DEVELOPMENT OF IMPACTS-BRC, VERSION 2.1*

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ABSTRACT

IMPACTS-BRC is a computer program developed to conduct scoping analyses for use in supporting rulemaking on petitions for exemption of waste streams from multiple producers. It was not initially intended for use on individual license applications for specific sites. However, the Federal Register, Volume 51, Number 168, specifies that IMPACTS-BRC be used to evaluate incoming license applications. This creates a problem since IMPACTS-BRC is not being used for its intended purpose. It is a generic code that is now being used for site specific applications. This is only a valid procedure if it can be shown that generic results from IMPACTS-BRC are conservative when compared to results from site specific models. Otherwise, IMPACTS-BRC should not be used.

The purpose of this work was to verify that IMPACTS-BRC works as specified in its user's guides (1,2,3). In other words, Sandia National Laboratories (SNL) has determined that the mathematical models given in the user's guide are correctly implemented into the computer code. No direct work has been done to verify that the mathematical models used in the code are appropriate for the purpose that they are being used. In fact, scrutiny of the groundwater transport models in IMPACTS-BRC has led us to recommend that alternate geosphere models should be used.

Other work carried out for this project included verifying that the input data for IMPACTS-BRC is correct and traceable. This was carried out, and a new version of the data with these qualities was produced. The new version of the data was used with the verified IMPACTS-BRC, Version 2.0 to produce IMPACTS-BRC, Version 2.1. Note that no code changes were made in the evolution to Version 2.1: performance differences between Version 2.0 and 2.1 are caused by the updated data.

INTRODUCTION

The Low-Level Waste Policy Amendments Act requires the U.S. Nuclear Regulatory Commission (NRC) to develop the technical capability for evaluating petitions to classify very low-level radioactive waste streams as Below Regulatory Concern (BRC). The NRC published a policy statement on BRC waste in the Federal Register, Volume 51, Number 168. This explicitly stipulates that IMPACTS-BRC shall be used to evaluate petitions for BRC classifications. It therefore provides a strong incentive to petitioners to use the code, although it does not require the code's use in a BRC petition. However, petitioners are requested, at a minimum, to provide NRC with the IMPACTS-BRC input data (2).

IMPACTS-BRC is a generic radiological assessment code that allows calculation of potential impacts to maximally exposed individuals, waste treatment and disposal workers, and the general population resulting from exemption of very low-level radioactive wastes from regulatory control (3). The code allows radiation dose calculations to be made of human exposure to the waste by many pathways and exposure scenarios. These scenarios encompass transportation, treatment, disposal, and post-disposal activities. Default environmental and populational parameters are included in the code for three geographical locations: a highly populated, humid Northeast site, a moderately populated, humid Southeast site, and a sparsely populated, arid Southwest site. Default parameters are also included that are representative of treatment and disposal facilities that allow calculation of radiation doses to workers on a generic basis. Several options are available to the user related to facility design and treatment options.

Because of the use of IMPACTS-BRC in the petition process and the potentially contentious atmosphere in which the code may be used, there is a strong requirement for the code to be as defensible as possible. To some extent, the defensibility of the code is linked to the adequacy of the verification that has been done to ensure that the code functions as specified in its documentation.

Independent review and verification of data in Version 2.0 input files was conducted, and code verification was performed on portions of the code that were not exercised by the existing sample problems. New sample problems have been developed to check the untested sections of the code, and the results of these tests also are discussed. The process of verifying the code and the data resulted in a new version of the code denoted IMPACTS-BRC, Version 2.1.

This paper is intended to summarize and gain more wide coverage for a soon to be published document: IMPACTS-BRC, Version 2.1 Code and Data Verification (4). The reader is referred to that document for more in depth discussion of the work presented here.

CURRENT ASSESSMENT AND VERIFICATION OF VERSION 2.0

An evaluation of Version 1.0 by O'Neal and Lee during the development of Version 2.0 showed that the sample

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problems distributed with the code allowed for verification of most, but not all, of the code. The evaluation of Version 2.0 by S. Cohen and Associates, Inc. (5) suggested the need for an additional verification of the data files used by the code. Details of this evaluation can be found elsewhere (4). The current assessment of IMPACTS-BRC was undertaken to remedy any gaps in the verification work carried out by O'Neal and Lee.

Data Verification

A review of data in the IMPACTS-BRC, Version 2.0 code was conducted. Data that could be compared to specific, accepted references (*e.g.,* fundamental dose conversion factors) were reviewed for correctness. However, many of the parameters used in IMPACTS-BRC do not have generic "correct" values (*e.g.,* retardation factors, transfer factors). For these parameters the data set was evaluated for traceability: the historical development of the code (1,2,3) was examined to identify when and by whom the parameter value was justified. An evaluation was also made to ensure that the most recent parameter recommendations were incorporated in the code. However, SNL did not compare this set of parameters to any other references to attempt to establish their conservatism.

The following parameter values for each radionuclide were traced historically through the development of the code (1,2,3):

- Radionuclides included in IMPACTS-BRC, Version 2.0
- Number of solubility classes included
- Solubility classes
- Soil-to-plant transfer factors
- Feed and water-to-meat transfer factors
- Feed and water-to-milk transfer factors
- Water-to-fish transfer factors
- Water-to-freshwater seafood transfer factors
- Waste-to-leachate partition ratio
- 1st and 4th set of retardation coefficients

The nuclide decay constants used in the code are consistent throughout all versions of the code; however, they were not referenced anywhere during the code's history. Consequently, they were recalculated using the half-lives given in Kocher and Eckerman (6) to produce compatibility with the dose conversion factors used in the code, which are based on those half-lives, and to ensure traceability.

The dose conversion factors for a volume source, were compared to the results obtained from the MICROSHIELD (7) computer code, which are listed in Table 7-6, pages 7-19 *to* 7-20 of O'Neal and Lee (3). The decay chains included in calculating the volume source dose conversion factor values are indicated in Table 7-6, page 7-9 of the IMPACTS-BRC user's guide (3).

The dose conversion factors for ingestion and inhalation were compared to the electronic tapes, DFINGEST.DAT and DFINHALE.DAT, received from Dr. Keith Eckerman at Oak Ridge National Laboratory. The tapes were taken from the ICRP/ORNL Dosimetry files assembled during the course of the calculations for ICRP-30 (8), Parts I-IV in preparation for the Federal Guidance Report 11 (9). The tapes include organ dose conversion factors needed for IMPACTS-BRC that were not included in the organ list published in Eckerman *et al.* (9). The tape values refer to a unit intake of the stated radionuclide, but include committed dose equivalent contributed by any daughter radionuclide produced from radioactive decay of the parent nuclide in the body. The dose conversion factors for inhalation are based on 1 micron activity median aerodynamic diameter size particles.

The dose conversion factors Ag-108m and Ag-110m were omitted from the Eckerman diskette. The ingestion and inhalation dose conversion factors for those radionuclides were compared to the dose conversion factor document by Eckerman *et al.* (9) (page 132 and page 163) for the organs included therein. These organs were lung, red marrow, bone surface, thyroid, and the effective dose equivalent. For the organs not included in the Eckerman document (*i.e.,* stomach wall, lower large intestine (LLI) wall, kidney, and liver) the dose conversion factors were compared with the values cited in the sample TAPE1.DAT in Volume II of the de Minimis documentation (2) and were found to be in agreement. Therefore, they were left unchanged.

The fundamental dose conversion factors for external exposure to an area source and for air immersion were compared to Tables A.1 and A.3 in the DOE dose-rate conversion document (6). For some nuclides, to obtain a dose conversion factor for the parent in a decay chain the dose conversion factor of the first daughter is added to that of the parent. These values are included in TAPE1.DAT. All TAPE2.DAT parameter values have been traced historically from Volume 1 of the de Minimis documentation (1).

The input data for IMPACTS-BRC is now in a form such that all parameters are traceable. Other items that could lead to the improvement of the code are discussed below. The current version of the code allows for only 85 radionuclides, and it is recognized that this list is inadequate for certain facilities. To incorporate an additional radionuclide involves replacing one of the nuclides in the standard list of radionuclides and all of the associated nuclide specific parameters. At the present time, this process is not trivial with many considerations necessary to ensure the substitution will allow the code to function as expected. Modifications also would have to be made to the data input preprocessor. It would be desirable to modify the current version of the IMPACTS-BRC code to allow for more flexibility on the part of the user to add radionuclides appropriate for their analysis, or conversely, to make the library large enough that all nuclides of interest are included.

Code Verification

In this section we describe the methods and results of the code verification work. The current verification effort was conducted according to the quality assurance procedures for this work given elsewhere (4). This involved production of an interim baseline version of the code using the updated (Version 2.1) input data, developed under the data verification component of the current project. All code verification efforts were conducted using the baselined 2.0 Version of the code with the updated Version 2.1 input data.

Write statements were added to the previously unverified sections of the baselined Version 2.0 of the code, which allowed for a line-by-line examination of the pertinent parts of the code. The modified code was then compiled with the Lahey FORTRAN F77L-EM/32, Version 4.0 compiler. The existing sample problems were rerun to ensure that addition of the write statements did not cause any spurious changes. This version of the code was then used for verification activities.

New test problems were developed; the intent of the test problems is to verify all previously untested mathematical models given in the reference documents (1,3) and ensure that they are implemented correctly. It is therefore unimportant for the problem to be completely meaningful, since the physics behind the mathematical model is not being tested under the current scope of work. Therefore, some unlikely combinations are included, such as Pu-236 present in an activated-metal BRC waste stream. This was done so that the unverified sections of the code could be tested in the most efficient manner. Three test problems were developed and the results from them are described below.

All previously untested portions of the code were exercised in this verification work. Deviations were discovered between the description of subroutine SPLICE in Oztunali and Roles (1) and its implementation in the code. We verified that the algorithm in the code is correct and that no changes should be made. An error was found in function XOQFC in the ASCII file normally distributed with the code. The error was not found in the code itself, and no changes to the code were necessary. Minor deviations were found between radionuclide concentrations calculated using subroutine CHNS and independent calculations for the Cf-252 chain. The differences are believed to be the result of slightly different half lives used in the two codes. No alterations to IMPACTS-BRC are recommended to address this issue. All other portions of the code were verified to be working correctly. No algorithm or coding changes to IMPACTS-BRC were necessary as a result of this verification effort.

IMPACTS-BRC, VERSION 2.1

Version 2.1 of IMPACTS-BRC was produced from Version 2.0 of the code with very minor revisions. These revisions include modifying the banner to print out the new version number and adding comments to detail our verification activities. No changes were made to the models in the code to produce Version 2.1. The only significant change to Version 2.1 is that it uses the 2.1 input data, which was produced during this project.

GENERAL COMMENTS ABOUT IMPACTS-BRC

In conducting our review of IMPACTS-BRC, we have several general comments about using the code for site-specific applications. Our primary comments pertain to possibly non-conservative models used in IMPACTS-BRC and the way uncertainties are addressed.

IMPACTS-BRC was derived from the Impacts Analysis Methodology for low-level radioactive waste (10). The Impacts Analysis Methodology (10) and its BRC update (11) were generated to support the Environmental Impact Statement for 10 CFR Part 61. They were developed to allow NRC to assess qualitatively the effects of various variables on the overall impacts of low-level waste disposal. The approach was clearly acknowledged to be used for scoping analyses, and it was not believed to be appropriate for site-specific applications. Similarly, the EPA developed the PRESTO (12) family of codes to conduct generic assessments for their 40 CFR Part 193 rulemaking on low-level waste (which has not yet been promulgated).

Both PRESTO and the Impacts Analysis Methodology were eliminated very early on in the development of the current NRC low-level waste performance assessment methodology, since they were specifically developed only for generic use in rule making, and they are considered inappropriate for site-specific applications.

Many of the models in IMPACTS-BRC are the same as those in the Impacts Analysis low-level waste methodology, and the models retain many of the same drawbacks. These drawbacks are:

1. The Impacts Analysis Methodology is demonstrably nonconservative compared to models in the current NRC low-level waste performance assessment methodology for the ground water pathways (13).
2. Most geosphere modeling cannot be done on a generic basis except through the use of very conservative (scoping) models (14) that bound the conceptual model uncertainty.
3. IMPACTS-BRC relies heavily on nonmechanistic "index" factors that reduce impacts by orders of magnitude; these factors cannot be justified for specific sites.
4. Use of nonphysical models and parameters in IMPACTS-BRC.

Some of the models in IMPACTS-BRC have dubious physicochemical bases. One example is the model for calculating the impact from bathtubbing of the disposal facility, which leads to overland flow that contaminates a nearby stream. The impact, H_2, is calculated using the equation

$$H_2 = \sum_i \sum_n \frac{f_0 \, C_{ni} \, f_i \, V_L \, M_0 \, 10^{(1-IA)} \, f_{2n} \, PDCF-7}{Q}$$

where

- f_0 = decay correction factor
- C_{ni} = concentration of the n^{th} radionuclide in the i^{th} waste stream (Ci/m^3)
- f_i = fraction of the total waste volume that is composed of the i^{th} waste stream
- V_L = volume of leachate released annually (m^3)
- M_0 = radionuclide-specific leach fraction
- IA = accessibility index
- f_{2n} = radionuclide retention in soil during overland flow
- PDCF-7 = pathway dose conversion factor (mrem m^3/yr Ci)
- Q = flow rate of the surface stream (m^3/yr)

Equation (1) is used to calculate the concentration of radionuclide in surface water, which can then be multiplied by the PDCF, and summed over all radionuclides to calculate an impact from this pathway. The assumptions necessary in using this equation are not discussed by Oztunali and Roles (1), therefore, a discussion is presented here.

One general problem with the IMPACTS-BRC code is the use of generic pathway dose conversion factors for site-specific applications. This approach is only appropriate as long as the pathways and usage factors in the model correspond to the conditions at the site. Hence, this approach cannot always be conservative, and there may clearly be cases for which the assumed pathways are inadequate. The conservatism of each pathway dose conversion factor must be evaluated for each specific site. The generic parameters and the unjustified assumptions used by the code should also be questioned. For equation (1), as an example, the assumptions made and the parameters used to calculate surface-water concentrations are doubtful.

The purpose of the numerator in the equation is to calculate the release rate of radionuclides into the stream. This release is then diluted by the stream flow rate to produce a surface-water concentration. This analysis assumes complete lateral mixing in the stream. While this approach may be appropriate for small streams, it is inappropriate for larger streams (15), since it will lead to calculation of nonconservative surface-water concentrations. Previously this limitation has not been acknowledged . We also note that the code cannot model lake concentrations, and that lakes have the potential to be net accumulators of radionuclides. Neglecting this potential accumulation is also not conservative.

Next, examine the parameters used in the numerator of equation (1) to calculate the radionuclide release rate to the stream. The combination $f_i C_{ni} M_0$ is used to calculate radionuclide concentrations in water in the disposal trench from concentrations in the waste stream. It assumes (1) complete dilution of the i^{th} waste stream by other wastes, and (2) some generic "leach fraction," M_0, that relates ground-water concentrations to solid concentrations. The complete dilution assumption is not conservative, but probably cannot be avoided because of the uncertainty about the distribution of waste in the disposal facility.

The leach fraction is another matter. Values for the leach fractions in the code were developed from data from the Maxey Flats' low-level waste disposal site. It is often argued that these values for leach fractions are conservative, *but there is absolutely no experimental or theoretical basis for this argument.* The leaching process depends heavily on the chemical and physical form of the waste, the geochemistry of the waste, soil, and ground water, and on the hydrological flow regime of the site. Leaching results from Maxey Flats depend in a complicated way on conditions at Maxey Flats, and other sites may bear no resemblance to these conditions. For example, at Maxey Flats, uranium moves very slowly. Consequently, it is assigned a low leach fraction in the IMPACTS approach. However, it is well known that uranium compounds are quite mobile at a number of existing DOE sites (16). This is a clear and demonstrable case in which the Maxey Flats' data are not conservative when used for a different site. In addition, chelating compounds cannot be excluded from consideration in BRC waste assessment, and the presence of chelating agents may increase leach rates even further. Furthermore, in developing the leach fractions, a number of dubious assumptions were required, so the Maxey Flats "data" are not as straightforward as they first appear (17). One of the most important pieces of missing information needed to generate the leach fractions is the inventory at the site. The quantities and forms of the inventory are not known with confidence at Maxey Flats, so the leach fractions are based on dubious estimates of the inventory (18). Current low-level waste leaching models assume that leaching from trash occurs through a "surface-wash" mechanism (19,15), which suggests that much higher release rates can be expected.

The leachate concentration is multiplied by the parameters V_L, $10^{(1-IA)}$, and f_{2n}. V_L was defined in Oztunali and Roles (1) in units of m^3, but it should be m^3/yr for dimensional consistency of the overall equation. The effect of the accessibility index, IA, in the code is to reduce release rates of activated metals by a factor of 10 for all situations. There is no experimental evidence for this ten-fold reduction in the release rate. Actual releases may be either more or less than those calculated using IMPACTS-BRC, and will depend on site-specific conditions. Sullivan and Suen (19) have suggested an alternate model for releases from activated metals. This model is a semiempirical approach that combines an established phenomenological analytical structure for corrosion rate with field data for underground corrosion as a function of soil properties. Limitations to the model are documented (15,19) and consist primarily of narrow empirical bases for parameters in the model. Nevertheless, the model is considerably more defensible than an arbitrary ten-fold reduction in release rates. The factor f_{2n} is the fractional amount of radionuclides retained by soils during overland flow. Two issues should be raised with regards to this parameter: (1) it is conventional to model sorption as a delay mechanism rather than a removal mechanism (the current approach in the code is not conservative), and (2) soil-radionuclide interactions cannot be quantified on a generic basis.

This examination of overland transport from the disposal trench in IMPACTS-BRC indicates that

- Parameters in the model have no physical or experimental basis.
- The model takes excessive credit for dilution and removal mechanisms at each step in the process.

Therefore, the model cannot be considered to be conservative on a generic basis, nor can it be considered either conservative or realistic for site-specific analyses.

These issues have been raised by examining only one of the many models in IMPACTS-BRC. It is expected that there are similar problems in other models in the code. Note that SNL's primary concerns are for the models for transport in the geosphere. These models have not been considered the most important for BRC waste disposal petitions. It has been more common for doses to the transportation worker to dominate the disposal scenario doses (20). It is therefore possible that addressing our concerns about these models will not substantially change previously calculated overall BRC doses.

On the other hand, doses for the ground water-to-well pathway almost always dominate postclosure doses in low-level waste disposal assessments (13). The system here is similar, except that inventories in BRC waste have lower concentrations, and the doses are compared against lower regulatory performance objectives. The ground-water transport analysis in IMPACTS-BRC is believed to suffer from the same defects as the overland transport analysis. Furthermore, many of the assessments of the relative importance of pathways have been carried out using IMPACTS-BRC. Given the probable nonconservatism of the geosphere models, these pathways may have been incorrectly identified as being insignificant. Consequently, these issues are of uncertain importance in relationship to the overall assessment of BRC wastes.

SUMMARY

All the data in the input files to IMPACTS-BRC have been verified. The verification was carried out by comparison of the data files with independent sources (6,9), tracing the data to earlier documentation of the code (1,2,3), changing the data to be consistent with the documentation, or identifying the data as untraceable. The new data, Version 2.1, has been produced under strict quality assurance procedures.

In addition to the data verification, SNL has conducted code verification on previously untested parts of IMPACTS-BRC. SNL has determined that the code implements the models correctly as documented in Oztunali and Roles (1), and that it performs as described in the code documentation (3). No changes were recommended to the code as a result of the code verification efforts.

SNL has produced IMPACTS-BRC, Version 2.1, which uses Version 2.1 of the data. Version 2.1 of the code differs from Version 2.0 only in the version number on the banner it prints in the output files and in some of the comment lines. IMPACTS-BRC, Version 2.1 was produced under quality assurance guidelines.

The purpose of the verification work was to produce a more defensible version of IMPACTS-BRC by ensuring that the data and the code were checked carefully for consistency with the literature. However, in SNL's opinion, the defensibility of the code is even more closely related to the defensibility of the underlying models than to its being produced under strict quality assurance guidelines.

Two areas of concern are identified in this paper. The first is concern about the lack of conservatism and the lack of physical bases for many models and parameters used in the code. The second area of concern is the approach taken toward uncertainty. The code appears to be intended to be used as a bounding analysis, but neither the models nor the parameters appear to bound the uncertainties. If, alternatively, an accurate estimate of impacts is desired, site-specific models must be used. Hence, IMPACTS-BRC, with its generic models and data sets, does not appear to produce either accurate site-specific results or conservative generic results.

It is possible that the modeling areas of concern will not greatly affect calculated doses from projected BRC waste disposal. However, we recommend that the models in the code and the overall approach to uncertainty analysis be reevaluated to ensure that conservative and defensible analyses are used.

RECOMMENDATIONS

In our view, evaluation of BRC petitions would be better conducted by identifying a suite of codes to conduct individual parts of the assessment. More than one code should be identified for each module of the methodology. This approach was used in the recently developed NRC/SNL low-level waste performance assessment methodology (13,21). One important advantage to this approach is that different models can be substituted into the analysis when they are appropriate. When greater uncertainties exist, more conservative models may be used.

The primary disadvantage to this approach is that a greater burden is placed on the applicant to justify the models and parameters used in the analysis. In other words, it is more work for the applicant since he must understand the site better. Again, the NRC's low-level waste performance assessment philosophy is to require a conservative analysis to be used, unless the applicant can demonstrate that less conservative approaches are appropriate (22). We believe that forcing the applicant to justify assumptions will result in better radiological assessments.

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