FINAL REPORT

Task 2: Computer Models

Radionuclide Soil Action Level Oversight Panel

July 1999

Submitted to the Radionuclide Soil Action Level Oversight Panel
in Partial Fulfillment of Contract between RAC and the Rocky Flats Citizen's Advisory Board

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TASK 2. COMPUTER MODELS

Abstract

This report discusses *Risk Assessment Corporation's* approach to soil action levels (SALs) in context with some computer programs that can be used to calculate them. A mathematical formulation is provided, along with an approach to uncertainty analysis with SALs. Dependence of SALs on exposure scenarios is emphasized. Two sets of scenarios are presented: (1) benchmark scenarios adopted by the Action Levels and Standards Framework for Surface Water, Ground Water and Soils (ALF) Working Group, consisting of members from the Department of Energy (DOE), the Environmental Protection Agency (EPA), the Colorado Department of Public Health and Environment (CDPHE), and Kaiser-Hill; and (2) some refined versions, which are provided for illustration and discussion. Five candidate computer programs were considered for their usefulness in estimating dose and SALs: RESRAD, MEPAS, GENII, MMSOILS, and DandD. RESRAD and GENII tentatively met the requirements set for future computations, which included not only appropriateness of the models implemented, but also the adaptability of the code to command-line execution from a front-end control program. This mode of operation would facilitate customized Monte Carlo analysis, and scripted preprocessing of input data and post-processing of output.

1. INTRODUCTION

This report considers specific computer models and methods that might be useful in the task of setting radionuclide soil action levels (RSALs) for the Rocky Flats Environmental Technology Site (RFETS). The models here reviewed are RESRAD, MEPAS, GENII, MMSOILS, and DandD. They are reviewed for their applicability to this task based on criteria discussed in Section 4. For the purpose of this report, RSALs are defined as radionuclide concentration (activity) levels in a contaminated layer in soil above which remedial action must be taken to prevent people from receiving an annual radiation dose greater than a specified dose limit. The Department of Energy (DOE) has performed calculations of soil action levels with the RESRAD program, which is a DOE product developed specifically for implementing the agency's approach to residual radionuclides in soil (DOE/EPA/CDPHE 1996). A part of the scope of this project is to review these calculations for choice of the parameters that were used in RESRAD, but the review is placed in the larger context of the scientific and technical appropriateness of the models and approach implemented in RESRAD, and whether other programs - or other models and approaches - might be preferred to the one followed by DOE. The parameter choices for RESRAD are a subject of Task 3. The goal of this report is a discussion and comparison of environmental assessment programs that might be used for developing soil action levels for RFETS; as required by the contract, the comparison includes RESRAD.

Before we can discuss the question of suitability of various computer programs for calculating soil action levels, we must make clear our conception of the task to which such programs would be applied. The goal is to protect people who may, in the near or distant future, come into contact with a site where radionuclides contaminate the soil at levels above background. Soil action levels are quantities, one or more per radionuclide, that are computed on the basis of environmental transport models, annual radiation dose limits, and formal assumptions (called exposure scenarios) about the nature and extent of *possible* contact that people *might* have with the site. For a single radionuclide, scenario, and dose limit, the soil action level is that concentration of the radionuclide in the soil that would lead to a maximum predicted annual dose equal to the annual dose limit. For multiple radionuclides, the criterion is more complicated. The concentration of each radionuclide is divided by the respective soil action level, as previously defined. The ratios are summed for all of the radionuclides, and if the sum exceeds 1 for one or more of the exposure scenarios, some action or special attention is indicated. Otherwise (the sum of ratios is less than or equal to 1), the interpretation is that no annual dose limit would be exceeded, and *by that criterion* the radionuclide levels are acceptable. If only one radionuclide is present, the sum of ratios reduces to a single ratio, but the interpretation is the same. Section 2 goes into detail about the definition of soil action levels, the environmental transport models, and the exposure scenarios.

.Our immediate point is that for each radionuclide in the soil, we calculate a quantity called a soil action level, which depends on environmental transport models, annual radiation dose limits, and exposure scenarios. As a matter of common practice, each soil action level is calculated deterministically, which is to say that it represents a single number, typically without indications of uncertainty. Similarly, when the ratios of radionuclide levels divided by

soil action levels are summed and compared with 1, the sum of ratios is itself a deterministic quantity, that is, a single number, with typically no indication of uncertainty.

Yet the movement of each radionuclide through environmental media and into possible contact with people is an uncertain process. Although this movement is fundamentally constrained by laws of physics, chemistry, and biology, models are, of necessity, empirical simplifications of reality, and much of the parametric information on which the models depend is not well known. Contemporary modeling practice explicitly recognizes this state of affairs by treating model parameters and state variables as probability (or uncertainty) distributions, and the calculation propagates the joint uncertainty in the parameters through to the endpoints of the calculation, which, in the case at hand, are the soil action levels and sum of ratios.

When uncertainties in soil action levels are considered, the decision is not so straightforward as in the deterministic case, when the sum of ratios is a single number that is to be compared to 1. When the calculation is stochastic (i.e., takes uncertainties into account), the sum of ratios is a distribution, and one must base a decision on *how probable it is* that the sum exceeds 1. If that probability is small, then one may be willing to forgo action, even though there is some acknowledged possibility that some annual dose limit could be exceeded (indeed, that possibility nearly always exists, even though many conventional calculations do not explicitly recognize it). Section 2.2 goes further into this question. We make the point here, however, that the development and interpretation of soil action levels should follow contemporary methods for incorporating uncertainty into environmental transport modeling. Accordingly, we consider the suitability of various computer programs to provide the necessary machinery.

This report summarizes and compares five prominent computer programs that are configured for environmental assessment: RESRAD, MEPAS, GENII, MMSOILS, and DandD. All of these programs have been developed with support from government agencies, and all have versions that install and execute under Microsoft® Windows 95 or NT. RESRAD, as we mentioned above, is intended to be used in connection with analyzing remediation of radionuclide-contaminated soils at DOE facilities. DOE generally grants access to RESRAD to DOE employees and contractors on DOE-funded projects. MEPAS, which was developed at Pacific Northwest Laboratories (PNL) and is now commercially marketed, is a large multimedia environmental transport program of extensive scope, which is applicable to radioactive and nonradioactive pollutants in many environmental media. GENII, also developed at PNL, is a highly modular radiological assessment system, which provides internal and external dose estimates for exposure through all pathways that are ordinarily considered in environmental radiological assessments. GENII has been under development for more than a decade and is unlikely to be modified further by its developers. MMSOILS, which was developed for the Environmental Protection Agency, is a large multimedia environmental transport program that was designed for screening assessments of chemical contamination. Although it does not treat radioactivity and decay chains, it was included in this review because it could possibly be useful for radionuclides in soils by using stable chemicals as surrogates for radionuclides and performing auxiliary decay-chain calculations external to the program. MMSOILS executables and source code are freely available from an EPA web server. DandD is currently under development by Sandia National Laboratory for the U.S. Nuclear Regulatory Commission (NRC).

We compare these programs with respect to features that are relevant to their possible use in computing soil action levels for the RFETS (Section 4). We draw on documentation distributed with the programs and on published comparisons by authors who participated in the development of the programs (Laniak et al. 1997; Mills et al. 1997). Comparisons of soil action levels developed with some of the programs is the subject of Task 5.

We hesitate to anticipate parameter uncertainties that may be dominant in methodologies for soil action levels until calculations have been done with site-specific data. However, we consider the level of uncertainty associated with the resuspension mechanism to be of sufficient concern that it should be raised in this report. This mechanism drives the inhalation exposure pathway and contributes to other pathways (such as deposition on garden vegetables and pasture grass) that could be considered in some scenarios. Models affecting this pathway were changed in RESRAD Version 5.75, although the calculations reported in the soil action levels document (DOE/EPA/CDPHE 1996) were performed with an earlier version of the program. We compare the previous and current versions of the models for this pathway in Section 4.2.3. Predictions of resuspension by the current version tend to be substantially lower than those of pre-5.75 versions.

2. SOIL ACTION LEVELS

Soil action levels may be defined for sites where radionuclides remain in soil at levels that detectably exceed background. Their purpose is to express a possibly complex set of criteria for action that would be taken to protect people who might be exposed to the radioactivity in the near or distant future. Once a set of soil action levels is calculated for the radionuclides of concern, that set may be combined in a sum of ratios with measured or hypothesized concentrations of the radionuclides in soil (each ratio is a soil concentration divided by the corresponding action level) to determine whether the criteria do (or would) call for action, given the measured or hypothesized levels. The soil action levels as defined do not depend explicitly on the actual radionuclide concentrations, because they are determined by using the transport models to calculate levels in soil that would give the limiting annual doses. Thus the same set of soil action levels might be used for determining the need for remediation (based on existing concentrations), planning the remediation (hypothesizing reductions that would result from proposed actions), and verifying that the remediation has been successful (using post-remediation survey results).

The soil action levels depend on four things:

(1) Predicted movement of the radionuclides through environmental media and into potential contact with people (environmental transport models and pathway analysis)

(2) Possible patterns of contact that hypothetical people are assumed to have with the radionuclides in the near or distant future; also, physiological characteristics that would affect the estimation of radiation dose that these hypothetical people would receive (exposure scenarios)

(3) Dosimetric models and data, including radionuclide-specific internal dose coefficients and dose rate factors for external exposure to gamma-emitting radionuclides; these models and data are used to estimate radiation dose to any hypothetical individual with known exposure to radionuclides in the environment (radiation dosimetry)

(4) Annual radiation doses that express protective thresholds for people who might be exposed to the radionuclides (annual dose limits).

The calculation of soil action levels requires environmental transport models (item 1) that consider the various environmental pathways from the source to people who might be exposed (item 2) and methods of radiation dosimetry (item 3) to estimate dose corresponding to the predicted exposure. The purpose is to enable us to see how to control the current levels of the radionuclides in the soil so that the annual radiation dose from these radionuclides to any person who might be exposed to them in ways foreseen in the scenarios (item 2) cannot exceed the annual dose limits (item 4). Section 2.1 presents details of the formulation of the soil action levels.

If the environmental transport models take parameter uncertainties into account, the soil action levels will be represented as a joint probability distribution (the term “joint” indicates possible correlation among the soil action levels), and the sum of ratios (radionuclide concentrations in soil divided by the corresponding soil action levels) is a one-dimensional distribution that must be compared with 1. In this case, we must ask what is the probability that the sum of ratios exceeds 1, and if that probability is acceptably small, one may be willing to accept that exceeding the annual dose limit would be highly unlikely, although possible. Section 2.2 goes into greater detail about uncertainty analysis for soil action levels.

Exposure scenarios are descriptions of characteristics and behaviors of hypothetical individuals who are assumed to have a specified pattern of contact with the radionuclides

originating in the soil at the site. Behaviors would include time regularly spent in one or more locations on or near the site or eating foods from contaminated sources (e.g., a family garden planted in contaminated soil). Characteristics include variables correlated with dose, such as average breathing rates or dietary habits (kg day^{-1} of various food types). Soil action levels may depend on one or more exposure scenarios. Section 2.3 includes additional discussion of scenarios and some examples that may be relevant to the RFETS soil action levels.

The reader is reminded that the validity of soil action levels rests on the information and assumptions that go into their calculation. The calculation anticipates the above-background presence (but not the concentrations) of specific radionuclides and considers only dose limits corresponding to those radionuclides, ignoring any others that may be present. The soil action levels depend on specific exposure scenarios, but the formulation of the scenarios may be quite arbitrary. Thus, it is possible to consider scenarios located in such a way that they would minimize dose from the site and to fail to formulate scenarios based on locations or other assumptions that would tend to maximize dose from the site. Even though the soil action levels do not depend on initial concentrations of the radionuclides of concern, it is recommended that all available information on the spatial distributions of initial radionuclide concentrations be considered as the exposure scenarios are formulated. Otherwise the resulting soil action levels may not impose the desired dose limitation. The implicit nature of soil action levels makes it possible for them to conceal models and assumptions that may not be appropriate for a particular site from users who do not have complete information about the derivation of the soil action levels.

The reader should also be aware that it is always possible, in principle, to avoid soil action levels altogether and to base remediation planning and verification on direct simulations with the data, models, and scenario definitions that would have been used to calculate the soil action levels. That is to say, given a set of measured or hypothesized radionuclide concentrations in soil, the environmental transport and dosimetric models are applied directly to these soil data to estimate annual dose over time to the subjects of the exposure scenarios and thus to determine whether or not dose limitations would be exceeded. Soil action levels need not be calculated at all, and this technique has been employed at various facilities analyzed in Task 1, including Maralinga, Australia, and the Nevada Test Site. This approach has the advantage that its explicit nature draws attention to the numerous elements that go into the estimation of dose as a function of initial concentrations of the radionuclides of concern. Reviewing these models, scenarios, and other data can cause the discovery of errors and assumptions that may not be appropriate for the site under consideration. The disadvantage is some added computational effort, although this disadvantage may have relatively less weight when uncertainties are introduced into the simulations. The current availability and speed of modern computers makes the direct calculation practical for virtually any technical group with the requisite knowledge, whereas decades ago, tables of hazard indices and action levels were essential for decision makers with little or no access to computing equipment that would have made direct computation possible. For example, in the 1960s and 1970s, the International Commission on Radiological Protection (ICRP) published tables of limiting air concentrations for radionuclides in occupational environments, based on dose limitation criteria, whereas contemporary ICRP publications emphasize dose coefficients, on the assumption that any reader has the means to use these coefficients to estimate dose from measured or hypothesized air concentrations of radionuclides.

2.1 Formulation

This section is intended primarily for specialists. It gives mathematical details about the formulation of soil action levels and their relationship to the models and scenarios. The general reader may wish to skip ahead to Section 2.2.

As we shall see in Section 3 and its subsections, it could be desirable to subdivide the RFETS into some number R of subregions, such that the concentration of each radionuclide can be treated as if it were spatially uniform in each subregion. Such a disaggregation would permit an improved representation of so-called hot spots and may offer some advantages in planning and verifying remediation steps. But for the initial discussion of the formulation of soil action levels, we consider a single uniformly contaminated region. At the end of this section, we indicate the more general forms of the formulas when multiple subregions are considered.

It is necessary to define a set of soil action levels for each of the exposure scenarios under study. For any set of radionuclide concentrations $(C_1,\mathsf{K}\ ,C_N)$ and scenarios indexed $s=1,\mathsf{K}\ ,S$, we can write a sum of ratios for each scenario s as

$$(\mathrm{SR})_s = \sum_{i=1}^{N} \frac{C_i}{(\mathrm{SAL})_{si}}, \quad s=1,\mathsf{K}\ ,S \tag{2.1-1}$$

where details of the computation of the denominators are given below. A simple geometric interpretation for $N = 2$ and $S = 1$ is shown in Figure 2.1-1. The $(\mathrm{SAL})_{si}$ will be calculated in such a way that the probability that $(\mathrm{SR})_s \le 1$ is equal to the probability that the dose limit for scenario s is not exceeded. But we must base our soil criterion on the probability that $\max_s (\mathrm{SR})_s \le 1$ (the notation $\max_s(\mathrm{SR})_s$ means the largest of the sums of ratios), so that we control all scenarios by controlling the ones for which potential exposure is maximum. In general, we allow both the numerators and the denominators in the sum in Equation. 2.1-1 to be uncertain quantities. The soil concentrations will come from a joint distribution based either on sampling or existing data. The denominators are based on applicable pathway calculations of dose for the respective scenarios, using Monte Carlo methods to estimate joint distributions. The term “joint” indicates the possibility that there may be correlations among the soil concentrations for different radionuclides, and the denominators may be correlated among scenarios that depend on common pathways (although as a practical matter, we may wish to treat different scenarios as if they were independent). The numerators and denominators will generally be independent.

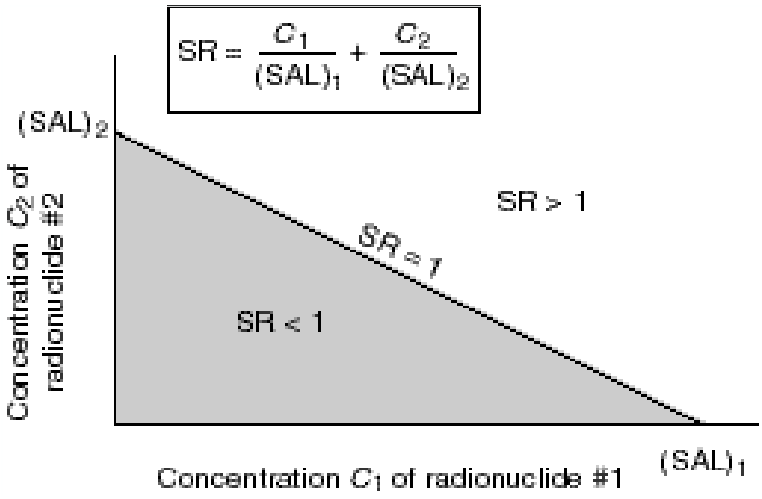

Figure 2.1-1. Geometric interpretation of the sum of ratios (SR) for two radionuclides (N = 2) and one scenario (S = 1). All points (C_1, C_2) on the line represent pairs of concentrations for which the sum of ratios equals 1. For all points in the shaded rectangle beneath the line, the pair of concentrations corresponds to a sum of ratios less than 1 and thus to annual doses that do not exceed the annual dose limit. The concentration pair for any point above the line would lead to an annual dose that exceeds the annual dose limit.

Let us define the transfer function T_{smi} as the quantity that converts a concentration C_i of radionuclide i in the soil to the dose estimate D_{smi}. The subscript s stands for the scenario, and m denotes the particular pathway. The transfer function is something that would be computed by an appropriate environmental transport model. The dose relation for a single radionuclide, scenario, and pathway is

$$D_{smi} = T_{smi} ? C_i \,. \tag{2.1-2}$$

Each scenario has a dose limit, and the dose limits are not necessarily the same for all scenarios. Let us denote the limit for scenario s by Δ_s. Then the requirement for the scenario is that

$$\sum_{i=1}^{N}\sum_{m=1}^{M} C_i T_{smi} = \sum_{i=1}^{N} C_i \sum_{m=1}^{M} T_{smi} \le \Delta_s \quad \text{for each } s = 1, \ldots, S \,. \tag{2.1-3}$$

If we divide Eq. 2.1-3 by the dose limit Δ_s and rearrange the second summation, the condition can be expressed as

$$\sum_{i=1}^{N} \frac{C_i}{\Delta_s \Big/ \sum_{m=1}^{M} T_{smi}} \le 1, \quad s = 1, \ldots, S \,, \tag{2.1-4}$$

and this shows us how to define the SALs for the scenarios:

$$(\mathrm{SAL})_{si} = \frac{\Delta_s}{\sum_{m=1}^{M} T_{smi}}, \quad s = 1, \ldots, S, \quad i = 1, \ldots, N \,. \tag{2.1-5}$$

Putting this expression into Equation 2.1-1 defines the scenario-dependent sum of ratios $(\mathrm{SR})_s$. The condition

$$(\mathrm{SR})_s \le 1, \quad s = 1,\mathrm{K}\ ,S \tag{2.1-6}$$

is equivalent to the dose-limitation condition of Eq. 3, in the sense that (2.1-3) holds for each $s = 1,\mathrm{K}\ ,S$ if and only if (2.1-6) holds for each $s = 1,\mathrm{K}\ ,S$. Thus, to achieve the required dose limitation, we must require that Equation 2.1-6 hold for all s, or equivalently

$$\max_s (\mathrm{SR})_s \le 1\ . \tag{2.1-7}$$

Of course this requires us to define a separate sum of ratios for each scenario. There is a way to avoid this. We may write

$$(\mathrm{SR})_s = \sum_{i=1}^{N} \frac{C_i}{(\mathrm{SAL})_{si}} \le \sum_{i=1}^{N} \frac{C_i}{\min_s (\mathrm{SAL})_{si}} = (\mathrm{SR})\ , \tag{2.1-8}$$

where the last equality in Eq. 8 defines a scenario-independent sum of ratios (SR). Now if we impose the condition

$$(\mathrm{SR}) \le 1\ , \tag{2.1-9}$$

Equation 2.1-9 implies that the inequality of Equation 2.1-7 follows, so that the dose limitation is met for all scenarios. But it does not work the other way, which is to say the following: there may be some sets of soil concentrations for which (2.1-7) would be satisfied but which would violate (2.1-9). Thus (2.1-9) (as defined by (2.1-8)) is a more stringent condition, which could impose lower soil concentrations. Using Equations 2.1-8 and 2.1-9 as the criterion also introduces a complication when we introduce probability and uncertainty.

We regard the C_i and the $(\mathrm{SAL})_{si}$ as uncertain quantities, and consequently we must interpret inequalities like (2.1-3) and (2.1-6) probabilistically. The probability that these equivalent inequalities hold is the probability — based on the uncertainty of the radionuclide concentrations and the environmental transport calculation — that the dose limitation for all scenarios will be collectively met. To estimate this probability, we sample from the joint distribution of the soil concentrations, and from the distributions of the scenario-dependent soil action levels (Equation 2.1-5); using Monte Carlo methods, this permits us to count the number of times during the run the inequality (2.1-4) holds for all scenarios *s.* Dividing this number by the total number of Monte Carlo cycles gives our estimate of the probability.

If we use criterion (2.1-9) instead, we can estimate the probability that the inequality (2.1-9) holds, but that probability is not the same as the probability that (2.1-7) holds (as we previously pointed out, inequalities (2.1-9) and (2.1-7) are not equivalent: (2.1-9) implies (2.1-7), but not the other way around). The probability of (2.1-7) will in general be larger than the probability of (2.1-9). This approach imposes a more stringent requirement and could require additional remediation to meet the criterion, given the scenarios, the dose limit numbers, and a specified probability that Equation 2.1-9 holds.

As we mentioned at the beginning of this subsection, it could be useful to consider a subdivision of the RFETS into some number *R* of subregions and to treat soil concentrations of radionuclides as being spatially uniform within any given region (we would hope to avoid this level of complexity). We conclude this section with the more general forms of the equations that define the soil action levels in such a multiple-source environment. We use the indexing variable $r = 1,\mathrm{K}\ ,R$ for the subregions ($R = 1$ corresponds to the previous case). For $R > 1$, we have a larger number of soil action levels: whereas in the previous formulation, there were *NS* (one for each radionuclide and scenario), now the number is *NSR* (one for each radionuclide, scenario, and source subregion). We add another index to the concentration $C_i^{(r)}$, and to the transfer function $T_{smi}^{(r)}$, and we define the soil action level as

$$(\mathrm{SAL})_{si}^{(r)} = \frac{\Delta_s}{\sum_{m=1}^{M} T_{smi}^{(r)}}, \quad i = 1,\mathrm{K}\ ,N, s = 1,\mathrm{K}\ ,S, r = 1,\mathrm{K}\ ,R \qquad (2.1\text{-}10)$$

and the sum of ratios for scenario s as

$$(\mathrm{SR})_s = \sum_{r=1}^{R}\sum_{i=1}^{N} \frac{C_i^{(r)}}{(\mathrm{SAL})_{si}^{(r)}}, \quad s = 1,\mathrm{K}\ ,S\ . \qquad (2.1\text{-}11)$$

Using this form of $(\mathrm{SR})_s$, we still apply Equation 2.1-7 as our criterion for dose limitation.

It is important to remember that the compact formulations shown in this subsection conceal a great deal of specific detail about the scenarios and environmental models. We describe a possible set of scenarios in Section 2.3. Sections 3, 3.1, and 3.2 outline a conceptual approach to environmental modeling for the site and the modes of exposure that would be relevant for the site and the scenarios.

2.2 Stochastic SALs

Uncertainty analysis is now regularly applied to environmental modeling. Parametric uncertainty is concerned with the propagation of uncertainty in parameter values through the simulations to the resulting estimates of concentrations in exposure media or to dose or risk. The usual tools are Monte Carlo techniques. In their simplest form, these techniques consist of assigning a probability distribution to each parameter that is treated as uncertain. The simulation is performed a large number of times (usually 1000 if practical), and at the beginning of each repetition, a number is sampled from the distribution associated with each parameter. This random set of parameter values is used to parameterize the model, and the corresponding result (say a dose) is calculated. The 1000 doses define an empirical distribution for the dose quantity. This distribution is considered an estimate of the quantity and represents the propagated uncertainty. Sometimes additional elaboration is necessary, such as the simulation of correlated subsets of the parameters. But the end product is an uncertainty distribution for each calculated quantity.

When the quantities to be calculated are soil action levels, there is no special difficulty in applying uncertainty analysis. The procedure produces an uncertainty distribution for each SAL. Each of these distributions is a marginal distribution of a multivariate joint distribution of the possibly correlated SALs. These correlations need to be preserved for the next step, which is combining the SALs with measured or assumed soil concentrations of the respective radionuclides by forming ratios: soil concentration divided by SAL. The ratios are summed as in the deterministic case, but in the stochastic case there are, say, 1000 sums of ratios, which define an empirical uncertainty distribution of the sum of ratios (SR) quantity. It is this distribution that is compared with 1 to determine the probability that 1 will be exceeded. If, for example, the value 1 occurs at the 95th percentile of the distribution, then the probability that the sum of ratios will exceed 1 is 5%, or one chance in 20. This might be accepted as a small probability of exceeding the dose standard imposed on the scenario from which the SALs were derived. This probability is associated with uncertainties in environmental data and models; it does not come from the scenario itself, which is considered fixed (Section 2.3). If the value 1 occurred at the 60th percentile of the sum of ratios distribution, the probability of exceeding the dose limit would be 40%, which anyone would likely consider large. In that case, some action or attention would be called for. Figure 2.2-1 is a schematic showing two sum of ratios uncertainty distributions corresponding to the two examples we have just given.

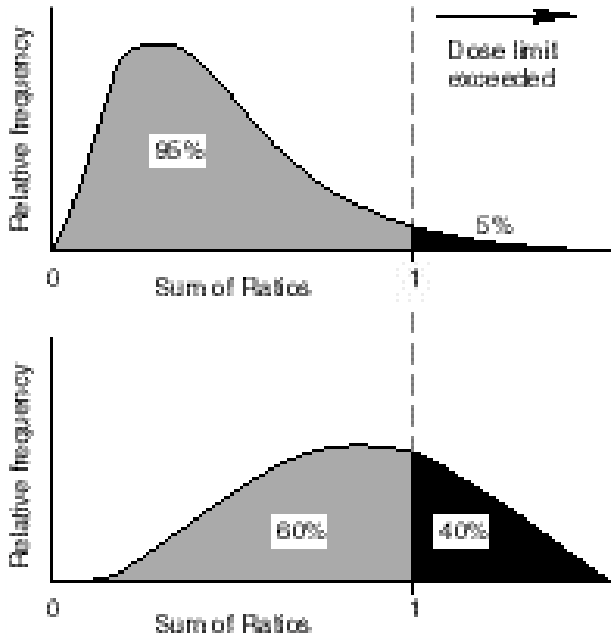

Figure 2.2-1. Schematic illustration of uncertainty distributions for the sum of ratios of soil concentrations divided by the corresponding soil action levels. In the top panel, the probability is 5% that the dose limit for a scenario would be exceeded. In the bottom, the probability is 40%.

2.3 Exposure scenarios

Exposure scenarios describe the characteristics and behaviors of hypothetical individuals who might have some contact with the radionuclides in the soil at the site. The people described by the scenarios live, work, or use the Rocky Flats site for recreational purposes. For the soil action level assessment, a succession of hypothetical individuals over time (for example, 1000 years) is considered. The scenarios represent a means to assess the behavior of radionuclides in the environment in terms of their impact on potentially exposed individuals. A goal for designing the scenarios in this study is that if the hypothetical individuals are protected by specified dose limits, then it is reasonable to assume that others will be protected. The reference scenarios are standards against which levels of radionuclides in the soil at the Rocky Flats site can be measured.

Each scenario represents a single individual with unique physical and behavioral characteristics. These characteristics include variables correlated with dose, such as average breathing rate or dietary habits. Behaviors include time spent indoors and outdoors or eating foods from contaminated sources (e.g. family garden). Exposure scenarios provide assumptions about the nature and extent of possible contact that people might have with the site. Because this study is prospective in nature and has the goal of protecting potentially exposed people from radiation, it may be appropriate to consider biasing some of the scenario parameters in a way that would increase estimated annual dose. However, we recommend that this practice be limited to include only the possible; for example, an individual breathing 24 hours a day at the maximum rate for an Olympic athlete during a strenuous performance is not credible and should not be used to establish an average breathing rate. But it may be appropriate to estimate average breathing rates to include

periods of strenuous activity, provided the number and lengths of these periods do not exceed what is reasonable.

For the RSAL assessment, some of the parameters are breathing rates for various activity levels and ages, soil ingestion rates for children and adults, fraction of time spent indoors and outdoors, and the potential use of or exposure to contaminated water from the area. Selecting appropriate parameters for the scenarios depends upon a thorough review of the scientific literature and fully considering the uncertainty (or variability) distributions of the relevant parameters. We use a wide range of references and studies to compile information on parameters. Subsequently, we can generate a distribution of values and sample from the distribution, using Monte Carlo techniques. This process considers the available studies equally. The distributions can be characterized with a central value such as the median and some measure of the spread of the distribution, such as the standard deviation or the 5th and 95th percentiles of the distribution. In developing a particular scenario and considering variability of a parameter within the population studied, we can use a high (or low) percentile of the distribution as needed to extend protection to a larger fraction of a potentially exposed population with characteristics similar to those of the scenario subject. Once a parameter value is selected from our distribution of values for use in the scenario, the scenarios are considered fixed just as standards are fixed as a benchmark against which to measure an uncertain value. Behavioral characteristics should be plausible and relevant to the exposure situations and the radiation protection objectives.

Scenarios provide a technical basis for focusing on those pathways and characteristics that are most important in the dose assessment. For example, for plutonium in soils at Rocky Flats, the inhalation pathway will likely prove important. The inhalation or breathing rate affects the transport of airborne contaminants to the respiratory tract and also influences their deposition onto surfaces of the airways and in the pulmonary region. As a result, it is important to exercise care in selecting breathing rate values for each scenario. We have compiled data from numerous published papers to provide perspective in the selection of suitable breathing rates. For soil ingestion, we have reviewed various studies on the unintentional and intentional ingestion of soil by children and adults (e.g., Kimbrough et al. 1984, Calabrese et al. 1990). Simon (1998) developed scenarios based on an extensive review of the literature. The selection of input parameters will be described fully in the Task 3 report for this project. The historic approach for estimating breathing rates over a specified time period is to calculate a time-weighted-average of ventilation rates associated with physical activities of varying time durations. A second approach for determining breathing rates for various populations is based on basal metabolism and measured food-energy intakes and energy expenditures. There is much variability in breathing rates with activity level and age and thus, it is more defensible to use a distribution of values from which to select the input breathing rates (using a high percentile, for example) for an individual scenario.

RAC is evaluating the three scenarios described in the report, *Action Levels for Radionuclides in Soils for the Rocky Flats Cleanup Agreement*, dated October 31, 1996 (DOE/EPA/CDPHE 1996), along with additional scenarios that we have proposed and described at the monthly Radionuclide Soil Action Level meetings. *RAC* believes strongly that it is important to describe the process behind the development of the scenarios, to provide the panel with a broad range of scenarios for evaluation, and to consider a number of likely scenarios before final scenarios are selected for the project. In our discussions with the panel, we have used several breathing rate studies as examples of the kinds of data that will be used to develop

uncertainty distributions for key parameters. In these meetings, we described the step-wise process to show how breathing rates can be selected based on activity levels and age, and how these values are summed over a specified time period (e.g. hour, day or year) to yield an annual breathing rate. This demonstration was important to understand that an annual inhalation rate for an airborne radionuclide is based on a weighted average rate, where the weights are determined from the times spent in different activities and at indoor or outdoor locations throughout the day.

We consider the three scenarios outlined in the current Rocky Flats Cleanup Agreement as workable scenarios for the current project. We have designed additional scenarios, too. In some cases we have proposed scenarios with only minor variations from the three current scenarios in the cleanup agreement. For others, we have outlined scenarios with different assumptions about lifestyles and living conditions. Once again, the objective in developing the scenarios is based on the rationale that if the hypothetical individual in the scenario is protected by specified dose limits, then it is reasonable to assume that others will be protected. During the course of designing the exposure scenarios, we had proposed seven additional scenarios. After many discussions with the panel, we focused on four of the proposed scenarios for future RSAL work. The exposure scenarios that are under consideration are described briefly here, beginning with the current Rocky Flats Cleanup Agreements scenarios. Table 2.3-1 summarizes some of the parameter values for those scenarios.

1. The future residential exposure scenario assumes that an individual resides onsite all year and grows and consumes homegrown produce. This person would be exposed to radioactive materials in soils by directly ingesting the soils, by inhaling resuspended soils, by external gamma exposure from contaminated soil and airborne radioactivity, and by ingesting produce grown in contaminated soil. This scenario is from the current Rocky Flats Cleanup Agreement.
2. The open space exposure scenario assumes the person visits the site 25 times per year for recreational purposes, spending 5 hours per visit at the site. The person would be exposed to radioactive materials in the soil by directly ingesting the soils, by inhalation of resuspended soils, and by external gamma exposure from the soils and airborne radioactivity. This scenario is from the current Rocky Flats Cleanup Agreement.
3. The office worker exposure scenario represents an individual who works a 40-hour per week, 50-week per year job indoors in a building complex at the site. It is assumed that this person would be exposed to radioactive material in soils by directly ingesting the soils, by inhaling resuspended soils, and by external gamma exposure from soils and airborne radioactivity. This scenario is from the current Rocky Flats Cleanup Agreement.
4. The resident rancher scenario assumes future loss of institutional control. The rancher is raising a family, maintaining a garden and leading an active life at the site, spending 24 hours per day, 365 days per year or 8760 hours at the site. Of that time, over 40% is spent out of doors. The potential pathways of exposure for this person include inhalation; eating produce from garden irrigated with groundwater, direct soil ingestion from outdoor activities, and direct gamma exposure from the soils and airborne radioactivity. The annual breathing rate is 10,800 m^3 per year, based on a time-weighted average of breathing rates and activity levels as described during the monthly RSALs meetings. *RAC* proposed this scenario for consideration at the January 1999 RSAL meeting.
5. Infant in rancher family is 0 to 2 years of age, and onsite 24 hours per day, 365 days per year, or 8760 hr/year. The infant's potential pathways of exposure include inhalation, some direct soil ingestion from outdoor activities, and direct gamma exposure from soils and airborne radioactivity. *RAC* proposed this scenario for consideration at the January 1999 RSAL meeting.
6. The child of the rancher family is assumed to be 5 to 17 years of age, and onsite 24 hours per day, 365 days per year, or 8760 hr/year. The potential pathways of exposure include inhalation, eating produce from garden irrigated with water from a stream on the site, direct soil ingestion, and gamma exposure from soils and airborne radioactivity. *RAC* proposed this scenario for consideration at the January 1999 RSAL meeting.
7. The current onsite industrial worker scenario assumes a person works onsite 8_ hours per day, 5 days per week, 50 weeks a year, or 2100 hours per year. It is assumed that 60% of the worker's time is spent outdoors. The potential pathways of exposure for this person include inhalation, direct soil ingestion from outdoor activities, and direct gamma exposure from the soils. The annual breathing rate is 3700 m^3 per year, based on a time-weighted average of breathing rates and activity levels for the time spent onsite. *RAC* proposed this scenario for consideration at the February 1999 RSAL meeting.

Table 2.3-1. Summary of Key Scenario Parameter Values for DOE and *RAC* Scenarios

	Current DOE/EPA/CDPHE scenarios			*RAC* recommended scenarios			
				Nonrestrictive	Restrictive		
Parameter	Resident	Open space	Office worker	Current site industrial worker	Resident rancher	Infant of rancher (new-born–2 y)	Child of rancher (5–17 y)
Onsite location				Present industrial area	East of present 903 Area	East of present 903 Area	East of present 903 Area
Time on the site (h d^{-1})				8.5	24	24	24
Time on the site (d y^{-1})				250	365	365	365
Time on the site (h y^{-1})	8400	125	2000	2100	8760	8760	8760
Time indoors onsite (h y^{-1})				900	3500	7740	6600
Time indoors onsite (%)	100	100	100	40	60	90	75
Time outdoors onsite (h y^{-1})	0	0	0	1200	5300	860	2100
Time outdoors onsite (%)	0	0	0	60	40	10	25
Breathing rate (m^3 y^{-1})	7000	175	1660	3700	10000	1900	8600
Soil ingestion (g)	0.2 for 350 d	0.1 per visit for 25 visits per y	0.05 for 250 d	0.20 for 250 d	0.20 for 365 d	0.20 for 365 d	0.20 for 365 d
Soil ingestion (g y^{-1})	70	2.5	12.5	50	75	75	75
Irrigation water source	Ground-water	NA[a]	NA	NA	Ground-water	NA	NA
Irrigation rate (m y^{-1})	1	NA	NA	NA	1	NA	NA
Onsite drinking water source	no	no	no	no	Ground-water	NA	NA
Drinking water ingestion (L d^{-1})	NA	NA	NA	NA	2	NA	NA
Drinking water ingestion (L y^{-1})	NA	NA	NA	NA	730	NA	NA
Fraction of contaminated homegrown produce	1	0	0	0	1	0	1
Fruits, vegetables and and grain consumption (kg y^{-1})	40.1	NA	NA	NA	190	NA	240
Leafy vegetables (kg y^{-1})	2.6	NA	NA	NA	64	NA	42

[a] NA = not applicable.

3. SITE CONCEPTUAL MODEL

By the term *site conceptual model*, we mean those features of the site that may be explicitly represented by mathematical models for the purpose of predicting dose and deriving soil action levels. The site conceptual model includes the source of the radioactivity, which in this case is the soil on the site with residues of radionuclides that with levels that exceed background by detectable amounts. The model considers the ways in which these radionuclides can deliver dose to people who might come onto the site, and mechanisms by which the radionuclides will move over time from surface soil into other environmental media (environmental pathways), where they may expose people. Thus, the scenarios must be considered part of the site conceptual model, to the extent that they define the receptors and exposure modes (e.g., inhalation, ingestion, or external exposure). The site conceptual model is less detailed than the mathematical models that provide specific formulas for calculating the behavior of the radionuclides over time (dynamic models) and for estimating dose from radionuclide concentrations in environmental media (dosimetric models). It provides a framework within which the mathematical models are organized. Sometimes the term is used to include all parametric information necessary to perform dose calculations. Some of the computer programs that perform the calculations have user-friendly modules that elicit from the operator the information that defines the conceptual site model (RESRAD, MEPAS, GENII). This section gives an overview of the *RAC* conceptual site model for radionuclides in soil at the Rocky Flats site.

Soil action levels are defined in terms of dynamic models that simulate the movement of radionuclide residues in soil through environmental media. They also depend on exposure scenarios, dosimetric models and data, and scenario-specific annual dose limits. The environmental models consider pathways that the radionuclides will follow from the soil to the potentially exposed individuals described by the exposure scenarios. The term *pathway* refers to the succession of environmental media through which the radionuclides move (for example, soil to air, soil to air to garden produce and pasture grass, or soil to surface water runoff to stream). We use the term *exposure mode* for the manner in which the exposure to body organs and tissues occurs. Inhalation, ingestion, and absorption through the skin are modes of intake that lead to exposure from an internally distributed source (internal exposure). External exposure is the result of a person's proximity to a contaminated medium outside the body (air, ground surface, water in which the person swims), such that gamma rays from the radionuclides in the medium deliver dose to the person's organs and tissues. Examples of pathways and corresponding exposure modes are inhalation of radionuclides that are resuspended from the ground surface; ingestion of contaminated soil, either directly or from produce; drinking contaminated surface water (e.g., from a stream that has received runoff from contaminated soil); and consuming animal products (meat or milk) from livestock that have grazed contaminated pasture or drunk contaminated water.

It is important to be as specific as possible about the nature of the models that simulate the movement of the radionuclides along the environmental pathways leading to possible exposure of people. There is no unique approach to the definition of these models: they can range from simple to complicated. The choice of definitions is usually indicated by experience, consideration of the site, and what is mathematically or computationally tractable. Pathways that can be shown to contribute negligibly to the endpoint of the calculation, relative to other pathways, can be omitted, but this must be done with care. Section 3.1 describes the pathways that are potentially relevant to the RFETS. The pathways depend on the exposure scenarios, which we described in Section 2.3. The models, coupled into a system, are treated as uncertain (principally through their parameters:

parametric uncertainty), and when we are given a set of measured or hypothesized concentrations of radionuclides in the soil, we apply Monte Carlo analysis to the sum of ratios to derive a distribution that tells us the probability that the dose limitations will be met.

3.1 Transport pathways

3.1.1 Availability of residual radioactivity in surface soil over time

The behavior of the radionuclides in the surface soil over time is clearly important because of the temporal scope of the scenarios (1000 years). Surface soil with adsorbed radionuclides is entrained into the air by wind action (resuspension) and eventually deposits again on the ground. The processes of resuspension and deposition exist in a quasi steady state cycle, with radioactivity being carried into a region and depositing there and local radioactivity being resuspended and carried away from the region. Over time, this cycle can alter the spatial distribution of radioactivity at the surface. Radioactivity is also removed from the surface soil over time by the action of water, at rates that depend on the amount of precipitation, properties of the soil, and the chemical forms of the radionuclides. Some of the radioactivity moves horizontally (runoff) to streams, and the remainder leaches downward, eventually (except for radioactive decay) crossing the water table and moving into the aquifer. Whatever effect the transport by surface water or groundwater may have on the scenarios that are chosen, it is necessary to take into account the fact that the fraction removed from the surface is no longer available as a source of external exposure or for resuspension. It is important that the transport models deal credibly with this dynamic behavior and persuasively quantify the uncertainties associated with it.

Our approach to multimedia modeling emphasizes the effort to preserve mass balance and to avoid deliberate biasing of environmental concentration estimates. This approach goes hand in hand with our treatment of uncertainty distributions. An example of an approach that would violate this principle is to estimate loss of radioactivity from surface soil by runoff and leaching without accounting for the complementary depletion of radioactivity in the surface soil reservoir. Such calculations can be defended as conservative, but the loss of mass balance accounting generally introduces difficulty into the analysis and interpretation of uncertainty, and we prefer to avoid this difficulty. Our alternative is to try to put the conservatism into the uncertainty distributions, preserving mass balance and minimizing bias. We stress that these are general guidelines, which require interpretation for specific application.

Thus, our conceptual site model treats the soil at any location of interest as a (primarily) vertical reservoir capable of representing distributions of different radionuclide concentrations over time. The model considers variable partitioning of each radionuclide into an aqueous (dissolved) and an adsorbed (adhering to soil) component. The first component moves with water that infiltrates the soil; the latter component is attached to soil matrix and mobile particles. Material attached to the soil moves by (1) surface weathering of the soil and (2) transferring from adsorbed to aqueous state when unsaturated water infiltrates the vadose zone. Radioactive ions also move from the aqueous state to attach to available sites on the soil matrix. The partitioning is usually characterized by a coefficient written as K_d, with units (mL g^{-1}). In environmental work, K_d is interpreted as the ratio at steady state of the radionuclide activity adsorbed on soil divided by the radionuclide activity remaining in solution. However, the steady state assumption is sometimes questionable in the

interpretation of process modeling. Narrower definitions of K_d are used in laboratory work, and criticisms of environmental soil modeling often turn on the use of this parameter and its different interpretations (Jirka et al. 1983).

We also need to mention the mechanism of colloidal transport, in which ions of the radionuclide attach to mobile submicron particles (colloids), which move by the action of water through intersticial spaces in soil and aquifers (Honeyman 1999). Recent investigations at the Nevada Test Site confirmed colloidal transport of $^{239+240}$Pu a distance of 1.3 km in groundwater. The ^{240}Pu:^{239}Pu ratio of the sample fingerprinted a particular underground nuclear test as the origin of the displaced plutonium (Kersting et al., 1999). The high affinity of plutonium for attachment to rocks has long supported assumptions of low mobility in predicting the movement of plutonium in soil and groundwater, but the introduction of colloidal transport models may eventually alter this pattern. No such explicit mechanism is included in any of the computer programs discussed in this report, and indeed, there is as yet no body of data that could credibly calibrate models of colloidal transport for the Rocky Flats site.

Given the initial amounts of radionuclides in the surface soil, the model predicts the evolving vertical distribution over time as the radioactivity is redistributed by the processes described above. At any subsequent time it is possible (in principle) to evaluate the predicted concentration in soil near the surface that would be available for resuspension, uptake through the roots of plants, direct ingestion, or exposing people to gamma rays from this external source. Not all computer programs handle the removal and redistribution mechanisms in the same way, and the results may differ.

3.1.2 Spatial disaggregation of soil

Contamination of the Rocky Flats reservation by some of the radionuclides of concern is far from uniform. Figure 3.1.2-1 shows the variation of ^{239}Pu concentrations along a transect eastward from the 903 Area, plotted from data of Webb (1996). Litaor et al. (1995) show contour plots of $^{239+240}$Pu concentrations in the soil. Programs such as RESRAD proceed on the assumption of a uniformly contaminated area (subject to variation within a factor of 3). For some scenarios it could be desirable to subdivide the site area into some number *P* of plots, each of which can be treated as having a uniform concentration of each radionuclide, but with concentrations varying from one plot to another. Such subdivision might be of assistance in the planning for remediation, because the effects of reducing the most contaminated plots by various amounts can be studied explicitly. However, given the relatively small area of the most highly contaminated soil, we would be reluctant to recommend this refinement without careful evaluation of any factors that might seem to indicate it. We have included equations for area disaggregation near the end of Section 2.1 for the sake of completeness.

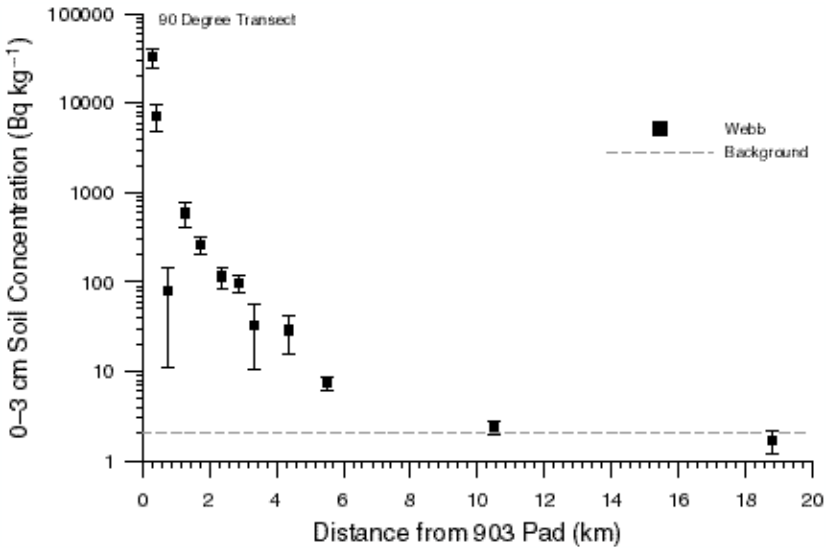

Figure 3.1.2-1. Plutonium-239 concentrations in soil (Bq kg^{-1}) at RFETS along a 90° transect (eastward) from the 903 Pad area. The data are from Webb (1996).

3.1.3 Resuspended contaminated soil

The experience of *RAC* in the Rocky Flats Dose Reconstruction project indicates that the inhalation of resuspended soil that was contaminated by plutonium from the 903 Pad is a potentially significant exposure pathway. Its importance depends on how the scenarios are defined, primarily with respect to location relative to the locations of highest contamination of $^{239+240}$Pu. In Section 2.3, we described a possible scenario that assumes eventual loss of institutional control of the site and that families establish homesteads west of Indiana Street, within the area most affected by the 903 Pad. Such a location (within the contour marked 10 Bq kg^{-1}) would maximize the inhalation exposure to resuspended plutonium, given the prevailing westerly winds, whereas locations west of the RFETS near Highway 93 would correspond to lower inhalation doses. It seems clear that this exposure pathway must be considered, whatever the decisions about scenarios might be.

A serious problem in dealing with any exposure pathway that depends on resuspended soil is the uncertainty introduced into the calculation by the inexact characterization of the mechanisms. Resuspension occurs as a result of wind action on available soil particles, at a rate that depends on wind speed, gross characteristics of the ground surface (roughness of the soil, vegetation, and other objects), and characteristics of the soil, such as size distributions of the particles and tendency of the soil to form less-erodible crusts. The resulting air concentration (which determines exposure by inhalation and external exposure to gamma rays from the diffused particles) depends not only on the resuspension rate but also on stability parameters for the atmosphere, which establish a vertical profile of concentration, and on the deposition rate at which the airborne particles return to the ground. Local levels of contamination borne by the resuspended particles are diluted by particles that entered the air at various distances upwind from the contaminated site. The complexity of this environmental system guarantees large uncertainties in predictions of process-level models for which parameters are difficult or impossible to quantify by direct measurements. (We use

the term *process-level* to refer to models that are formulated in terms of the processes of fundamental physics, chemistry, and biology, as opposed to *empirical* models, which may summarize many complicated processes in a few directly measurable parameters. This is an oversimplification since most models are empirical at some level, but the distinction is sufficient for this discussion.)

Langer (1986) reports measurements of airborne ^{239}Pu and airborne dust at heights of 1, 3, and 10 m from November 1982 through December 1984 (measurements at 3 m covered a shorter period). The dust-collection and wind-measurement apparatus was placed 100 m southeast of the former East Gate of the plant, near the 903 Pad, and less-detailed measurements of airborne ^{239}Pu were also taken from three samplers near the former East Gate. Both the dust and radioactivity measurements give a crude indication of particle size distributions. A relatively long record of this kind provides what may be the most useful information for calibrating empirical models of resuspension from the field east of the 903 Pad, although this information is still very limited and must be applied with care. But these measurements do provide long-term averages of ^{239}Pu air concentrations that likely approach the maximum for the site. These measurements implicitly take into account the dilution from upwind dust of low contamination, whereas modeling this dilution is a highly uncertain exercise. Krey et al. (1976) used air and soil sampling data from three sites in the field east of the 903 Pad to estimate that only 2.5% of the respirable dust came from local resuspension. This result cannot be considered generically applicable because of uncharacteristically high precipitation during the sampling period, but it does illustrate the point.

The computer programs under investigation approach the resuspension mechanism in one of three ways (in some cases, the user is offered an option of more than one method). (1) *Mass loading*, in which a measured or hypothesized concentration of airborne dust (g m^{-3}) is multiplied by the local concentration of radionuclide on resuspendable soil particles (Bq g^{-1}) to produce an estimate of airborne radioactivity concentration (Bq m^{-3}). (2) *Resuspension rate* (m^{-2} s^{-1}), which may be estimated as the air concentration of dust at a reference height (g m^{-3}) times an average deposition velocity (m s^{-1}) divided by the mass of resuspendable particles per unit area (g m^{-2}). (3) *Resuspension factor*, which may be defined as the air concentration of dust at a reference height (g m^{-3}) divided by the mass of resuspendable particles per unit area (g m^{-2}). The resuspension factor has units m^{-1} (or g m^{-3} airborne per g m^{-2} of resuspendable soil particles) and is equal to the resuspension rate divided by the average deposition velocity. These three approaches to resuspension modeling must be handled with some care. Used without adjustment, they incorporate a tacit assumption that the calculated air concentration of radioactivity-bearing dust is undiluted by uncontaminated dust from upwind. The resuspension factor, for example, is interpreted as the air concentration of dust per unit areal mass of resuspendable particles. This very definition tempts one to impute the local air concentration entirely to the local supply of available particles. But under the usual windy conditions, this assumption would be approximately valid only for large uniform areas upwind from the reference location, and the same is true when the particles are assumed to be contaminated with radioactivity.

All three of these approaches require quantification from the analyst or from default values or formulas supplied by the programs. In this respect, the mass loading approach is perhaps the most direct, requiring as its parameter the very air dust concentration that we seek to estimate. The parameter estimate should be based on measurements taken at the site

and averaged over as long a period as possible. The measurements of Langer (1986) indicate a mean total dust concentration of 47 $\mu g\ m^{-3}$ with standard deviation 9.0 $\mu g\ m^{-3}$ at the 1-m height for the period November 1982 through December 1984. This total quantity, however, includes a substantial fraction of particulate mass in a size range that is not regarded as respirable (59%). If the coarsest category of particles is discarded, the mean concentration is only 19.2 $\mu g\ m^{-3}$. Most of the resuspended plutonium activity (81%) at the 1-m level is associated with the coarse (non-respirable) particles, leaving only 19% associated with respirable particles. We cite these data to illustrate the point that one should consider the question of the size distribution of the airborne dust and the distribution of plutonium activity over the airborne particles in order to make credible estimates of inhalation dose. The computer programs that implement mass loading do not exercise this judgment, although default values of some parameters may be supplied. Another complication is that air samplers lose efficiency as the particle aerodynamic diameter increases, and the efficiency loss is aggravated by the high wind events that cause much of the resuspension. Thus the measurements taken at Rocky Flats are subject to uncertainties of interpretation, and these uncertainties need to be quantified and incorporated into the calculation.

An approach to resuspension rate estimation is given by Cowherd et al. (1985) in an EPA report. Equations are provided for wind-driven resuspension associated with infinite and limited reservoirs of resuspendable particles. The parameterizations for the EPA models are given in detail, with instructions for coarse particle-size measurements in the field. The report also treats resuspension by mechanical means, such as vehicular traffic. The methods presented are intended to provide a "first-cut, order-of-magnitude estimate of the potential extent of atmospheric contamination and exposure resulting from a waste site or chemical spill, within the 24-hour emergency response time frame." Variants of these models are incorporated into MEPAS, with the necessary graphs and figures from Cowherd et al. (1985) reproduced in the MEPAS documentation. But by use of the front-end technique described in Section 4.1, these resuspension rate models can also be used in connection with other assessment programs, such as RESRAD, that do not implement the models. When this approach is taken, the resuspension model is programmed as part of the front-end script program, which calculates the resuspension rate and passes the information to RESRAD (or any other program with which a front end is used) through an input file. The EPA models will be compared with other resuspension approaches in the work for Task 5 (Independent Calculation) and a recommendation will be made. Our present reference to the variety of approaches is not intended to make the selection prematurely, but rather to stress the point that the available programs, as they stand, are merely tools. Whichever tool is chosen must be coupled with judgment, research, and due consideration of site-specific characteristics to produce a persuasive assessment.

The resuspension pathway affects several components of radiation dose: (1) inhalation, (2) external gamma dose from airborne particles, and (3) deposition onto foliar surfaces of food and fodder crops, thus affecting the ingestion dose from consumption of local produce and animal crops. For oxides of plutonium in the soil and a scenario such as the resident rancher or hypothetical future resident, that is located in the field east of the 903 Pad, the resuspension-inhalation exposure mode is likely to be the dominant component of annual dose. Therefore, it is much more important to formulate credible approaches to modeling the resuspension mechanism and quantifying its uncertainty for the Rocky Flats site than it is to

devote too much time and attention to debating relative merits of one computer tool over another.

3.1.4 Groundwater and surface water transport

In calculating the proposed soil action levels (DOE/EPA/CDPHE 1996), the groundwater and surface water pathways were dismissed because (1) surface water features (Woman and Walnut Creeks) on the site are perennial and would not provide a reliable year-round water source for an individual living on the site and (2) surface aquifers underlying the site do not produce enough water for domestic or agricultural use. In addition, the aquatic food pathway was eliminated because the streams are not capable of sustaining a viable fish population. In this section, we will discuss these assumptions and the rationale behind them, and we will examine the ramifications of dismissing the groundwater and surface water pathways in the assessment.

3.1.4.1. Overview of surface and groundwater hydrology at the RFETS. Groundwater and surface water hydrology is discussed in the Sitewide Hydrologic Characterization Report (DOE 1995). The following material was paraphrased from this document and a White Paper that discussed the vertical contaminant migration potential at the RFETS (DOE 1996).

Three hydrostratagraphic units have been defined for the RFETS. Listed in descending order these units are the Upper Hydrostratagraphic Unit (UHSU), the Lower Hydrostratagraphic Unit (LHSU) and the Laramie-Fox Hills Aquifer Hydrostratagraphic Unit (LAHU). The UHSU consists of all surficial geological deposits and Arapahoe Formation sandstones that are in hydrologic connection with overlying surficial deposits, and weathered Laramie Formation claystone bedrock. These geologic units contain the uppermost aquifers underlying the RFETS. The LHSU consists of all unweathered Arapahoe and Laramie Formation bedrock and strata including upper Laramie claystones and confining beds. The LAHU consists of all unweathered lower Laramie Formation sandstone and Fox Hills Sandstone strata that comprise the regional Laramie–Fox Hills aquifer system. The LAHU forms the upper confining bed and the 7000+ ft thick Pierre Shale forms the lower confining layer.

The UHSU extends from the surface to a depth of about 35–60 feet. Small, mostly unconfined aquifers are present in the UHSU within the alluvium, colluvium, and valley-fill alluvium that make up the unit. Hydraulic conductivity in these units span 5 orders of magnitude. The geometric mean value for the Rocky Flats alluvium, colluvium, and valley-fill are 2.06×10^{-4}, 1.15×10^{-4}, and 2.16×10^{-3} cm s^{-1} respectively. These aquifers are not considered viable for drinking water or irrigation because their well yields are quite low, typically ranging from 0.05 to 2 gallons per minute in isolated areas. Water flow is typically from west to east-northeast and follows the surface topography. Aquifers terminate where they intercept the ground surface at incised surface drainage features such as Woman and Walnut Creek and at the contact between the Rocky Flats alluvium and bedrock unconformity. Surface discharge is typically manifested in the form of a seep. There is also vertical movement downward into the LHSU.

The LHSU is composed mainly of claystone and siltstone with a few discontinuous sandstone lenses. Thickness is estimated to range between 850–870 feet. Vertical migration of infiltrating waters from the UHSU into and through the LHSU is limited by the low

vertical hydraulic conductivity of this unit. Laboratory tests of core samples indicate a hydraulic conductivity ranging from 1×10^{-6} cm s^{-1} near the top of the unit to 1×10^{-7} cm s^{-1} near the bottom. Fracturing, however, can significantly increase the effective hydraulic conductivity in a relatively impermeable porous medium such as the LHSU. Fracture zones have been observed in the UHSU and LHSU and provide a viable means of moving groundwater from the UHSU to the Laramie–Fox Hills aquifer system. Faulting has also been postulated as a potential groundwater transport pathway from the UHSU and LHSU to the LAHU.

The LAHU is composed of fine to medium grained sandstone separated by a few claystone beds in the upper portion. Thickness ranges from 200 to 220 feet for the "A" and "B" sandstone that comprise the lower interval of the Laramie formation, and 80 feet for underlying Fox Hills sandstone unit. The Laramie–Fox Hills aquifer system is the target of most water wells in the vicinity of Rocky Flats because this aquifer provides sufficient water for domestic and industrial uses. Recharge to the aquifer takes place along the foothills west of the RFETS where the permeable sandstone beds of the formation are folded up and exposed. The permeable sandstone generally dips eastward toward the center of the Denver Basin.

Surface water features at the RFETS include Walnut and Woman Creeks and several ditches that provide irrigation water. Walnut and Woman Creeks are perennial and generally respond to seasonal fluctuations in precipitation, recharge, groundwater storage, and stream and ditch flow.. In the past these creeks drained into and Standley Lake, respectively. As of 1992, Walnut Creek, which previously flowed into the Great Western Reservoir, was diverted around Great Western Reservoir. By 1996, Woman Creek no longer flowed from the site directly into Standley Lake.

3.1.4.2. Implications of ground and surface water pathways on soil action levels. In an analysis of the vertical contaminant migration potential at RFETS (DOE 1996) it was concluded that the upper Laramie Formation confining beds have a sufficient amount of hydrologic and geochemical integrity to provide long-term protection of the Laramie–Fox Hills Aquifer from contamination at the RFETS. After reviewing this document and its supporting calculations, we agree with their conclusion but do not see this as a reason to discontinue research in this area or to dismiss entirely groundwater issues at the RFETS. The analysis leaves open other potential water transport pathways, and the possibility of colloidal transport may be important. Most notably, these potential pathways include lateral transport in the UHSU and discharge to surface water features followed by migration to downstream reservoirs. Additionally, direct usage of the UHSU aquifers could also be considered. One may also argue that under an exposure scenario that assumes subsistence conditions, a water well that produces 2 gallons per minute (such as has been observed in the UHSU) would be adequate to provide drinking water and perhaps water for a few head of livestock and some limited irrigation. Failure to address these pathways quantitatively leaves open the question of their potential importance.

It is well beyond the scope of this project to address the groundwater pathway in any substantial way other than through a simple screening exercise. Sophisticated groundwater modeling is difficult and time consuming, requiring substantial quantities of field data to characterize subsurface hydrologic units. We examine a conservative calculation in order to address the question of whether or not the pathway can be ruled out of the current analysis. We activate the groundwater pathway model in the RESRAD simulations, using the site

conceptual model and parameter values developed and documented in the proposed soil action level document (DOE/EPA/CDH 1996). The RESRAD conceptual site model assumes that a scenario subject uses groundwater derived from the UHSU for drinking water and some irrigation. The default RESRAD water ingestion rate of 510 liters per year was used in the analysis. Parameter values used in the assessment were reviewed and appear to be reasonable based on the information provided in the hydrogeologic characterization reports (DOE 1995).

Results for Tier 1 Action Level (85 mrem) residential exposure scenario are shown in Table 3.1.5-1. Note that action levels changed only for ^{241}Am, ^{241}Pu, and ^{234}U. In the case of ^{241}Pu, the ingrowth and ingestion of ^{241}Am is what caused groundwater ingestion doses to outweigh doses from external sources and inhalation. In the case of ^{234}U, ingestion doses are substantially higher than doses from external radiation. Dose from external radiation made up most of the total dose for ^{235}U and ^{238}U, and therefore groundwater ingestion doses had little impact. In the case of ^{241}Am, ingestion doses are substantially higher than inhalation or external doses. The highest doses for radionuclides where inclusion of the groundwater pathway made a difference (^{241}Am, ^{241}Pu, and ^{234}U) occurred 202, 222, and 379 years from the start of the simulation respectively. Highest doses when the groundwater pathway was ignored occurred at year 0 except for ^{241}Pu, which occurred 15 years from year 0. For the radionuclides whose action levels changed when the groundwater pathway was included, the differences in the times of maximum dose reflect the transit time from the source to the aquifer. For the radionuclide given the most attention (^{239}Pu), the soil action level remained unchanged.

Table 3.1.5-1 Soil Action Levels for the Residential Exposure Scenario at the 85 mrem Level Including and not Including the Groundwater Pathway

Radionuclide	Soil Action Level without Groundwater Pathway (pCi g^{-1})[a]	Soil Action Level with Groundwater Pathway (pCi g^{-1})
^{241}Am	215	110
^{238}Pu	1529	unchanged
^{239}Pu	1429	unchanged
^{240}Pu	1432	unchanged
^{241}Pu	19830	3370
^{242}Pu	1506	unchanged
^{234}U	1738	660
^{235}U	135	unchanged
^{238}U	586	unchanged

a. Source: DOE 1996a

The results of this exercise suggest that the rationale for dismissing groundwater as a viable pathway should perhaps be investigated further. The ongoing activities of the Actinide Migration Panel and other studies involving plutonium mobility should shed additional light on this subject. However, the results of these studies will not be available in time for completion of this work. For the purpose of calculating soil action levels, we will include the

groundwater ingestion pathway for at least one of the scenarios using a model with a level of complexity similar to the one implemented in RESRAD. A more detailed evaluation is not possible with the time and budget constraints of this project. We use the principle that by protecting scenario subjects who live and use water onsite, we are protecting all other potential users because transport of activity away from the site will result in lower exposure concentrations because of dilution and dispersion.

As shown by the preceding example, the inclusion of the groundwater pathway had little impact on the overall soil action levels except for the radionuclides noted, and we expect that this will be true in future simulations because inhalation and external doses tend to outweigh ingestion doses for most nuclides. We should caution that the results this assessment of groundwater are subject to reinterpretation based on any new findings from actinide migration studies and additional investigations performed for site remediation purposes.

3.2 Exposure Modes

The exposure modes described in this section have already been mentioned in previous sections to illustrate exposure pathways. The basic modes are inhalation and ingestion (internal exposure) and exposure to an external medium containing beta- and (primarily) gamma-emitting radionuclides. Other possible modes for internal exposure are absorption of a radioactive compound through intact skin or introduction of radioactivity into blood or by contact of a radioactive chemical with an open injury.

All types of radiation from radionuclides are significant for internal exposure. For external exposure, the dominant radiation type of a radionuclide permits some generalizations. Alpha-emitting radionuclides are not ordinarily a significant external source. Some beta emitters in high enough concentration in close proximity to a subject for a sufficient time can produce short-term damage to the skin, but beta rays have limited penetration in tissue and their dose is usually confined to a layer within a few millimeters of the skin surface. Gamma emitters produce penetrating rays that are capable of delivering energy (dose) from an external source to all parts of the body. The magnitude of the gamma dose received depends on the concentration of the gamma-emitting radionuclide in the source medium, its energy spectrum (higher energy photons tend to distribute their energy more deeply in tissue than lower energy photons), the geometry of the medium, the duration of the exposure, and the distance of the subject from the source medium.

Practical dose estimation is accomplished by means of dosimetric databases, consisting mainly of *dose coefficients* (sometimes called *dose conversion factors*) and other factors that relate the various kinds of exposures to the dose received per becquerel (Bq) of a radionuclide taken into the body or the dose rate per unit concentration of a radionuclide in an environmental medium to which a subject is exposed. These dosimetric factors are computed by specialists, who use models of physical and biological processes to simulate the interaction of radiation with tissue and the dynamics of metabolism of radioelements and compounds by organs of the body. Dose may be estimated by multiplying an intake rate (such as the breathing rate of someone inhaling a radionuclide suspended in the air, or the daily amount of a radionuclide that is being consumed with water and food) by the appropriate dose coefficient (intake per day times effective dose per unit intake = committed dose per day) and by the duration of the exposure; or by multiplying the concentration of a radionuclide in an exposure medium (such as the air) by a dose factor that gives dose rate per unit

concentration of the radionuclide in air (= dose received per day) and by the duration of exposure. There is a difference of interpretation between the internal and external dose estimates just indicated by example. When a radioactive chemical is taken into the body, time is required for the chemical to be translocated to the internal organs, metabolized, and excreted. During this process, the organs and tissues are exposed to the radionuclide and receive dose, but the amount of dose depends in part on the time required for metabolic processes and radioactive decay to remove the material from the body. For some radionuclides, the time over which the dose from a single intake accumulates is measured in years, and accordingly, we speak of the *committed* dose that will result from the intake (although some radionuclides have short half-lives and are quickly removed by radioactive decay, and some radioelements and compounds have biochemical properties that cause them to be rapidly removed from the body). External dose, on the other hand, is delivered at a practically instantaneous rate as long as the subject is exposed to the medium in which the radionuclide (or other source) is distributed.

Dose can be estimated for any organ that absorbs energy from ionizing radiation. The *effective dose* is a concept promoted by the International Commission on Radiological Protection (ICRP), which gives a nonlocalized definition of dose that is roughly proportional to the risk of radiation-induced cancer in *some* organ or tissue; the proportionality is achieved by weighting the equivalent dose to each internal organ with a relative risk coefficient for the organ (ICRP 1977). The effective dose is not to be confused with whole-body dose, which lacks this more refined connection to cancer risk.

All radiological assessment computer programs that we consider have databases of internal dose coefficients and external dose rate factors for each of a large library of radionuclides, including the relevant plutonium and americium isotopes for the Rocky Flats site and the decay products. The databases are similar among the programs, to the extent that they are based on published guidance from the International Commission on Radiological Protection (ICRP), particularly for internal dosimetry. The tables of internal dose coefficients provide alternative sets of numbers for different element-specific solubilities for both inhalation and ingestion. External dose rate factors are taken from Federal Guidance Reports such as Eckerman and Ryman (1993).

4. CANDIDATE COMPUTER PROGRAMS

4.1 Introduction

We originally selected for review five candidate computer programs that were developed for environmental risk assessment. The criteria for selection included the following:

(1) Presumed correctness of the models implemented by the programs, as indicated by their general acceptance, logical correspondence with features of the site, treatment of exposure pathways, and consistency with the available site data
(2) Amount and quality of validation that has been carried out and documented, and suitability for validation with local data
(3) Quality of program documentation and availability of source code
(4) Platform (i.e., computer and operating system) and (if source code is made available) programming language
(5) Flexibility of operating features, particularly the possibility of bypassing the user interface in order to invoke the computational part of the program and specify input and output files from the command line.

We confined the selection to programs that are generally comparable to RESRAD and that are (or are likely to be) widely used. In accordance with the contract, we include RESRAD as one of the candidates (it would have been included in any case). The other programs are MEPAS, GENII, MMSOILS, and DandD. All five have been (or are being) developed under sponsorship of one or more federal agencies, and to the best of our knowledge, the development project for each program has been carried out under formal quality assurance (QA) protocols.

The five criteria listed above were formulated before we made final decisions about the selection and before we began to procure code and documentation, install the executables on computers, and explore ways in which each program could be used. We have been allowed to see the source code for RESRAD. Source code is distributed with MMSOILS and GENII. We were not granted access to source code for MEPAS, but some version of DandD source code may be available, though it was not yet available to us as this report was prepared. It is not and was never our intention to carry out detailed reviews at source code level. We were primarily concerned with ways of executing the programs as indicated in item (5). We felt the need to be able to use scripting programs to manage Monte Carlo selection of parameter sets, to permit initialization calculations of relative abundances of plutonium and americium isotopes, and to invoke each of the five programs from the command line through the scripting program, passing each parameter selection prior to execution. This mode of operation permits us to apply Monte Carlo methods to programs that have no internal provision for them. Even with RESRAD, which has a beta-test version of a Monte Carlo facility, the built-in version is not entirely satisfactory for our purposes. RESRAD, MMSOILS and GENII are adaptable to this approach.

All five of the programs can be installed and executed under some version of the Microsoft Windows operating system (95 or NT, and presumably 98; by compiling the FORTRAN source code, we have executed MMSOILS under the Linux operating system, which is a variant of Unix; the instructions downloaded with MMSOILS indicate the installation procedure for DOS or Windows). Thus all of the programs would be widely accessible.

Comparative studies of three of these programs (RESRAD, MMSOILS, and MEPAS) have been made by groups including members who participated in their development (Laniak et al. 1997; Mills et al. 1997).

As this Task 2 report was nearing completion, a relevant report by the National Council on Radiation Protection and Measurements was released (NCRP 1999). NCRP Report No. 129 extends the NCRP series on screening limits, and this latest installment directly addresses radiation doses from exposure to contaminated surface soils. The report hypothesizes eight exposure scenarios and provides extensive tables of parameter values, screening limits, and dose estimates, with estimated uncertainties. The timing of the release of NCRP Report No. 129 did not permit us to prepare any substantial commentary on its relationship to this project. The reader should bear in mind that NCRP Report No. 129 is about screening limits. These limits are based on an annual effective dose limit of 25 mrem for exposure to a particular site, and this limit refers to the maximum dose to any exposed individual within a period of 1000 years. The screening limits (units Bq kg^{-1}) correspond to soil action levels for the NCRP-defined exposure scenarios, although the "action" envisioned in the screening context would likely consist of some level of site-specific reassessment. As we move forward with the project, we will continue to evaluate NCRP Report No. 129 for any implications that its methods and data might have.

This project's Request for Proposals (RFP) expressed concern for validation of the programs to be considered. We feel that it is necessary to go into some detail about procedures usually (but not always) termed *validation* and *verification* as applied to models and computer programs. We wish to be as clear as we can about what can and cannot be assumed with regard to procedures that are labeled with these terms.

4.1.1 Verification of Computer Programs

We believe it is necessary to make a distinction between the terms *validation* and *verification* (and the corresponding verbs) when they are applied to computer software. We need to go into some detail about these concepts, because one term is frequently used in place of the other, and usage is not uniform. Validation enters prominently into the project contract, and we need to strive for a clear understanding of what is possible in this regard and what is not.

Verification refers to procedures that try to ensure that a program is correctly coded, which is to say that it faithfully implements the mathematical descriptions of the models that define it, that it correctly translates input information furnished by the operator into all parameter values and control information required for calculations, that it detects inadmissible entries in the input, and (given admissible input) that it produces output that is in correct correspondence with the input. A process of verification would be perfect if one could somehow prove that for any set of admissible input data, the program will provide the output that the mathematical models and the algorithms imply, and that any inadmissible input data will be flagged. Computer scientists study verifiability as an academic subject and endeavor to develop methods for proving that a given program does what it is intended to do. As a practical matter, verification is an empirical process of systematic testing at many levels during development, investigating apparent anomalies reported by users, and making corrections as required. A reality that must be accepted is that all complex software is imperfect to some degree; in the vernacular of the trade, it has "bugs." The amount and

quality of testing that a programming project can afford depends on the intended use of the software and the seriousness of the probable consequences, should it malfunction. When failure may cause injury, loss of life, property damage, or misallocation of significant sums of money, then extensive testing is necessary, and its cost must be supported. Different levels of criticality are formalized in QA procedures for software. The length of time a computer code has been used is perhaps a more important factor. Codes with a long track record of performance have had many of their bugs pointed out by users and corrected by the developers. Users have also compared code output to their own hand calculations or results from other codes that perform comparable calculations. Taking this longevity into account, a user may gain confidence that the code is performing in a satisfactory way.

4.1.2 Validation of Computer Programs

Validation is an entirely different concept from verification. Validation also entails testing, although it is testing of a different kind. We will point out here that validation also has a special meaning in the realm of computer code quality assurance (QA). In this context, validation of a program is the process by with all of its modules are tested together, as a whole. The test is satisfactory if the requirements identified in the software specification and requirements documents are met. The present discussion does not address this narrower meaning of computer code validation. Instead, we consider model validation — that is, the collective ability of the mathematical models encoded in the computer program to predict the behavior of contaminants in the environment.

Abstractly, a computer program is considered valid for a specified predictive application if its results can be shown always to approximate acceptably their real-world counterparts. Thus, if we know how much uranium was released from a nuclear facility during a particular period and we have air monitoring data for uranium for that period, then using the known releases and an atmospheric diffusion model, we can predict air concentrations at the locations of the monitoring stations and compare the predicted concentrations with the measured values (if we assume that no other source of airborne uranium is distorting the measurements). If the approximation is acceptable, we have validation of the model for the period and the monitoring locations. Like verification, validation is necessarily imperfect (indeed, in a strict sense, it is impossible; *invalidation* would be decisive if the predictions and observations did not agree, but a claim of *validation* is merely a finding of no contradictory evidence, which leaves open the question of whether such evidence still might exist). The testing is specific rather than general: it is useless to declare that a computer program "has been validated," without specifying the particular comparisons that have been carried out. In our experience, validation of software that is applied to environmental assessments needs to be site-specific, and conclusions of any comparison must be drawn very cautiously. In the uranium example just mentioned, we might be willing to extend our tentative confidence in the model to other locations within the assessment domain that are not much farther from the facility than the monitoring stations, and we might accept predictions for other periods when we have data on releases but no monitoring data. But if we used the model to predict deposition of uranium on the ground near the facility without having measurements of uranium concentrations in the soil, for example, we would probably be going beyond the validation exercise that we have described, and although deposition rates are proportional to

air concentrations, the predicted deposition rates would not gain the same credibility from the exercise as the predicted air concentrations.

The interpretation of validation exercises is never entirely clean. Consider once again the example of predicting uranium concentrations in air. Our calculations involve more than the computer program: there are the estimates of the uranium releases, which are subject to error, and there are meteorological data, which may or may not be accurate for the locations and period for which they were applied. It is possible for errors in the data to compensate for errors in the model, giving apparently good results and encouraging us to trust a program that intrinsically might not be an acceptable representation of the processes we are simulating. Alternatively, errors in the data could make an acceptable model look bad. When we must depend on data that are available, it is practically impossible to implement rigorous designs that might remove these confounding effects. We must generally be satisfied with making as many tests of two or more correlated functionalities (e.g., diffusion and deposition, if we have data for both) as possible, in the hope that good agreement of predictions and data will be persuasive at an admittedly subjective level.

There are processes for which validation would require measurements spanning impractically (or impossibly) long time intervals. The rate of removal of plutonium from surface soil is a relevant example for which many years of data — possibly a century or more — at the same set of locations would be required for validating some relevant parameters of RESRAD for Rocky Flats, when the intent is to use scenarios spanning 1000 years.

The computer programs themselves sometimes thwart validation efforts. When the computed results must be interpreted as spatial or temporal averages, and the only data available for comparison are specific to a small part of the assessment domain, or represent only a brief period, then the comparisons may be meaningless. There are instances when the program does not output those quantities that would be used for comparison; this is often the case when the desired endpoint is dose or risk, but for validation, we may need predicted concentrations of radionuclides in air, soil, or water.

We do not wish to convey the impression that we believe the kinds of comparisons usually called *validation* are not important. On the contrary, we include them whenever we believe they can contribute to the level of confidence we and others might have in the application of a computer program that we are using. But we stress the point that in no circumstances should any computer program be considered “validated” in the abstract so that its output is implicitly trusted. In our view, validation is a process involving a specific problem (e.g., an environmental assessment involving specified scenarios and pathways at a particular site), analysts, other interested parties, a computer program, and sets of data that can be interpreted as exogenous inputs, parameter values, and outcomes of processes simulated by the computer program. When the people involved can agree that persuasive correlations of predictions and data have occurred, then we may consider the program to be validated with respect to the processes, data, and other specifics (e.g., location and time) that have been tested, but always bearing in mind that our sense of caution should increase as we apply the program to conditions different from those of the tests. A decisively negative result of a validation process is also a useful result (although often considered an inconvenient one), in that it points to something that is wrong about the program, the data, or the interpretations that have been made; but such a result usually produces further analysis and eventually another set of tests. And we must add that in some cases, a satisfactory validation

(by which we mean that it reaches an accepted result, affirmative or negative) may not be possible.

Given the inherent difficulties of validation, one often has to supplement it with other approaches. Uncertainty analysis, appropriately applied, leads to results that quantify possible errors that derive from lack of knowledge or variability of parameters. Uncertainties about the proper structure of the model are more difficult. The temptation is to try to broaden the "space" of models from which the one in question has been drawn and to extend the uncertainty calculation to a representative set of possible replacements from this space of models (Draper 1995). But this approach has immense conceptual and technical difficulties. A more pragmatic option is to accept model structures that have been affirmatively validated in a variety of similar problems as provisionally correct but with magnitudes of uncertainty indicated by a broad range of experience. For example, in atmospheric diffusion calculations, the straight-line Gaussian plume model is widely used in environmental applications, although this model is based on assumptions that are technically too simple for most of those applications. But experience and experiment indicate that for particular categories of predictive use, the Gaussian plume can be associated with corresponding uncertainty distributions. For example, from a review of numerous sets of experimental data, Miller and Hively (1987) concluded that for flat terrain, away from coastal areas, the Gaussian plume can predict annual averages of concentrations within a factor of two 90% of the time out to a distance of 10 km and within a factor of four with 90% probability somewhat beyond that distance. Such information must be applied with care and skill, but it provides an empirical representation of atmospheric diffusion and some level of confidence in the model; the cost is the stated uncertainty. This illustration, however, should not be interpreted to mean that the straight-line Gaussian plume model is applicable with knowable uncertainty to any atmospheric diffusion problem. It is not, and we know of no model that is.

Some scientists object to the use of the terms *verification* and *validation* (which are sometimes used interchangeably in the sense in which we have used the latter) in connection with numerical models of complicated and incompletely understood open systems (i.e., depending on incompletely specified initial and boundary conditions and exogenous information). Oreskes et al. (1994) criticize definitions given by DOE and the International Atomic Energy Agency (IAEA) in which validation implies that a model or program correctly represents a physical system, and these authors correctly emphasize that such a claim "is not even a theoretical possibility." They would prefer the use of more neutral language, replacing *verification* and *validation* with terms that indicate judgment and contextual interpretation of model performance.

4.2 RESRAD

The U.S. Department of Energy (DOE) and Argonne National Laboratory (ANL) have developed the computer program RESRAD (RESidual RADioactivity) for the purpose of performing calculations related to meeting the Department's criteria for residual radioactivity. The program originally (1989) implemented site-specific guidelines (called soil action levels in this report) based on a dose assessment methodology consistent with DOE Order 5400.5 (DOE 1993).

The most recent version of RESRAD for which we received executable code from ANL (Version 5.82, transmitted to us in October 1998) differs in some important respects from older versions that are still in use; in particular, it differs from the version of RESRAD that was used in the preparation of the action levels document (DOE/EPA/CDPHE 1996). Thus RESRAD is not uniquely defined for this study, and we must distinguish among versions of the program in discussing it and in considering it for possible use. In Sections 4.4.3 and 4.6.3, comparisons of GENII and RESRAD, and DandD and RESRAD, respectively, were made using Version 5.61 of RESRAD.

4.2.1 RESRAD overview

The manual for Version 5.0 (Yu et al. 1993), which was distributed with Version 5.82, does not correspond to the more recent graphic user interface (GUI) implementation. A user's guide for the latter, which is a replacement for Chapter 4 in the manual (Yu et al. 1993) is now available from ANL or from the web site http://www.ead.anl.gov/resrad. DOE has directed ANL to discontinue distribution of RESRAD versions for the DOS operating system, the most recent of which was Version 5.62. Some of the information we received seemed to suggest that there might be incompatibilities of DOS versions with contemporary Windows operating systems. However, we have tested Version 5.61 in a command window under Windows NT and encountered no problems with it. However, a major algorithmic change affecting the Windows versions of RESRAD (beginning with Version 5.75) has been made in the area factor for the resuspension of soil particles (Chang et al. 1998). The difference in predicted doses and soil action levels can be significant. We will discuss the change in a later section.

The manual for RESRAD (Yu et al. 1993 with replacement for Chapter 4) is written with reasonable clarity and is a good compromise between encyclopedic detail (which nevertheless would sometimes prove helpful) and readability. Five chapters (and a sixth of references) provide introductory material, a rather good discussion of the pathway analysis implemented by RESRAD, a definition and discussion of *guidelines* for radionuclides in soil (the RESRAD and DOE term for what this report has called soil action levels), a user's guide for the program keyed to the earlier version 5.0 (for which the previously mentioned replacement is available), and a discussion of the "As Low as Reasonably Achievable" (ALARA) process. A set of appendices provides detailed information on the models and approaches incorporated into RESRAD (some of the information in Appendix B is made obsolete by the presentation of Chang et al. (1998)). A substantial index should be high on the list of priorities for this manual, and we would recommend breaking the user's guide (Chapter 4) into a separate document, which can more easily be kept current with new releases (a replacement for this chapter has been issued for the Windows versions of RESRAD).

The basic model that RESRAD implements is the family farm or homestead with soil and possibly surface water and groundwater contaminated with residual radionuclides. However, pathways (inhalation, external gamma radiation from soil and airborne radioactivity, soil ingestion, drinking water, ingestion of vegetables, meat, and milk) can be individually switched on or off to permit the treatment of other scenarios. RESRAD begins with an assumed initial mixture of radionuclides in an unsaturated soil compartment called the contaminated zone (CZ), which is a slab of finite area that may or may not be isolated from

the surface by a cover layer (for applications at the Rocky Flats site, the contaminated zone has no cover layer; it is assumed to extend from the surface to a depth of 15 cm). In general, the contaminated zone is a proper subregion of the unsaturated zone. The unsaturated zone may be partitioned into as many as five independently parameterized strata to simulate soil zones with different transport characteristics, and the contaminated zone may be contained in one of these layers or intersect two or more of them. Initial radionuclide concentrations of radionuclides in the saturated zone (groundwater) may also be included. RESRAD simulates the removal of radioactivity from the contaminated zone by leaching, moving it vertically into groundwater, and by runoff into streams or ponds. If the water pathway is activated, contamination of drinking water at a central or peripheral well site is estimated, and contaminated groundwater may be mixed with contaminated surface water for drinking, household use, irrigation, and watering livestock.

Radioactivity from the contaminated zone may be resuspended by a mass-loading model; separate resuspension pathways are implemented for inhalation exposure and for foliar deposition on crops and animal fodder. External doses from exposure to gamma emissions from the contaminated zone and the resuspended contaminated soil particles are estimated. Beginning with Version 5.60, the external radiation field calculations incorporated refinements for the finite area and volume (with possibly irregular shape) of the contaminated zone, in contrast to previous methods that assumed semi-infinite distributions of radioactivity in source media (Kamboj et al. 1998).

As we have pointed out in Section 3.1.3, resuspension of contaminated soil at Rocky Flats should not be treated as a routine matter, and there are several approaches that need to be considered. As noted above, versions of RESRAD beginning with 5.75 represent the area factor for resuspension in a more elaborate way that potentially produces dose and soil action level estimates that differ significantly from those of earlier versions. RESRAD does not include a conventional atmospheric transport model for estimating remote air concentrations and foliar deposition (e.g., at locations away from the contaminated zone on the Rocky Flats site), but the manual gives some guidance for carrying out auxiliary calculations if they are required. However, the new approach to the area factor for resuspension (Chang et al. 1998) does make use of the Gaussian plume model, but the use of this model is confined to estimation of the area factor and thus effectively applies the Gaussian plume model only to a receptor at the downwind boundary of the contaminated zone.

Ingestion pathways for crops, meat, milk, and direct ingestion of soil are included in RESRAD, with the assumption that the food for people and fodder for animals are grown in the soil of the contaminated zone. Thus these plants are subject to radionuclide uptake through the roots and surface contamination by foliar deposition by resuspended contaminated soil. The dose conversion factors that are applied to the ingestion pathways correspond, by default, to the most readily absorbed (i.e., most soluble) form of each radionuclide that is available in the database. This means that the largest available value of the gut absorption parameter f_1 is used. For isotopes of plutonium, the RESRAD default assumption is $f_1 = 10^{-3}$, which means that approximately 1/1000 of the plutonium activity that passes through the small intestine is absorbed into body fluids and translocated to systemic organs, principally bone. Less soluble forms of plutonium, such as oxides, would correspond to $f_1 = 10^{-5}$. The analyst can decline the RESRAD default and opt for a dose conversion factor with a smaller value of f_1 from the database (provided one is available;

10^{-5} is available for plutonium). For material incorporated into plant tissue by root uptake, an argument may be made that the process favors an ionic state of the nuclide, but for oxides of plutonium that deposit on plant surfaces, $f_1 = 10^{-5}$ is likely the more realistic choice. However, the assumption of the more soluble form is a common one for screening calculations.

Area factors for crops, meat and milk account for fractions of the quantities consumed that come from inside the contaminated area, as opposed to the remainder, which is assumed to be produced elsewhere and uncontaminated. The default assumption is that at most half of the produce consumed is raised within the contaminated area; for meat and milk the fraction increases linearly to 1.0 as the area of the contaminated zone increases to 20,000 m^2. The analyst can change these default values.

Foliar deposition and retention is based on a simple steady-state model. The deposition rate is computed as the air concentration of radioactivity and a deposition velocity that depends on the assumed physico-chemical state of the material (0 m s^{-1} for relatively inert gases, 10^{-2} m s^{-1} for halogens, and 10^{-3} m s^{-1} for everything else; these values appear to be hardwired into the program). An interception fraction determines how much of the deposition flux is retained on the plant (this value may be changed), and the amount is decreased over the holdup time according to a first-order weathering rate parameter with a default value that corresponds to a half-time of about 2 weeks. The model also depends on the crop yield for the type of food (produce, fodder for meat, or fodder for milk). The air concentration on which this pathway depends is based on a mass loading model that is similar to but evaluated separately from the one for inhalation, because the effective air concentration for inhalation depends on times spent indoors and outdoors.

RESRAD has in common with the other computer programs considered in this report — except MMSOILS — the capability of performing its calculations for radionuclides that belong to possibly long and complex decay chains. This capability involves solving generalizations of the well-known Bateman equations of decay and formation of radioactive progeny, combined with first-order removal of radionuclides and decay products from environmental compartments. Although mathematically routine, the computational details are quite tedious and susceptible to errors from loss of significant digits if the strategy is not carefully managed. For the radionuclides present in the Rocky Flats soils, the decay chains are non-trivial and make ad hoc calculations tedious.

RESRAD also provides virtually exhaustive output, summarizing all input data and database numbers and providing nearly every breakdown of output by pathways, radionuclides, dose, and concentration in media that might be desired.

4.2.2 Code acquisition

Argonne National Laboratory sent us Version 5.82 of RESRAD for Windows October 13, 1998, together with the manual for Version 5.0, with no notification of availability of updated documentation. Our request for the DOS version was declined, in a letter stating that the DOS version was no longer distributed. On October 23, 1998, the Rocky Flats Citizen Advisory Board received the computational part of the source code for Version 5.62, accompanied by a letter to Mr. Tom Marshall, Chairman, from W. Alexander Williams of the DOE Office of Eastern Area Programs, Office of Environmental Restoration, Germantown, MD. In the letter, Dr. Williams states that the computational code for Versions

5.61 and 5.62 is identical. He cautions that Versions 5.61 and 5.62 were written for the DOS operating system and are no longer distributed. Windows versions of RESRAD 5.61 and 5.62, he states, "were available for test and evaluation, [but] these versions may not be compatible with newer releases of the WINDOWS operating system." He alludes to "changes made in RESRAD to accommodate the changing computer platforms." Although the letter emphasizes changes that relate to the compatibility of RESRAD with different versions of the Windows operating system (presumably Windows 3.1 vs. Windows 95/98/NT), it makes no mention of the algorithmic differences between versions 5.62 and later versions beginning with 5.75. As we pointed out in Section 4.2.1, these algorithmic differences affect the resuspension pathway, in particular, and the resulting estimates of dose and soil action levels in potentially significant ways. We were not provided with computational source code for Version 5.75 or later.

We have developed an initial front-end program that performs preliminary calculations related to contemporary levels of plutonium, americium, and their decay products in the soil east of the 903 Pad. This front-end program writes files for RESRAD to read and then initiates the execution of RESRAD. The front-end program can execute RESRAD repeatedly in Monte Carlo fashion to obtain distributions of estimated radionuclide concentrations or annual doses to exposed scenario subjects. This particular front-end program is intended for use with the contemporary (unremediated) levels of radionuclides; variant versions will be prepared that will calculate soil action levels. Such a front-end approach permits us to substitute alternative resuspension mechanisms that RESRAD does not incorporate, as discussed in Section 3.1.3. Details of the front-end programs will be given in the Task 5 report.

If the questions of algorithmic inconsistency between the RESRAD documentation and the program can be resolved satisfactorily, we believe RESRAD can be used as the primary tool for investigating the benchmark (and possibly other) scenarios of use of the Rocky Flats site and the establishment of the relationship between radionuclide levels in the soil and annual dose standards (soil action levels, in particular). Factors that weigh in favor of RESRAD are (1) its continuing support by DOE, (2) its longevity, with a corresponding base of experience and understanding of its strengths and limitations, (3) its extensive well-formatted output, and (4) its design that permits us to separate the calculating engine from its graphic user interface and control it from a front-end scripting program. RESRAD has no monopoly on these features individually, but collectively it achieves a marginal lead over GENII, the other program that was not eliminated from consideration for this project. The inconsistencies in the distributed materials for RESRAD, however, are troubling. The fact that DOE does not choose to make the source code generally available for public inspection is also a negative consideration. If the source code were made available on a web site for downloading, it is our opinion that the useful feedback from a variety of users and programmers would result in developmental improvements and user confidence that would far outweigh whatever concerns the agency might have regarding unauthorized substitutions of code in compliance calculations.

With the reservations noted previously regarding the inter-version changes in mechanical resuspension of contaminated particles, the models offered by RESRAD are generally appropriate for application to the benchmark scenarios defined by the soil action levels document (DOE/EPA/CDPHE 1996) and to others constructed for purposes of

illustration or likely to be proposed as alternatives to the benchmark set. However, as with any environmental models, they should be applied with a healthy amount of skepticism.

Use of RESRAD should not exclude the use of other similar tools or ad hoc programs when their use is indicated for comparisons needed to shed light on questions of the performance of the environmental models. This choice of a tool should not be allowed to substitute a computer program for the underlying mathematical models and scenario definitions, which are paramount. As our comparison of RESRAD and GENII illustrates (Section 4.4.3), more or less equivalent calculations can be performed with a variety of programs or combinations of programs, provided the mechanisms are understood and differences of implementations are properly allowed for. On the other hand, it is entirely possible to make erroneous calculations with the tool of choice. We must stress the continuing involvement of professional people who have experience with environmental assessments, the relevant models, and the appropriate computing tools. Despite the early expectations of the regulatory agencies, it does not seem possible to package all of this knowledge, once and for all, in a canonical computer program and prescribe its parametric application to all sites and situations without further analysis.

4.2.3. Changes in the area factor for resuspension

We have previously alluded to algorithmic changes in RESRAD, beginning with Version 5.75, that affect the resuspension mechanism. Given the importance of resuspension in the Rocky Flats context, these changes are of potentially substantial significance.

Discussion of these changes and the related mechanisms is of necessity somewhat technical. The changes involve the calculation of the area factor, which affects resuspension predictions. The area factor accounts for the dilution of locally contaminated airborne dust by uncontaminated dust resuspended from outside the contaminated area. Larger (smaller) area factors correspond to larger (smaller) predictions of airborne contamination, which would produce larger (smaller) predictions of dose by inhalation and by external exposure to airborne gamma-emitting radionuclides. Bearing these relationships in mind, some readers may prefer to refer primarily to Figure 4.2.3-1 for a sense of the extent to which the changes might reduce RESRAD predictions of air concentration.

To understand the meaning of an area factor for resuspension, we must consider a process of suspension, balanced by deposition, of uniformly contaminated soil that occurs upwind from a receptor location at which we are interested in the air concentration. If the upwind fetch is infinite, we would anticipate a larger air concentration of radioactivity at the receptor point than would occur if the contaminated region were finite (which is what we are assuming in applications of RESRAD). The strategy in RESRAD is to estimate an air concentration that would correspond to an infinite region and correct it by multiplying it by a factor that represents the ratio of concentration due to the finite area divided by the concentration due to an infinite fetch. A value equal to this ratio must, of course, be derived in a round-about way, because the numerator of the ratio is the very concentration that we are trying to calculate. It is this ratio that is called the *area factor* for resuspension.

Before Version 5.75, RESRAD used an area factor (AF) that can be derived from a simple box model of the resuspension and deposition process (see, for example, Hanna et al. (1983), Chapter 9). If $\sqrt{A}$ is taken as the linear dimension of the contaminated region in the

direction of the wind, where A is the area, the ratio defined in the previous paragraph can be shown to be

$$\mathrm{AF} = \frac{\sqrt{A}}{\sqrt{A} + \mathrm{DL}} \qquad (4.2.3\text{-}1)$$

where DL is a dilution length that depends on the deposition velocity, the mean wind speed, and the mixing height (height of the atmospheric layer over which the concentration is averaged). RESRAD generically used a default value of 3 m for the dilution length, although it should be considered a highly variable parameter (3 is the geometric mean of 0.03 and 250 m, corresponding, we are told, to surface roughness and the height of the stable planetary boundary layer, respectively; see Chang et al. (1998)).

In what the developers of RESRAD consider a more refined approach, they have developed an area factor that considers vertical and crosswind diffusion as represented by a Gaussian plume model, with gravitational settling estimated by Stokes's law (using a tilted plume to account for depletion) and wet deposition using a scavenging model. These models introduce additional parameters, such as the size distribution of aerodynamic diameters (1 to 30 μm is the size range considered in studying the variability of the area factor), particle density, rainfall rate, raindrop size, wind speed, and the dispersion coefficients σ_y and σ_z as functions of atmospheric stability and distance from the source. The point source of the Gaussian plume is integrated over the finite contaminated area, while the receptor is kept fixed at the midpoint of the downwind boundary. The corresponding concentration for an infinite area is obtained by increasing the area of the square source region until the receptor concentration converges to a maximum value.

Reference values are assumed for some of the parameters, namely rainfall rate (100 cm year^{-1}), particle density (2.65 g cm^{-3}), atmospheric stability (Pasquill-Gifford class D, which typically occurs almost half of the time), and raindrop diameter (1 mm). The model is represented by a logistic regression curve, which was fitted to data generated by calculations for a grid of points in the parameter space. The function is

$$\mathrm{AF} = \frac{a}{1 + b(\sqrt{A})^c} \qquad (4.2.3\text{-}2)$$

where A is the area of the contaminated zone and each of the parameters a, b, and c is a function of the particle diameter (μm) and wind speed (m s^{-1}). The functional correspondence for a, b, and c is shown in Table 4 of Chang et al. (1998).

Wind speed is available as an input to RESRAD, but particle aerodynamic diameter is not. The dose conversion factors for inhalation in the RESRAD database are based on activity median aerodynamic diameter 1 μm, and the RESRAD developers have chosen to fix the particle size parameter at this value for the present. Chang et al. (1998) compare the old and new area factors (Equations 4.2.3-1 and 4.2.3-2, respectively) in a series of plots in their Figure 5, for values of the particle diameter ranging from 1 μm to 30 μm. Using the plot corresponding to 1 μm and the curve for wind speed = 5 m s^{-1} (the average for the Denver area is about 4 m s^{-1}), with a contaminated area of 10^4 m^2, the old factor exceeds the new by roughly a factor of 6; for 100 m^2, the old area factor is more than 10 times the new one. Lower wind speeds correspond to lesser discrepancies, and higher wind speeds would give larger ones. Larger areas would correspond to better agreement between the two area factors.

Figure 4.2.3-1 shows a comparison of the old and new area factors for particle diameter 1 μm plotted against $\sqrt{A}$ for several values of the wind speed.

In reading the documentation of Chang et al. (1998), we could not be certain that the distinction between physical and aerodynamic particle diameters was being consistently observed. In the form of Stokes's law that is quoted, the physical diameter is the correct interpretation. But if the tabulations are then based on physical particle diameters, a physical diameter of 1 μm would not correspond to an activity median aerodynamic diameter of the same numeric value, but rather to a median diameter of about $\sqrt{2.65}\ 1.6$ (given the assumed density of the particles). The language should be clarified.

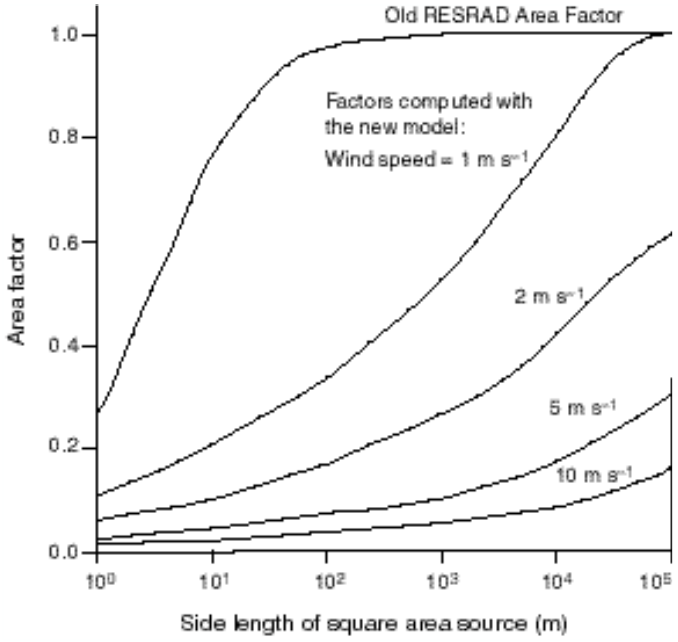

Figure 4.2.3-1. Comparison of the old and new RESRAD area factors for particle size 1 μm, plotted against the side length of a square contaminated area. The new area factor is shown for several values of the wind speed. This figure was redrawn from Chang et al. (1998).

A potentially more serious criticism concerns the generic use of this area factor in assessments at various locations with different circumstances. Perhaps in anticipation of this point, Chang et al. (1998) present a series of sensitivity calculations, varying pairs of parameters, and showing results separately for particle diameters 1, 10, and 30 μm. The variable pairs are wind speed and rainfall rate; wind speed and particle density; and wind speed and atmospheric stability. In each case, the relative area factor (perturbed divided by nominal) is plotted against the side length of the area source. The greatest variations from the nominal case occur for variations involving particle density (from 1.325 to 5.– [illegible] g cm^{-3}) and for high wind speeds in unstable air. Most variations of the relative area factor are within a factor of two, and none is as large as a factor of three.

The presentation of this sensitivity analysis may tempt a reader to the conclusion that the uncertainty introduced into resuspension-dependent quantities by the area factor is some composite of the variability shown in the figures. However, the sensitivity analysis

demonstrates only the propagation of parameter variations; it does not necessarily deal with uncertainty in the models themselves relative to the real environment. For example, Miller and Hively (1987) reviewed numerous applications of the Gaussian plume model to cases where such variables as the release rate, wind speed, atmospheric stability, and downwind concentrations were monitored or could be considered known. At best, the predicted annual-average concentrations agreed with the observations to within a factor of two when the terrain was regular and the meteorology unexceptional (i.e., $0.5 \leq$ predicted / observed ≤ 2); in cases of irregular terrain or (for example) coastal meteorology, the reported annual-average uncertainty was a factor of ten. Generic application of a Gaussian plume model should involve consideration of these uncertainties. Of course, the application of the Gaussian plume to the area factor differs in scale and detail from conventional predictions of concentration downwind from a source, and in some part the uncertainty may derive from parametric uncertainties, but it seems to us that we cannot assume *a priori* that the model is intrinsically more reliable for deriving the area factor than the study of Miller and Hively (1987) has shown it to be for conventional applications.

Another point that can be raised regarding the models used to derive the area factor is that the representation of dry deposition by the Stokes's-law gravitational settling model is at best an approximation that ignores the partial dependence of the particle behavior on micrometeorological variables. For particles with aerodynamic diameter near 1 μm, Stokes's law may not be an adequate parameter for total deposition for purposes of the area factor.

It is not our intent to criticize the RESRAD developers. The models and parameters that they have applied to estimate the area factor are well known and frequently invoked. Their approach is rational from a research standpoint, their analysis seems thorough, and we are appreciative of the well-organized numerical explorations they have provided in Chang et al. (1998). Our reservations have more to do with objections to generic application of assessment models. The developers consider this formulation of the area factor more realistic than the older version that was based on a simple box model (Equation 4.2.3-1), and that may be true. But in any assessment, the analyst should be weighing the appropriateness of any factor that enters into the calculations for the site in question and integrating each factor into the composite uncertainty picture. We certainly agree with the last sentence in Chang et al. (1998): "However, if measurement data are available, the measured air concentrations [*sic*] data should be used in RESRAD analysis." The user's manual should clarify just how this is to be done; we assume it would involve supplementary off-line calculations based on RESRAD output. We will be making use of such measurements in the calculations for Task 5.

In general, one can expect Versions 5.75 and newer of RESRAD to predict lower annual resuspension-dependent doses and correspondingly larger radionuclide soil action levels, with the extent of the discrepancy depending on the values supplied for the mean wind speed and the area of the contaminated zone. For application to the Rocky Flats site, we cannot make a more definite statement at this time, until an appropriate area for the field of contamination is determined. In regard to the version of RESRAD that will be applied, there is some ambiguity about the intentions of the regulatory agencies. The soil action level document (DOE/EPA/CDPHE 1996) presents RESRAD parameters and computed soil action levels that appear to correspond to an earlier version of the code (perhaps 5.61 or 5.62). This was probably the most recent version available at the time that document was prepared. But if the assessment were to be carried out in a purely formal manner, with the newer

version of the code being substituted and executed with the same set of parameters, the foregoing analysis indicates that a possibly important change in the predictions would occur.

4.3 MEPAS

The Multimedia Environmental Pollutant Assessment System (MEPAS) was developed at Pacific Northwest Laboratory under DOE sponsorship. Offered as a commercial product by Battelle Memorial Institute under a technology-transfer agreement with DOE, MEPAS is the most ambitious of the programs considered here. It advertises applicability to both chemical and radioactive pollutants, with computation of human health risk for carcinogens and hazard quotients (sometimes called hazard indices) for noncarcinogens. MEPAS includes air transport models in addition to surface water and groundwater transport, and it treats all major exposure pathways (Buck et al. 1995). As we mentioned in Section 3.1.3, MEPAS incorporates variants of the EPA models for particulate suspension by mechanical and wind-driven erosion (Battelle Memorial Institute 1997). The MEPAS documentation that we have reviewed does not indicate an intrinsic Monte Carlo capability for uncertainty analysis.

Battelle Memorial Institute declined our request for permission to examine portions of the MEPAS source code. Absent special instructions, such access would be necessary to allow us to discover how to circumvent the graphic user interface and prepare a front-end interface program to provide Monte Carlo simulations and initial calculations. Accordingly, we cannot give further consideration to MEPAS at this time for application to the Rocky Flats site soil contamination. This decision was taken for reasons of practical necessity; it does not deny the potential applicability of the MEPAS models to the problems we are considering. However, it is not clear that MEPAS would offer any decided advantage over RESRAD or GENII for the specific calculations that we are considering. The wealth of models and options that MEPAS offers would likely be wasted, for the most part.

Considerable effort has gone into benchmarking MEPAS with RESRAD and MMSOILS (Laniak et al. 1997; Mills et al. 1997). In response to our request for source code access, we were sent the report of Cheng et al. (1995), which presumably is a more detailed account of the work reported by Laniak et al. (1997) and Mills et al. (1997), and what appears to be a prepublication copy of a report without a cover page, with the title *Test Plan and Baseline Testing Results for the MEPAS Saturated Zone (Aquifer) Transport Model*. These reports did not reach us in time to permit a proper examination of them, and we do not comment further on them at this time.

4.4 GENII

At the direction of the U.S. Department of Energy in 1988, the Hanford Environmental Dosimetry Upgrade Project was undertaken by Pacific Northwest Laboratory to incorporate the internal dosimetry models recommended by the International Commission on Radiological Protection into updated versions of the environmental pathways models used at Hanford. The resulting second generation environmental dosimetry computer codes were compiled in the Hanford Environmental Dosimetry System — Generation II or GENII (Napier et al., 1988). The GENII system was developed by means of tasks designed to provide a state-of-the-art, technically peer-reviewed, documented set of programs for calculating radiation doses from radionuclides released to the environment.

4.4.1 Code overview

The GENII system was designed to address exposure and dose resulting from both routine and accidental releases of radionuclides. Doses may be calculated on an annual, committed, or accumulated basis. Transport pathways include air, soil, biotic, surface water, and to a limited extent, drinking water. Pathways of exposure include direct or external exposure via water (swimming, boating, and fishing), soil (surface and buried sources), and air (semi-infinite and finite infinite cloud geometries), inhalation pathways, and ingestion pathways. The inhalation pathway includes direct inhalation of material released to the air from a facility or operation, and inhalation of resuspended contamination from the soil. Ingestion pathways include soil, and transfer of radioactivity from soil to food products (produce, milk, meat, and poultry), and contaminated drinking water.

GENII includes options for calculating both near-field and far-field (some refer to near-field as onsite and far-field as offsite) exposure scenarios. In a near-field scenario, the focus is on the doses an individual could receive at a particular location as a result of initial contamination or external sources at that location. A far-field scenario considers the doses received by an individual or a population exposed to radioactivity that has been released and transported from a location remote from the receptor. The two types of scenarios are not mutually exclusive, and any given scenario may have components of both the near- and far-field scenarios.

The proposed soil action levels developed for the RFETS are essentially based on a near-field scenario. The RESRAD code is not capable of addressing directly what GENII defines as a far-field scenario, and therefore, GENII appears to have an advantage as a model that may provide dose estimates to off-site individuals. Far-field scenarios in GENII include chronic and acute atmospheric releases, and chronic and acute surface water releases. Doses from ingestion of contaminated groundwater may be calculated in GENII, but groundwater concentrations must be computed externally to the code, using a model suited to that type of computation or direct measurements.

Source term input to GENII may be in the form of effluent release rates to various environmental media (air, soil, or water), or initial contamination levels in these media. The code allows for environmental transport calculations to be performed externally to GENII and the results input by way of a dispersion factor or a user-defined concentration value in an environmental medium. Radioactive decay and formation of decay products are handled within the code. Half-lives, dose conversion factors, and animal and plant uptake factors are stored for a library of 251 nuclides. In addition, the decay chain is automatically constructed once a parent nuclide is selected, and decay and formation of progeny are calculated for the entire decay chain over time.

The GENII package of codes was developed under a stringent QA plan based on the American National Standards Institute (ANSI) standard NQA-1 (ASME 1986) as implemented in the PNL Quality Assurance Manual PNL-MA-70[1]. All steps of the code development have been documented and tested. Extensive hand calculations have been performed and are available for review on request

[1] Procedures for Quality Assurance Program, PNL-MA-70. This is a controlled document used internally at PNL. Information regarding the manual may be obtained from Pacific Northwest Laboratories, Richland, Washington.

4.4.2 Code features relevant to calculating soil action levels for Rocky Flats

GENII models the same pathways that are included in the RESRAD simulations that were used in the soil action levels document (DOE/EPA/CDPHE 1966). These pathways are resuspension and inhalation of contaminated soil, inadvertent soil ingestion, transfer of radioactivity into homegrown produce and animal products, and external exposure of the subject to surface soil contamination and contaminated airborne particles. Two resuspension models are available in GENII: a mass loading approach that is similar to the one in RESRAD Versions prior to 5.75, and a time-dependent method developed by Anspaugh et al. (1975). The Anspaugh model was calibrated to empirical data that showed a decrease in the amount of resuspended material over time. It appears that the Anspaugh model is not applicable to the Rocky Flats environs because it applies only to the first 17 years following a deposition event. In the case of the soil at Rocky Flats, the contamination has been there for more than 30 years.

External exposure in GENII is calculated using a modified version of the ISOSHIELD code (Engel et al. 1966). The ISOSHIELD code uses the commonly accepted techniques of Rockwell (1956) or other standard references for computing exposure rates from isotopes distributed in various geometric configurations. The calculation considers the initial photon, energy spectrum, material properties in the source region, air, and any shielding materials placed between the source and receptor (such as a cover layer of soil), and mass attenuation and build-up within the source and shield materials. Exposure rates (in Roentgen per hour) are converted to effective dose equivalents using the energy-dependent surface-dose to organ-dose conversion factors derived from information in Kocher (1981). Organ weighting factors were obtained from ICRP 26 (ICRP 1977).

Two models are available for ingestion of contaminated crops. These models are a chronic exposure model and an acute exposure model. The chronic exposure model assumes a constant source of contamination released to the model domain. The acute model assumes an initial contamination level in soil and water that is not replenished over time. The acute model appears to be appropriate for the Rocky Flats site, because the site will be shut down and release no additional radioactivity (other than what is currently present) to the environment. The acute model of GENII is conceptually similar to the PATHWAY model (Whicker and Kirchner 1987) but uses fewer inputs. It includes the processes of root uptake, recycling of contamination on the plant surface with the surface soil, redistribution due to tilling, and translocation of contamination from non-edible to the edible portions of the plant. GENII also includes models for calculating transfer of radioactivity from the soil to animals and animal products, such as milk meat, eggs, and poultry. These pathways were not considered in the original conceptual model defined for the proposed soil action levels, but it is conceivable that alternative scenarios might include them.

GENII also considers an on-site groundwater pathway like RESRAD. However, RESRAD computes transport from the source, through the vadose (unsaturated) zone, and into the aquifer while GENII only allows the user to input a previously measured or modeled groundwater concentration, and dose calculations are performed on that basis. In RESRAD, the groundwater model consists of relatively simple representations of subsurface aqueous flow and transport and does not consider off-site transport of contamination in the aquifer.

The internal dose conversion factors provided in GENII are calculated based on the models for dosimetry reported in ICRP Publication 30 (ICRP 1979–1982). These models for

dosimetry were coded into the INTDF code to allow for dose to be calculated on an annual (as opposed to committed) basis for different commitment periods. While this is an important feature of the GENII code, the need to calculate dose at this level of detail is not necessary for meeting the dose requirements for soil action levels. The annual dose limit specified for the soil action levels includes the 1-year effective dose equivalent from external radiation sources and the 50-year committed effective dose equivalent from one year's exposure to internal (inhalation and ingestion) sources. Therefore, only the dose conversion factors representing the 50-year committed dose equivalent are needed for this calculation.

4.4.3 Code acquisition and testing

The GENII computed dose system and documentation, version 1.485 was obtained from the Radiation Safety Information Computational Center (RSICC) at Oak Ridge National Laboratory. The code was written in FORTRAN, and source code was provided in the distribution. The code was installed on a personnel computer running under Windows 95© and MS DOS© version 6. Primary input to the GENII software package is through an ASCII input file that may be prepared using a menu-driven pre-processor written in BASIC called APPRENTI. Other files containing dose conversion factors, environmental transport factors, and default parameter values are required for execution and are stored in the GENII default subdirectory. These files may be modified by the user using a standard ASCII text editor.

In order to test the code and observe its performance, we set up a GENII simulation assuming the same conceptual model that was used to define the proposed soil action levels for the resident exposure scenario at the Rocky Flats site (DOE/EPA/CDPHE 1996). These results could then be compared to the RESRAD Version 5.61 results, permitting us to highlight differences in the transport, exposure and dosimetry models used between the two codes. Key input parameters applicable to both codes are described in Table 4.4.3-1. Dose conversion factors used in GENII assumed the same lung clearance class and gut absorption fraction as in the RESRAD simulations used to develop the soil action levels reported in DOE (1996). This required several GENII simulations, because in any given GENII simulation, all radionuclides are assumed to have the same lung clearance class and gut solubility. Plant-to-soil concentration ratios were left at their respective default values for each code. Results were normalized to their dose per unit concentration in surface soil (mrem (pCi $g^{-1})^{-1}$) or their dose-to-soil ratio (*DSR*) for ease of comparison.

Table 4.4.3-1. Key Input Parameters for the Proposed SAL Conceptual Site Model[a]

Parameter	Value	Units
Area of contamination[b]	>1250	m^2
Thickness of contaminated zone	0.15	m
Density of contaminated zone	1.8	g cm^{-3}
Time of assessment (time after institutional control)	0	years
Inhalation rate	7000	m^3 y^{-1}
Mass loading factor	2.65×10^{-4}	g m^{-3}
External gamma shielding factor	0.8	---
Fruits, nonleafy vegetables & grain consumption	40.1	kg y^{-1}
Leafy vegetable consumption	2.6	kg y^{-1}
Soil ingestion rate	70	g y^{-1}
Lung clearance class for americium	W	---
Lung clearance class for plutonium and uranium isotopes	Y	---
Gut absorption fraction, plutonium isotopes	1.0×10^{-5}	---
Gut absorption fraction, americium isotopes	1.0×10^{-3}	---
Gut absorption fraction, uranium isotopes	5.0×10^{-2}	---
Mass loading for foliar deposition	1.0×10^{-4}	g m^{-3}

[a.] from DOE (1996), Attachment I

[b.] Area of contamination in GENII is only defined in terms of less than or greater than 1250 m^2

The results (Tables 4.4.3-2 and 4.4.3-3) indicate that there is not much difference between the *DSRs* calculated with the two codes for the inhalation and ingestion pathways. However, significant differences were noted for the external exposure pathway and in particular, for ^{238}U and ^{241}Pu. The *DSRs* for these two nuclides were significantly smaller for the GENII simulations compared to those of RESRAD Version 5.61. It is not clear whether these differences were due to the photon transport and attenuation models employed in the codes or the methodology to convert exposure rate to effective dose equivalent. Differences as high as 12.4% were also noted in the ingestion pathway for uranium and americium isotopes. These differences may be attributed to differences in the terrestrial food chain models and perhaps to a smaller extent to the dose conversion factors used. The inhalation pathway showed the least amount of difference between the *DSRs* calculated with the two codes. The maximum difference between GENII and RESRAD *DSRs* was 2.9% for ^{242}Pu. Because both codes use virtually identical resuspension models that make use of the mass loading factor, the difference between the two results can mostly be attributed to their respective dose conversion factors. In terms of the *DSR* for all pathways of exposure (external, inhalation, and ingestion), differences >5% were noted only for the uranium isotopes. For the most part, RESRAD provided a more conservative estimate of dose, except for ^{241}Am and ^{234}U, where GENII ingestion doses were higher compared to those calculated by RESRAD. In general, inhalation was the dominant pathway; however ingestion was equally important for the uranium isotopes. According to RESRAD Version 5.61, external exposure was the most important pathway for ^{238}U.

Table 4.4.3-2. Dose-to-Soil Ratios (*DSR*, mrem (pCi $g^{-1})^{-1}$) for RESRAD V. 5.61 and GENII

Radio-nuclide	RESRAD				GENII Results			
	External	Inhalation	Ingestion	Total	External	Inhalation	Ingestion	Total
Am-241	.0344	.0811	.282	.397	.0230	.0800	.310	.413
Pu-238	.00012	.0526	.00384	.0566	.00010	.0520	.00370	.0558
Pu-239	.00023	.0563	.00401	.0605	.00022	.0550	.00380	.0590
Pu-240	.00012	.0563	.00401	.0604	.00010	.0550	.00380	.0589
Pu-241	.00001	.00091	.00006	.00098	2×10^{-10}	.00089	.00006	.00095
Pu-242	.00010	.0536	.00381	.0575	.00008	.0520	.00360	.0557
U-234	.00032	.0241	.0249	.0493	.00030	.0240	.0280	.0523
U-235	.583	.0225	.0235	.629	.390	.0220	.0260	.438
U-238	.100	.0216	.0237	.145	.00014	.0210	.0260	.0471

Table 4.4.3-3. Percent Difference[a] Between the DSRs for RESRAD V. 5.61 and GENII

Radionuclide	External	Inhalation	Ingestion	Total
Am-241	33.10%	1.40%	−10.06%	−3.98%
Pu-238	16.67%	1.20%	3.60%	1.39%
Pu-239	3.51%	2.29%	5.20%	2.49%
Pu-240	14.38%	2.29%	5.20%	2.51%
Pu-241	100.00%	1.82%	7.20%	3.62%
Pu-242	17.32%	2.89%	5.44%	3.09%
U-234	4.76%	0.50%	−12.39%	−5.98%
U-235	33.07%	2.14%	−10.61%	30.33%
U-238	99.86%	2.64%	−9.79%	67.57%

a. [(DSR (RESRAD) – DSR (GENII)]/DSR (RESRAD)

4.5 MMSOILS

Developed for screening analysis of hazardous waste sites, MMSOILS was developed by the EPA's Office of Research and Development, National Exposure Research Laboratory, Ecosystems Research Division, Regulatory Support Branch and is currently available from EPA's web site in Version 4.0. Written in FORTRAN-77 and distributed with full source code and documentation, the MMSOILS program may be implemented under Windows or Unix operating systems. The accompanying documentation, which includes a user's guide and descriptions of the models, is detailed and extensive (EPA 1996).

The MMSOILS goal is estimation of human exposure and health risk from chemically contaminated hazardous waste sites. Collectively, the models of MMSOILS provide a multimedia tool that simulates chemical transport in the atmosphere, soil, surface water, groundwater, and the food chain. It treats inhalation of airborne volatile and particulate materials, drinking contaminated water, ingestion of soil, and consumption of crops and animal products that were produced on contaminated land. The program includes a Monte

Carlo mechanism for propagating parameter uncertainties into estimates of exposure and risk. MMSOILS has been benchmarked with RESRAD and MEPAS (Laniak et al. 1997; Mills et al. 1997).

It is possible to apply MMSOILS to radionuclides in the soil, but the program has no mechanism, beyond simple radioactive decay, for dealing with decay chains. Allowing for the possibility that we might be able to simulate this mechanism by pre- and post-processing methods, we included MMSOILS in the list of programs to be considered. But as a practical matter, given the time constraints of this project, such an approach would not be satisfactory. In these circumstances, we must rule out the use of MMSOILS for estimating dose and developing soil action levels for the Rocky Flats site.

4.6 DandD

The software package *Decontamination and Decommissioning* (DandD) was designed by the U.S. Nuclear Regulatory Commission (NRC) as a user-friendly analysis tool for NRC rulemakers and facilities under NRC regulation seeking decommissioned status. The code incorporates the information contained in NUREG/CR-5512, Volume 1, and helps NRC licensed facilities determine the level of cleanup required to allow the release of their property for unrestricted use.

4.6.1. Code overview

DandD was designed as a screening level analysis program to provide a simplified estimate of the dose to an average member of a carefully specified critical screening group (Daily 1999). The estimate is designed to be "prudently conservative" but is not designed to be used as an estimate of actual dose (NRC 1992).

The DandD code includes four exposure scenarios: building renovation, building occupancy, drinking water, and residential. For the residential scenario, the pathways included are external exposure, inhalation, drinking water ingestion, ingestion of food grown from irrigated water, land-based food ingestion, soil ingestion, and fish ingestion. The pathways are hard-wired into the scenarios and can only be removed from consideration by zeroing the annual intake of any given product.

Input parameters for each of the DandD scenarios have default values that were selected in such a way as to be "prudently conservative" (NRC 1992). The default values were chosen for a select and limited population group, and are not intended to represent the average over an entire population. DandD does allow modification of each parameter value within a limited range. Parameter values that are outside the range of allowed values are not accepted as input to the code. These ranges were selected using an analysis done by Sandia National Laboratory in 1997 and 1998. NRC warns that use of this conservative generic approach requires a great deal of professional judgment and common sense (NRC 1992). The intent of the code is to account for the majority of potential land and structural uses, and the code is designed to overestimate the most probable annual dose.

Doses calculated with DandD are total effective dose equivalent (TEDE) estimates, which include annual effective dose and committed dose equivalent during each year. The dose reported in the output of the calculation is the committed dose for the year of maximum total committed dose. This is comparable to the dose limit input in RESRAD (e.g. for the Rocky Flats calculation, 15 or 85 mrem according to the scenario being considered).

Source term input to DandD is strictly in the form of initial concentrations of radionuclides in soil. Radioactive decay and progeny ingrowth are calculated within the code. Half-lives, dose conversion factors, and organ specific dose conversion factors are not available as inputs within the code and remain fixed throughout the calculations. In keeping with the "prudently conservative" goal of the code, the chemical form of the radioactive material that would confer the largest dose is assumed to exist in all cases. For plutonium, this means that the most soluble form of plutonium is assumed, and the dose conversion factors used by DandD correspond to this form (clearance class W for inhalation and $f_1 = 10^{-3}$).

It is important to point out that DandD is in Version 1.0 and has not yet undergone extensive scrutiny or use. Documentation that accompanies the code has not been published, nor has the source code been publicly released. This makes it difficult to use the code and even more difficult to make confident statements about how the code functions. The release of this documentation is not scheduled to occur within a time that would allow consideration of DandD for use in this project. *RAC* has requested and awaits receipt of all code documentation and source code material upon its publication.

We have gone forward with our analysis of this code in a limited fashion to show some of the limitations of the code in its present form for application to this project.

4.6.2. Code features relevant to calculating soil action levels for Rocky Flats

DandD models most of the same pathways as RESRAD, but some of the details about the pathway analyses have been difficult to determine without supporting documentation.

Resuspension and inhalation of contaminated soil are modeled in DandD using a mass loading model that appears to be similar to the one in RESRAD Versions earlier than 5.75, but using an additional level of detail. DandD partitions residential scenario annual activity into three different categories that are accompanied by three different mass loading factors and three different breathing rates. The three categories are indoor, outdoor, and outdoor gardening. We do not have information about how area factors are handled.

The contamination of vegetables, fruits, and roots is represented by two mechanisms: foliar mass loading of resuspended soil and root uptake of contaminated soil. The most significant difference between the way RESRAD and DandD model contamination of food products from contaminated soil has to do with the soil to plant resuspension and deposition pathway.

DandD assumes a constant ratio between radionuclide concentrations in plants and soil, using a default mass loading value of 0.1 pCi g^{-1} dry plant per pCi g^{-1} dry soil. This parameter value means that plant foods are assumed to be 10% soil by weight, a rather high estimate. DandD further applies a translocation fraction of 1.0 for contamination deposited on leafy vegetables, which means that all of the soil deposited on the leaves is integrated into the edible portions of the plant.

The RESRAD model assumes a constant deposition rate with removal controlled by a first-order weathering constant (NRC 1998). The deposition and removal are assumed to occur over the entire growing season. For radionuclides without a high degree of root uptake, like plutonium, the mass loading factor in DandD dominates the ingestion dose and the total dose for the year of maximum dose. This factor seems to be controlling the dose from

radionuclides without a high degree of root uptake and causing doses calculated with DandD to be higher than those calculated with RESRAD.

4.6.3. Code acquisition and testing

The DandD Version 1.0 windows-based executable file was downloaded from the NRC web site. Supporting documentation has been requested from NRC but not yet received. The code was written in the FORTRAN programming language, and *RAC* expects to receive the source code upon its release for public distribution later this month. Input to the DandD code is provided by the user through a graphic user interface.

To test and observe the performance of the DandD code, we attempted to reproduce the hypothetical residential scenario used at Rocky Flats to calculate soil action levels (DOE 1996). This was somewhat difficult to do, as a result of the variant definitions of inputs between the two codes and the fact that some parameters used in the Rocky Flats analysis were outside the allowed distributions of parameter values in DandD or were treated as constants by DandD and could not be altered. The difference between the results are highlighted below, but the reasons are not always known, since the documentation has not yet been published and the models are not transparent.

Table 4.6.3-1 shows some of the key parameters used in each calculation. Since the DandD code uses Class W (soluble) plutonium for inhalation and a gut adsorption fraction for ingestion of 10^{-3}, the Rocky Flats RESRAD calculation was changed so that solubility class matched the DandD values (RESRAD Version 5.61 was used). This was the only change necessary to make in the Rocky Flats calculation. All further changes were made to the DandD input parameters.

Because it is not possible to inactivate pathways in DandD the way it is in RESRAD, a number of parameters were set to zero to simulate this. To match the DOE Rocky Flats RESRAD calculation, the parameters that control the pathways for meat, milk, poultry, and aquatic food ingestion, as well as the ground and surface water pathway, were set to zero.

Table 4.6.3-1. Key Input Parameters for the RESRAD V 6.1 to DandD Comparison

Parameter	RESRAD value	DandD value
Thickness of contaminated zone	0.15 m	0.15 m
Density of contaminated zone	1.8 g cm^{-3}	1.8 g cm^{-3}
Time of assessment (after shut down)	0	0
Inhalation rate	7000 m^3 y^{-1}	0.8 m^3 h^{-1}[a]
Mass loading factor for inhalation	2.65 x 10^{-5} g m^{-3}	2.65 x 10^{-5} g m^{-3}
Fruit, nonleafy vegetables & grain consumption	40.1 kg y^{-1}	40.1 kg y^{-1}
Leafy vegetable consumption	2.6 kg y^{-1}	2.6 kg y^{-1}
Soil ingestion rate	70 g y^{-1}	0.095 g day^{-1}[b]
Lung clearance class, americium	W	W
Lung clearance class, plutonium isotopes	W	W
Lung clearance class, uranium isotopes	Y	Y
Gut adsorption fraction, americium	1.0 x 10^{-3}	1.0 x 10^{-3}
Gut adsorption fraction, plutonium isotopes	1.0 x 10^{-3}	1.0 x 10^{-3}
Gut adsorption fraction, uranium isotopes	5.0 x 10^{-2}	5.0 x 10^{-2}

[a]DandD input units shown; this converts to the same value as the RESRAD parameter.
[b]DandD input units shown; this converts to half the RESRAD parameter, but DandD parameter distributions would not allow the RESRAD value, so the calculation was run with this input and soil ingestion dose from DandD was multiplied by 2.

An important parameter that could not be reconciled between the two codes is the mass loading for foliar deposition. As described above, the pathway for contamination of plants from resuspension of contaminated soil is quite different between the two models. In creating dose to soil concentration ratios for RESRAD and DandD for Table 4.6.3-2, the DandD code was run twice for each radionuclide using the above parameters. In the second run, the value for the foliar mass loading was reduced from the default value by a factor of 10 to display the large effect that this parameter has on the outcome of the calculation. Foliar mass loading in DandD is in units of picocuries per gram of dry plant matter per picocurie per gram of dry soil. The impact of this change on the dose to soil concentration ratio is shown in Table 4.6.3-2. Even with the factor of 10 reduction, the total dose to soil concentration ratios are still significantly higher for DandD than RESRAD. Table 4.6.3-3 shows the percent difference between the dose to soil concentration ratio for RESRAD and DandD.

Without the appropriate documentation, it is not possible for us to acquire a proper understanding of the models and parameters employed in DandD. This lack of available documentation precludes further consideration of DandD in this analysis.

Table 4.6.3-2. Dose-to-Soil Concentration Ratios (DSR, mrem (pCi $g^{-1})^{-1}$) for RESRAD and DandD

			RESRAD		
Radionuclide	External	Inhalation	Plant ingestion	Soil ingestion	Total
Am-241	.0344	.0796	.0269	.255	.396
Pu-238	.00012	.0703	.0237	.224	.318
Pu-239	.00023	.0769	.0262	.248	.351
Pu-240	.00012	.0769	.0262	.248	.351
Pu-241	.000015	.00148	.00051	.0048	.0068
Pu-242	.00010	.0737	.0249	.235	.334
U-234	.00032	.0237	.0051	.0198	.0489
U-235	.583	.0221	.0048	.0187	.628
U-238	.100	.0212	.0049	.0188	.145

			DandD			
Radionuclide	External	Inhalation	Plant ingestion (ML = 0.1)	Plant ingestion (ML = 0.01)	Soil ingestion	Total (ML = 0.01)
Am-241	.0443	.147	4.3	.445	.252	.89
Pu-238	.00015	.13	3.75	.37	.222	.73

Pu-239	.00029	.142	4.17	.419	.246	.81
Pu-240	.00029	.142	4.17	.419	.246	.81
Pu-241	.00005	.00279	.0829	.00834	.00484	.016
Pu-242	.00013	.136	3.96	.398	.232	.77
U-234	.00041	.0439	.347	.0472	.0297	.11
U-235	.748	.0407	.328	.0445	.0186	.85
U-238	.11	.0393	.329	.0446	.0185	.22

Table 4.6.3-3. Percent Difference[a] Between the DSRs for RESRAD and DandD

Radionuclide	External	Inhalation	Plant ingestion (ML=0.1)	Plant ingestion (ML=0.01)	Soil ingestion	Total (ML=0.01)
Am-241	−28.8%	−84.7%	−15800%	−1550%	1.18%	−125%
Pu-238	−26.7%	−84.9%	−15800%	−1490%	0.89%	−129%
Pu-239	−20.6%	−84.7%	−15800%	−1490%	0.81%	−131%
Pu-240	−145%	−84.7%	−15800%	−1490%	0.81%	−131%
Pu-241	−263%	−88.5%	−15800%	−1490%	−1.04%	−136%
Pu-242	−27.5%	−84.5%	−15800%	−1490%	1.28%	−131%
U-234	−28.9%	−85.2%	−6690%	−824%	0.51%	−125%
U-235	−28.3%	−84.2%	−6690%	−821%	0.54%	−35.4%
U-238	−13.0%	−84.9%	−6690%	−818%	1.59%	−51.7%

[a][DSR(RESRAD) – DSR(DandD)] / DSR(RESRAD)

5. CONCLUSIONS AND RECOMMENDATIONS

It seems clear from the tests and comparisons reported in Section 4 that either RESRAD or GENII could be adapted for purposes of the project. Because of its earlier stage of development and still limited documentation, DandD cannot be counted on in the time available for this project. In addition, the strong orientation of DandD to screening calculations would make it less suitable for the kind of assessment that is envisioned for Rocky Flats. MEPAS and MMSOILS were ruled out on other practical grounds.

RESRAD and GENII are based on similar models, for the most part, and the agreement of their results for the same scenario is not really surprising. The change in the RESRAD area factor for resuspension beginning with Version 5.75 is a complication. We have confined our comparisons to pre-5.75 versions of RESRAD. It is possible to circumvent the resuspension area factor with the earlier versions of RESRAD, thereby permitting the substitution of other resuspension models, but this may be more complicated with the new algorithm.

We want to emphasize one last time that none of these computer programs can guarantee the "right answer." It could be argued that there is no such thing. These programs are tools, which, in the hands of careful analysts, can be useful for carrying out the relevant computations for an assessment, or when used in the absence of proper analysis can produce misleading information. It now appears that either RESRAD or GENII applied with experience, skill, careful consideration of site conditions and data, and with proper interpretation and communication of the results, can help to complete a persuasive assessment of the RFETS. Analysts will have make adjustments for the differences in the two programs, but used properly, they should lead to similar results. RESRAD provides a more complete listing of database quantities in its output, and some of its defaults regarding inhalation solubility classes and gut absorption factors for the radionuclides considered in a run are more easily changed by the operator. For the assessment at hand, it seems fair to say that RESRAD is the more convenient tool, but GENII may have conceptual or operational advantages in other situations.

When RESRAD is applied to the resuspension pathway, we recommend that it be with full awareness of the effect of the area factor. As we mentioned in Section 3.1.3, measured air concentrations of some of the radionuclides in the source term are available, and careful consideration should be given to using these measurements or calibrating the model to them. This approach may require manipulating the input parameters so that the area factor is effectively 1. Similar manipulations will be required if alternative resuspension models are to be substituted. With some auxiliary calculation, it may also be possible to make RESRAD more useful for application to off-site scenarios.

We want to suggest that everyone concerned with this assessment pay less attention to soil action levels and instead concentrate on the relationship between particular measured or hypothetical sets of radionuclide concentrations in soil and the predicted maximum annual dose to each scenario subject. When uncertainties in environmental parameters are introduced, soil action levels will become more cumbersome to deal with and will offer little, if any, advantage.

We have some recommendations for DOE and the developers of RESRAD. We are aware that the evolving Windows graphic user interface (GUI) is intended to make the program more accessible to a variety of users, but this greater utility comes at a cost to some potential users. It often is desirable to link programs together, with outputs from one becoming inputs to another. The procedure is usually implemented by writing scripts, which are control programs for the process (Unix operating systems are particularly hospitable to this approach). But a GUI defeats script-driven executions. We are not suggesting that the GUI be eliminated, because it is probably the preferred access for the majority of users, but we

do urge DOE and the RESRAD developers to facilitate a way of bypassing the GUI and launching RESRAD from the command line.

The pieces for this mode of interaction are already in place. The GUI is currently implemented as a separate program, which interacts with the user and the database files and ultimately writes input files for a separate program, RESMAIN3, which the GUI executes through the operating system. RESMAIN3 is the computational engine for RESRAD and is executable from the command line. It reads two auxiliary files, which provide information needed for dynamic allocation of storage arrays, and it reads a data input file specified from the command line (the GUI writes this file, and Version 5.82 gives it the filename extension RAD). RESMAIN3 writes the results of the calculation to a set of files with the extension REP ("REPort"). The data input file is formatted in conformity with the FORTRAN NAMELIST input protocol, in which variables to be initialized in the program are listed by name in the input file and equated to the desired values. By preparing this file with the necessary names and values (a somewhat tedious undertaking) and adjusting the auxiliary file DIMENSON.DAT appropriately, a user can execute RESMAIN3 without invoking the GUI program.

Our recommendation is (1) that this launching mechanism be preserved in future versions of RESRAD, and that its relative independence of the GUI be maintained, so that the program can be launched directly from the command line or from a scripting program, without invoking the GUI front-end, and (2) that the procedure be documented so that users desiring to prepare the NAMELIST-formatted input file, make the modifications in DIMENSON.DAT, and run RESRAD from a script or wishing to run some preprocessing program on the input can do so. Primarily, the documentation should explain how each dimension value in the file DIMENSON.DAT is derived. It should explain the details of the auxiliary files KIFLG.DAT and KIFLG30.DAT (which are related to the decay chains). And it should define every variable in the NAMELIST-formatted input file, with units, and indicating conditions under which the variable is or is not used by RESRAD. There may also be other information that would be useful. This documentation could be printed in an appendix of the user's guide or it could be made available on the RESRAD web site.

We also recommend that DOE consider releasing the source code for RESRAD, making it available for downloading from a web site. We believe this change of policy would have three advantages: (1) Analysts using Unix workstations could recompile the code to function on their platforms, at least with command-line launching as we described in the previous paragraphs (having not seen the source code for the GUI, we do not know how difficult the conversion would be for that module). (2) Analysts with a good knowledge of programming can often resolve puzzling and subtle questions about what is being computed by referring to the source code. (This point is not intended to suggest that the developers do not support RESRAD and try to answer users' questions; as far as we know, the program is well supported.) (3) Experience seems to indicate that many useful suggestions for improving the program and the models it implements would come from programmers and analysts whose participation is currently precluded. In cases where there is particular concern about the authenticity of numbers imputed to RESRAD, it seems that some protocol could be developed that would require "final" or "official" results to be produced with a DOE-provided executable.

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