of dose through the given pathway.

Example:

NuclideID	StatID	Total	FarmPathway	DrinkingWaterPathway	PondPathway
22	1	6.31501720090655	0.115859163824551	0	0
22	2	7.8054251335416	1.60627683958954	4.58202776252917E-11	2.85148594600873E-10
22	3	6.45835541172811	0.259211517137271	4.58225232183848E-13	2.85164307648308E-12
22	4	0.181999388536105	0.181998907034963	4.58202549880339E-12	2.8514843624432E-11
22	5	6.60386781823706	0.404729170853565	2.0587002001501E-30	1.40541955425932E-29

ExternalPathway	InhalationPathway	SecIngestionPathway	IrrigationPathway
6.19876318636059	4.77371614627895E-06	3.57355296801155E-04	0
6.19876318636059	1.01873605162395E-04	3.57355296801155E-04	1.80156990512671E-10
6.19876318636058	2.33529283291658E-05	3.57355296801154E-04	1.80162625031057E-12
4.77739405288454E07	1.95202543764743E-05	2.25863862366848E-11	1.80156933666473E-11
6.19876318636059	4.61932408044741E-05	3.57355296801155E-04	8.92814968327486E-30

datBldDoseSummary, datResDoseSummary

These tables contain a single record with the TEDE quantile value report for comparison against the dose limit based on the most recently calculated dose distributions (these distributions are stored in the *datBldTotal* and *datResTotal* tables).

[Tcrit] is the critical dose value reported for comparison.

Example:

Terit
4.32114734947361E-03

datBldHistNucMean, datResHistNucMean, datBldHistNucStdDev, datResHistNucStdDev, datBldHistPathMean, datResHistPathMean, datBldHistPathStdDev, datResHistPathStdDev

These tables contain history data. If the option is turned on to collect this data (*bld/resSettings*.[SaveHistory] = True), then the *histNucMean* tables will contain the average total dose broken down by individual nuclides for each time step. The *bld/resHistPathMean* will contain the average dose broken down by pathways. The standard deviations are stored in the *NucStdDev* table.

Example: Table *datResHistNucMean*

Time	AllIsotopes	Nuc6
1	16.772316845586	16.772316845586
2	2.66008144165796E-21	2.66008144165796E-21
3	1.7170072754837E-29	1.7170072754837E-29

Three time steps were run for each of the Monte Carlo simulations. [AllIsotopes] contains the average over all simulations of the total dose for all contaminants combined. In this example, there was only one contaminant. The average over all simulations of the total dose for this contaminant is recorded in [Nuc6]. The field name [Nuc6] identifies that contaminant as having parameter ID 1006. This can then be referenced in the *appNuclide* table, where this corresponds to Na 24.

Example: Table *datResHisPathMean*

Time	ExternalPathway	InhalationPathway	FarmPathway
1	16.7610990285165	4.58142219584829E-07	1.11875676527068E-02
2	2.65868079721869E-21	6.5950796285523E-29	1.39585266728979E-24
3	1.71610396991989E-29	4.24355366503163E-37	9.00209152594661E-33

Again, the total dose due to each of the pathways is averaged over all Monte Carlo simulations, and is listed for each time step. The standard deviations are stored in the *HistPathStdDev* table.

datBldHistNucStdDev: see *datBldHistNucMean*.

datBldHistPathMean: see *datBldHistNucMean*.

datBldHistPathStdDev: see *datBldHistNucMean*.

datBldInitSurface

[Vector] is the vector number corresponding to simulation.
 [AllIsotopes] is unused.

The remainder of the fields will contain the initial surface concentration of a nuclide or progeny for simulation identified by vector number [Vector]. The field names will correspond to [nukeID] in table *appNuclides*.

Example:

Nuc187 corresponds to nuclide ID 187, or U 232. The initial surface concentration of U232 at the beginning of simulation number two was 1052.

Vector	AllIsotopes	Nuc187	Nuc173
1		1052	1081
2		1160	1191
3		1248	1282

datBldNucIndex, datResNucIndex

These tables contain the field indices for each of the nuclides with reported doses. These tables are used by DandD to locate doses in the pathway.dose tables for individual radionuclides.

[NuclideID] is a unique nuclide identifier that matches the [Source] field of the *appCandCDecode* table.
 [OutputFieldID] is the index of the field containing the dose value in the dose value tables (e.g., the *datBldExternalPathway* table) where [OutputFieldID] = 1 corresponds to the first field.

Example:

NuclideID	OutputFieldID
23	2

datBldSurface

This table is formatted identical to table *datBldInitSurface*. However, the data in this table is the surface concentration of the nuclide at the time of peak dose.

datBldTmax, datResTmax

These tables contain the time (in years) at which the calculated maximum TEDE occurs for each parameter sample. The building occupancy scenario is only simulated for one year; however, the table is generated for this scenario to accommodate possible extensions.

[Vector] is a unique sample vector index that ranges from 1 to the number of samples.
 [Time_of_Maximum] is the time (in years) at which the calculated TEDE reaches its maximum value.

Example:

Vector	Time_of_Maximum
1	1
2	1
3	6
4	1
5	6
6	1

datBldTotal, datResTotal

These tables contain the calculated combined dose values along the various exposure pathways for each parameter sample vector. The total dose for all nuclides, and the dose due to individual nuclides, are stored. The structure is the same as that of the pathway dose tables *datBldXXXPathway* and *datResXXXPathway*.

datBldXXXPathway, datResXXXPathway

These tables contain the calculated dose values along the individual exposure pathways for each parameter sample vector. A separate table, denoted by XXX, is created for each pathway.

For the residential scenario,

XXX = DrinkingWater, External, Farm, Inhalation, Irrigation, Pond, SecIngestion;

while for the building occupancy scenario,

XXX = External, Inhalation, SecIngestion.

Each table contains the total dose along the pathway at the time of peak dose and the contributions of the component nuclides:

- [Vector] is a unique sample vector index that ranges from 1 to the number of samples.
- [AllIsotopes] is the total dose along the pathway due to all isotopes.
- [Nuci] is the pathway dose from nuclide *i*.

Example:

Vector	AllIsotopes	Nuc23
1	3.52192694572157E-08	3.52192694572157E-08
2	2.21202219082726E-08	2.21202219082726E-08
3	5.94394714605343E-03	5.94394714605343E-03
4	3.85410853236806E-10	3.85410853236806E-10
5	3.19504183051653E-03	3.19504183051653E-03

datResConcStats: see *datBldConcStats*.

datResDoseStats: see *datBldDoseStats*.

datResDoseSummary: see *datBldDoseSummary*.

datResHistNucMean: see *datBldHistNucMean*.

datResHistNucStdDev: see *datBldHistNucMean*.

datResHistPathMean: see *datBldHistNucMean*.

datResHistPathStdDev: see *datBldHistNucMean*.

datResInitSoil

This table is formatted identical to table *datBldInitSurface*. However, the data in this table is the initial soil concentration of a nuclide or progeny for simulation identified by vector number [Vector]. The field names will correspond to [nukeID] in table *appNuclides*.

datResNucIndex: see *datBldNucIndex*.

datResSoil

This table is formatted identical to table *datBldInitSurface*. However, the data in this table is the soil concentration of the nuclide at the time of peak dose.

datResTmax: see *datBldTmax*.

datResTotal: see *datBldTotal*.

datResWater

This table is formatted identical to table *datBldInitSurface*. However, the data in this table is the water concentration of the nuclide at the time of peak dose.

datResXXXPathway: see *datBldXXXPathway*.

D.2.4 Error Information Tables (err tables)

errCorrelationErrors

This table describes warnings and errors detected by the LHS preprocessor that prevent the correlations specified in *bldCorrelations* or *resCorrelations* from being implemented. This table is only created and populated if warning or error conditions are detected. If the table exists when the LHS processor is called, it will be deleted.

- [ParameterID1] identifies one of the pair of correlated parameters.
[Code1] is the error code for this parameter:
if 0, there is no problem.
if 1, then the parameter is a Constant or Derived parameter, and is not sampled.
If 2, the parameter was not found. This implies an internal inconsistency among the parameter tables.
- [ParameterID2] identifies the other correlated parameter.
[Code2] is the error code for this parameter.

Example:

ParameterID1	Code1	ParameterID2	Code2
3	0	42	2

errSampleBoundaryViolations

This table describes parameter value warnings and errors detected by the LHS postprocessor. This table is only created and populated if one or more of the model parameter values generated by LHS fall outside the “hard” or “soft” limits defined in the appropriate tables (e.g., *appParameter*). If the table exists when the LHS processor is called, it will be deleted. The dose model can be executed, following user notification, if only the soft limits are exceeded. Exceeding either hard limit should preclude execution of the dose model.

- [ParameterID] identifies the parameter whose bounds were exceeded in one or more samples.
[SoftLowerLimit] is True if the soft lower limit was exceeded, and False otherwise.
[SoftUpperLimit] is True if the soft upper limit was exceeded, and False otherwise.
[HardLowerLimit] is True if the hard lower limit was exceeded, and False otherwise.
[HardUpperLimit] is True if the hard upper limit was exceeded, and False otherwise.

D.2.5 Sampling Result Tables (par tables)

parBldBasicSampleValues, parResBasicSampleValues

These tables hold values for the sampled basic model input parameters for each sample vector generated by LHS. These tables are created and filled by the LHS pre/postprocessor function. Basic model parameters that are known not to vary from sample to sample are stored in the *parBldConstantValues* or *parResConstantValues* table.

[Vector] is a unique sample vector index that ranges from 1 to the number of samples.
 [parameter_i] is the value of parameter *i*. The specific parameter name depends on the scenario, and on whether the parameter can vary from vector to vector.
 The field name matches the [Symbol] field in the *appParameter* table.

Example:

Vector	SFI	PD	RFR	CDO	CDI
1	0.58474815	0.232044	0.00000166272	0.000000256544	1.56421803488E-07
2	0.58474815	0.0206941	0.000000215785	0.00000444799	1.58842615689E-06
3	0.58474815	0.233635	0.00000556082	0.000000166557	1.15857215757E-07

parBldConstantValues, parResConstantValues

These tables hold the values for the basic model input parameters that are known to be invariant from vector to vector. This determination is made at the time parameters are sampled based on the distributions currently assigned to the parameters.

[ParameterID] is the parameter identifier.
 [Value] is the constant value.

Example:

ParameterID	Value
10	1
11	0.1
12	0.1

parBldFieldIndex, parResFieldIndex

These tables describe the locations in which the sampled parameter values have been stored by the LHS postprocessor. They are created by the LHS pre/postprocessor function.

[ParameterID] is the parameter identifier.
 [Varies] is a logical flag which is -1 if a separate parameter value is stored for each sample vector. If the value is zero, the fixed value for the parameter is stored in *parBldConstantValues* or *parResConstantValues*.
 [FieldID] is the zero-based index of the field containing sampled values for this parameter if the parameter is variable (if [Varies] is -1). Values for this parameter are stored in the indexed field of the table containing values for this parameter type (either *parXXXBasicSampleValues*, *parXXXSourceSampleValues*, or *parResElementSampleValues*).
 [Minimum] is the minimum sampled value.
 [Maximum] is the maximum sampled value.
 [HasRange] if -1, the parameter varies from one vector to another. If zero, the parameter values do not change from one vector to another.

Example:

ParameterID	Varies	FieldID	Minimum	Maximum	HasRange
3	0	0	1.4	1.4	0
4	-1	1	0.000000927394	0.0000187132	-1

parBldSourceSampleValues, parResSourceSampleValues

These tables hold the input source specification for the dose models for each sample vector generated by LHS. These tables are created and filled by the LHS pre/postprocessor function.

[Vector] is a unique sample vector index that ranges from 1 to the number of samples.
 [nuclide_i] is the source concentration of nuclide *i*. The specific nuclide names depend on user specification.

parResBasicSampleValues: see *parBldBasicSampleValues*.

parResConstantValues: see *parBldConstantValues*.

parResElementSampleValues

This table contains the values for the element-dependent parameters for each sample vector generated by LHS and each chemical element appearing in the source term decay chain.

[Vector] is a unique sample vector index that ranges from 1 to the number of samples.
 [NuclideParameterNameID] is the identifying number of the parameter category matching the *appElementParameterNames* table.
 [element] is the parameter value for the element corresponding to the field name.

Vector	NuclideParameterNameID	Ni
1	0	51.4315958409505
1	1	0.0144274
1	2	5.06598505778435E-02

parResFieldIndex: see *parBldFieldIndex*.

D.2.6 Sensitivity Analysis Tables (sen tables)

senBldSelectedPvalues, senResSelectedPvalues

[Vector] is the vector number corresponding to simulation number.

The remainder of the fields will contain the value of variables used for the simulation identified by vector number [Vector]. The field names will correspond to the [Symbol] field in tables *senBld/ResSensitiveParams*.

Example:

This table shows that during simulation number one, Rfo* had a value of 0.0000101235.

Vector	RFo*	Rfo	232U+C
1	0.0000101235	0.0000734183	8624.3004
2	0.000010886	0.000115646	9503.931
3	0.0000106881	0.0000136194	10223.7438

senBldSensitiveParams, senResSensitiveParams

These tables are created by the DandD software for sensitivity analysis. There is one entry in this table for each of the uncertain variables.

- [ParameterID] identifies the parameter ID. It matches with [ParameterID] in *appNuclides*, *appParameter*, etc.
- [Symbol] is the symbol used to identify this parameter from within the modeling codes.
- [Description] is a detailed description of the parameter.
- [Default] is 0 (False) if the parameter value is different than the screening (default) value.
is -1 (True) if the parameter value is the same as the default value.
- [Units] are the units associated with the parameter value.
- [KSProb] are the results of the Komolgorov-Smirnov (K-S) test for sensitivity.
- [Sensitive] is 0 (false) if 1 - [KSProb] <.95. In other words, False if varying parameter values do not affect TEDE values significantly.
is -1 (True) if varying parameter does affect TEDE value.
- [Selected] is -1 (True) if parameter has been selected for analysis; zero (False) otherwise.
- [Committed] is a boolean indicator (-1 or 0) used by the DandD software to indicate if the selection of a parameter should be retained.

Example:

ParameterID	Symbol	Description
4	RFo*	Effective resuspension factor during the occupancy period = RFo * FI
287	Rfo	Resuspension factor for loose contamination
1188	232U+C	Concentration of 232U+C

Default	Units	KSProb	Sensitive	Selected	Committed
0	1/m	2.954970987048E-04	-1	-1	-1
-1	1/m	0.711234867572784	0	-1	-1
0	nCi/m**2	4.57946978948964E-11	-1	-1	-1

senResSelectedPvalues: see *senBldSelectedPvalues*.

senResSensitiveParams: see *senBldSensitiveParams*.

D.2.7 User Settings Tables (usr tables)

usrSettings

This table contains a single record consisting of session settings. It is initialized when the session is created. Some fields can be modified by the user during the session.

[Title] is the session title.
[Description] is the description of the session.
[Version] is the database version used for compatibility checking by the interface.
[Scenario] indicates the current scenario selected by the user at the time the session file was closed. The value of this field matches with a value of *appSenario.SenarioID*.

Example:

Title	Description	Version	Scenario
My First Session	details are typed here	2.1.0	Building Occupancy

D.2.8 Other Tables

These tables are used by the software as scratch workspaces, and are not relevant to the site specification or results; *resScratchImportCon*, *usrScratch*.

D.3 References

Beyeler, W.E., W.A. Hareland, F.A. Duran, T.J. Brown, E. Kalinina, D.P. Gallegos, and P.A. Davis, 1999.
"Residual Radioactive Contamination From Decommissioning, Parameter Analysis, Draft Report for Comment," Sandia National Laboratories, NUREG/CR-5512, Volume 3, October 1999.

APPENDIX E TABLES OF TECHNICAL DATA

E.1 Introduction

This appendix contains auxiliary information on data tables needed to calculate annual total effective dose equivalents (TEDEs) for the residual radioactive contamination scenarios defined in Kennedy and Strenge (1992) with differences as described in Appendix A (taken from Wernig et al. (1999)). These tables cannot be changed by the user of the DandD software. The data in these tables can be reviewed through the DandD graphical user interface (see Section 4.3.8).

E.2 Radioactive Decay Data

The radioactive decay chain table contains decay data for the master list of radionuclides. The decay chain representations in the table are taken from International Commission on Radiological Protection (ICRP) Publication 38 (ICRP, 1983). The table contains a data set for each radionuclide or chain, except natural thorium and natural uranium, for which dose factors are calculated from entries for the radionuclides in the decay chain. For single-member chains (i.e., no progeny), the table contains the radionuclide name, decay half-life, and atomic number. Decay chains having progeny also contain listings for each chain member, including the radionuclide name, decay half-life (explicit members only), atomic number, and branching information.

The chains in the radioactive decay chain table are organized by atomic number of the decay chain parent. Within each decay chain, members follow according to their decay sequence. The treatment of progeny radionuclides as implicit or explicit is indicated by the presence of a value for the radioactive half-life. Implicit radionuclides have no value for the radioactive half-life, while explicit radionuclides have the half-life listed. The table also includes a chain member position index for each explicit radionuclide, with the parent always having position 1. The position indices are used to indicate the decay sequence, which is necessary when branching occurs. Implicit radionuclides have no chain member position index because they are not included in the decay calculations performed by the decay processor.

The branching information listed in the table defines the sequence and fraction of parent decays that result in the production of each chain member. The branching fractions defined for each member indicate the source of production of the chain member. This con-

vention is the opposite of the usual method of defining the fractions for the parent and an indication of the radionuclides produced by the parent decay. A chain member may be produced by one or two precursor chain members. The decay chain table contains the following information:

- index of the first precursor (if any) for the chain member,
- fraction of first precursor decays that result in production of the chain member,
- index of the second precursor (if any) for the chain member, and
- fraction of second precursor decays that result in production of the chain member.

The decay fractions for implicit progeny represent the total fraction of explicit precursor decays that result in production of the implicit progeny. The atomic number as provided in the radioactive decay database is used as a cross-reference index with other element-specific data.

E.3 Dose Equivalent Factors

External dose conversion factors and internal committed effective dose equivalent (CEDE) factors were obtained from existing Federal Guidance published by the Environmental Protection Agency (EPA), implementing the recommendations of the ICRP. This table provides a complete listing of these factors.

E.3.1 External Dose Rate Conversion Factors

The external dose rate conversions were obtained directly from the EPA Federal Guidance Report No. 12 developed by Oak Ridge National Laboratory (ORNL) (Eckerman and Ryman, 1992). These factors provide the external effective dose equivalent by summing the product of individual organ doses and organ weighting factors over the body organs. These factors are consistent with ICRP 26 (1977) guidance; however, they are inconsistent with the concept of deep dose equivalent, as defined by the NRC (see Appendix F of Kennedy and Strenge, 1992). For purposes of this generic study, the EPA factors are judged to be an adequate representation of the external dose because skin is not considered as one of the organs. For most radionuclides,

the numerical difference between the effective dose equivalent evaluated without skin and the deep dose equivalent will be a few percent. If skin were included, the difference would likely be greater for radionuclides with low photon energies. The external dose rate conversion factors from the EPA are used to determine factors for the source conditions used for this study: 1) infinite surface (thin-layer) contamination (for surface sources in the building occupancy scenario), and 2) volume contamination in a 15-cm-thick slab source (for surface-soil sources used in the residential scenario). The table contains the external dose conversion factors for exposure to surface and volume sources. These factors are in units of

- Sv/d per Bq/m² for external exposure to surface sources and
- Sv/d per Bq/m³ for external exposure to volume sources.

E.3.2 Inhalation and Ingestion Dose Conversion Factors

For inhalation and ingestion of radioactive materials, unit CEDE conversion factors were obtained from EPA Federal Guidance Report No. 11 (Eckerman, Wolbarst, and Richardson, 1988). This Federal Guidance Report supersedes previous Federal Radiation Council (FRC) guidance and, in addition to listing CEDE conversion factors per unit intake, it presents values for derived annual limits on intake (ALIs) and derived air concentrations (DACs). The unit CEDE conversion factors for inhalation and ingestion from the EPA references are included in the table for the radionuclides considered in this application. These factors are in units of Sv/Bq inhaled or ingested.

E.4 Residential Soil Characteristics

Several input parameters represent characteristics of the surface soil or the soil of the unsaturated layer. These parameters include porosity, infiltration rate, and saturation ratio. Rather than sample independently from distributions of these parameters, the dependence of these parameters is represented by first sampling soil texture then selecting an appropriate distribution for the soil characteristics. These soil characteristics include porosity, hydraulic conductivity, and a shape parameter “b” for the soil moisture retention curve.

The model input parameters are then calculated from these soil characteristics as described in the on-line references for the hydrologic parameters.

A common method of describing and quantifying soil texture is the U.S. Department of Agriculture (USDA) soil textural classification (Soil Survey Staff, 1997). This classification was used by Meyer et al. (1997) to represent the variability of a number of soil hydrologic properties that are related to porosity and saturation ratio. The USDA soil textural classification is also reported in a variety of available electronic databases for the United States.

Normal distributions of porosities (assumed to be equivalent to saturated water content) are given in Carsel and Parrish (1988). They are reported based on the 12 Soil Conservation Service textural classifications and a compilation of data for each of the textural classes. The soil characteristics table contains the means and standard deviations for these normal distributions.

Distributions of saturated hydraulic conductivity are given in Carsel and Parrish (1988). They are reported based on the 12 Soil Conservation Service textural classifications. Carsel and Parrish (1988) fitted distributions from a class of transformed normal distributions. Meyer et al. (1997) refitted the distributions of Carsel and Parrish (1988) to distributional forms that are more commonly used and more easily constructed—either lognormal or beta. The lognormal distribution is completely specified by the mean and standard deviation while the beta distribution is completely specified by mean, standard deviation, and range (upper and lower limits of the distribution). The soil characteristics table contains the parameters for these distributions for each of the 12 soil types.

Campbell (1974) derived a relationship between unsaturated hydraulic conductivity and saturation ratio that includes a curve fitting parameter “b” related to pore size distribution. Meyer et al. (1997) derived a relationship for “b” using soil water retention parameters considered in Carsel and Parrish (1988). Using this relationship, Meyer et al. (1997) constructed distributions for “b.” The soil characteristics table lists the parameters for these distributions for each of the 12 soil types.

See DandD’s on-line reference for hydrologic parameters for more information on how this data is used.

E.5 Residential U.S. Bureau of Reclamation Percolation Fractions

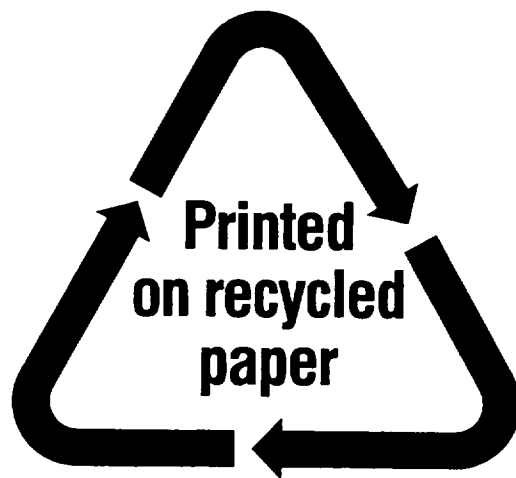
The U.S. Bureau of Reclamation (USBR) has developed an empirical relationship between soil permeability and the proportion of water that percolates beneath the root zone (USBR, 1993). The percolation fraction table contains the permeability-percolation fraction pairs that define this relationship. This relationship is used to derive the default distributions for saturation fraction and infiltration rate.

See DandD's on-line reference for hydrologic parameters for more information on how this data is used.

E.6 References

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11. ABSTRACT <i>(200 words or less)</i> The Decommissioning and Decontamination (Dand D) software package developed by Sandia National Laboratories for the Nuclear Regulatory Commission (NRC) provides a user-friendly analytical tool to address the dose criteria contained in NRC's Radiological Criteria for License Termination Rule (10 CFR Part 20 subpart E). Specifically, Dand D embodies the NRC's screening methodology and Dand D are part of a larger decision framework that allows and encourages licensees to optimize decisions regarding alternative actions at their site, including the collection of additional data and information. The screening methodology employs reasonably conservative scenarios, fate and transport models, and default parameter values and parameter distributions to allow the NRC to quantitatively estimate the risk of terminating a license given only information about the level of contamination. A licensee has the option of specifying only the level of contamination and running the code with the default parameters or, if site-specific information is available, modifying scenario pathways or providing site-specific parameter distributions and then calculating dose. Version 2.1 of the software allows probabilistic (Monte Carlo) dose assessments and incorporates a new and improved Microsoft Windows standard user interface.												
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