COMPARISON OF COMPUTER CODES AND APPROACHES USED AT DOE SITES TO MODEL INTRUSION SCENARIOS

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ABSTRACT

Computer codes and scenarios used to evaluate intrusion scenarios at U.S. Department of Energy (DOE) sites are compared and discussed. The primary objective of this paper is to provide a comparison of the assumptions used in previous disposal site performance assessments and identify differences in the approaches and areas where it would be appropriate to recommend a standardized approach. The task is comprised of two steps: a benchmark study of GENII and PATHRAE-EPA (the two most commonly used computer codes at DOE sites) and a comparison of assumed values for selected input parameters from scenarios used in performance assessments at five DOE sites as well as the U. S. Nuclear Regulatory Commission (NRC). Differences in assumptions made at DOE sites and NRC guidance are identified to provide examples of DOE Headquarters Performance Assessment Task Team efforts to foster consistency in performance assessment approaches and interpretation of results across the DOE system. The importance of understanding differences in default assumptions in computer codes and their applicability is emphasized, because GENII, PATHRAE-EPA, and other similar computer codes are applied to a variety of sites within DOE and other regulatory environments.

INTRODUCTION

The U.S. Department of Energy Headquarters (DOE-HQ) established a Performance Assessment Task Team (PATT) to integrate the activities of sites that are preparing performance assessments (PAs) for the disposal of newly generated low-level waste (LLW), as required by Chapter III of DOE Order 5820.2A (1). The PATT is comprised of representatives from each of the DOE sites that are actively disposing of LLW, representatives from DOE-HQ, and a liaison from the U. S. Nuclear Regulatory Commission (NRC). The PATT's charter is to recommend policy and provide guidance to DOE-HQ on issues that impact PAs. The recommended policy and guidance provided by the team will improve the consistency of approaches (where applicable) and interpretation of results across the DOE system.

One of the first tasks undertaken by the PATT was to examine all aspects of a PA to find areas where consistency could be improved without impacting the credibility of the analyses. For example, groundwater modeling is strongly driven by site-specific considerations; therefore, efforts to standardize groundwater modeling would likely compromise the credibility of the calculations. Based on this evaluation, intrusion scenarios were judged the area most likely to be amenable to some level of standardization. The PATT established a subteam to evaluate the approaches and computer codes used to model intrusion scenarios at DOE sites. The goal of the subteam was to identify areas where differences exist and provide recommendations on areas where standardization may be appropriate. This paper summarizes two activities of the subteam: performing a benchmark study of the GENII (2) and PATHRAE-EPA (3) computer codes for similar sets of inputs and comparing assumed input values for selected parameters from scenarios used by DOE sites to address the inadvertent intrusion criteria of DOE Order 5820.2A. An important consideration during the comparison was to identify differences in default parameters assumed in the two computer codes. These comparisons had not been conducted previously and were considered essential to meet the goals of the subteam.

BENCHMARK STUDY OF GENII AND PATHRAE-EPA COMPUTER CODES

An initial consideration for the benchmark study was to use a value of one for most inputs. However, a number of input values were difficult to change in GENII or PATHRAE-EPA (especially for the ingestion pathway). For example, some inputs are part of the source code (hard-wired) in PATHRAE-EPA, and GENII uses binary libraries for some inputs. For this comparison, the subteam did not change source code or protected (binary) libraries. Based on this policy, some of the "unchangeable" inputs were set at the default values used in PATHRAE-EPA or GENII (as appropriate) for the study. Fortunately, during this comparison no inputs for a given parameter were "unchangeable" in both computer codes.

One example of "unchangeable" inputs in PATHRAE-EPA is the use of hard-wired values for the mixing depth and area of spreading for excavated wastes (waste inventory is the input), whereas GENII uses initial soil concentrations as input. To account for this difference, the input waste inventories for PATHRAE-EPA were scaled to force the initial soil concentration to be one (the valued used in GENII). Another example was that the dose conversion factors for GENII are maintained in a binary library, whereas PATHRAE-EPA requires the user to input the dose conversion factors. Thus, for the study, dose conversion factors from GENII were used as input for PATHRAE-EPA.

A relatively consistent set of inputs for PATHRAE-EPA and GENII was generated based on the above constraints. The primary inputs were set to identical values. While a number of secondary inputs are included in the two codes, their complete consideration would have required more time than was productive for this task. The goal of the benchmark study was for the results to agree within ±10%. Thus, if necessary, secondary input data for the two codes were investigated and made consistent until the results agreed within ±10%. Each pathway is discussed independently in the following subsections.

Inhalation Pathway

The inhalation pathway comparison was straightforward, and other than using the default dose conversion factors from GENII, it appeared that any values could be used for the other parameters in a test case. An additional case was run with PATHRAE-EPA to compare with hand calculations, and the results were identical. The hand calculations provide an exact comparison for the computer code. Input parameters required for the scenario included soil concentration, soil density, exposure time, breathing rate, and dose conversion factor. Additional parameters that may be used include respirable fraction and fraction of dust from onsite.

Ingestion Pathway

Ingestion was more complicated than inhalation for a variety of reasons including different foods that need to be considered (e.g., leafy vegetables, produce, and meat), exposure results from a sequence of transfer factors (e.g., soil to plant to human and soil to plant to animal meat to human), and transfer factors can be modeled using different assumptions (e.g., stored feed versus fresh forage and composition of stored feed). The method used to select pathways considered in the benchmark study is discussed in the following paragraphs.

The comparison was more complicated because the categories of food used by PATHRAE-EPA and GENII are different. PATHRAE-EPA considers only leafy vegetables and produce, while GENII considers leafy vegetables, root vegetables, grain, fruit, and eggs. In order to simplify the comparison, the values used for leafy vegetables and produce in PATHRAE-EPA were input into leafy vegetables and root vegetables in GENII. Comparisons of the meat and milk consumption pathways were more difficult because of differences in the codes. For example, stored feed is all grain in GENII, but PATHRAE-EPA uses a hard-wired proportion of grain and pasture grass. Because of this and other complicating factors, the meat and milk pathways were not considered in the initial comparison. Thus, the exposure route considered in the comparison was soil to leafy vegetables and produce to humans. Inputs for this exposure route included soil concentrations, dry-to-wet ratios for plant uptake factors, plant uptake factors, delay times between harvest and consumption, consumption rates, and dose conversion factors.

A difference in the approach for considering uptake of Carbon-14 (^{14}C) was identified in the two codes. PATHRAE-EPA assumes no plant uptake of ^{14}C and GENII includes plant uptake. Given this assumption, PATHRAE-EPA will always predict a dose of zero for ingestion of ^{14}C. Ng et al. (4), the NRC (5), and Sheppard et al. (6) indicate that ^{14}C in the soil can be taken up by plants; therefore, ^{14}C uptake should be included in PA models. This is a significant finding, because ingestion of ^{14}C can be a major contributor to the overall dose. PATHRAE-EPA will allow uptake of ^{14}C, if any identifier other than "C-14" is used in the input deck (e.g., "C-14X").

A subtle error was identified in the PATHRAE-EPA manual. The manual indicates that a wet weight soil to plant uptake factor should be used as input, when in reality it should be a dry weight. Dry to wet weight conversion factors are hard-wired into PATHRAE-EPA. Although the differences in results due to using the wrong factor are relatively minor, the error needs to be identified. For the benchmark study, the hard-wired dry to wet weight conversion factors from PATHRAE-EPA were used as the inputs for the GENII runs. A deficiency related to GENII was that references for some of the default parameters were not clearly identified. Also, when comparing intrusion scenarios without groundwater contributions, the user must be sure that leaching from waste is turned off or set at the same value in the two codes. GENII also considers resuspension of radionuclides onto leaves by rain splash; when comparing results with PATHRAE-EPA this feature should be turned off.

External Exposure Pathway

The external exposure pathway produced the greatest differences when the results from GENII and PATHRAE-EPA were compared because different methodologies are used to calculate external exposure. GENII incorporates ISOSHLD (7) dose calculation program into its structure, while PATHRAE-EPA uses an infinite plane approximation. Due to the fundamental differences in the models used by the two computer codes, it was determined that further efforts to obtain agreement between the codes would be of little benefit.

Summary of Benchmark Study Results

Input files were constructed for GENII and PATHRAE-EPA based on the above considerations for each of the pathways. Results were obtained for five radionuclides that typically contribute a large proportion of the predicted dose from LLW disposal facilities at DOE sites: Cesium-137 (^{137}Cs), Iodine-129 (^{129}I), Technetium-99 (^{99}Tc), Plutonium-239 (^{239}Pu), and Strontium-90 (^{90}Sr) (Cobalt-60 (^{60}Co) was substituted for ^{99}Tc for the external exposure pathway). Table I illustrates that the results of the benchmark runs agreed within the preset criterion of 10% for all five radionuclides for the inhalation and ingestion pathways. Because the desired level of agreement was obtained, further fine tuning to account for subtle differences in the codes was not attempted. It should be noted that the relatively close agreement was expected for the ingestion and inhalation pathways because the models used by the codes are relatively similar. More important than the actual comparison of results was the information obtained about differences in the default assumptions in the codes. Additional discussion of some of the assumptions in the codes is provided in the following section.

Although acceptable agreement was obtained for the inhalation and ingestion pathways, the results of the comparison for the external exposure pathway were not acceptable. Table I illustrates the large deviation in results for the external exposure pathway predicted by the two computer codes. Also, note that results for ^{14}C were not included in Table I for any pathway. The results for ^{14}C were based on fundamentally different models for ingestion and external exposure. In both cases, the predicted doses were zero in PATHRAE-EPA and non-zero in GENII. The differences in ^{14}C assumptions are discussed further in the following section.

TABLE I

Comparison of Relative Doses Predicted by GENII and PATHRAE-EPA

Ingestion (Leafy Vegetables and Produce)	Normalized GENII Dose	Normalized PATHRAE-EPA Dose
^{90}Sr	1.0E+0	9.2E-1
^{99}Tc	8.7E-2	8.7E-2
^{129}I	2.9E-1	3.0E-1
^{137}Cs	3.3E-2	3.2E-2
^{239}Pu	5.8E-3	5.8E-3
Inhalation		
^{90}Sr	2.6E-4	2.5E-4
^{99}Tc	1.1E-5	1.0E-5
^{129}I	1.9E-4	1.8E-4
^{137}Cs	3.6E-5	3.6E-5
^{239}Pu	6.2E-1	6.2E-1
External Exposure		
^{60}Co	1.3E-5	2.8E-5
^{90}Sr	2.8E-5	1.6E-3
^{129}I	2.2E-3	4.2E-1
^{137}Cs	1.7E-1	4.2E-1
^{239}Pu	1.3E-4	5.8E-3

COMPARISON OF ASSUMED MODELS AND INPUTS

The second objective of this effort was to compare data and scenarios from the different sites. The post-drilling and post-excavation scenarios are considered here. The post-drilling scenario assumes that a well is drilled through a disposal facility, causing waste to be exhumed. Subsequently, the waste is mixed with surrounding clean soil at the surface upon which crops are grown and cattle are raised. The dose results from ingestion of contaminated crops, beef, and milk; inhalation of contaminated dust; and external exposure. The post-excavation scenario is identical except that waste is exhumed through excavation of a house basement to a depth that intersects the depth of burial. These scenarios were chosen because they provide maximum dose estimates relative to other scenarios (8). Consequently, the dose estimates from these scenarios typically determine waste concentration limits in classification schemes.

The parameter with the widest range of inputs and largest apparent impact on the results was the soil dilution factor. The dilution factor is a function of the volume of waste exhumed and the volume of surface soils in which the waste is mixed. Table II lists the dilution factors used at different sites and by the NRC. Although Table II indicates general agreement among all sites for the excavation scenario, the agreement results from a fortuitous combination of inputs, because individual inputs to determine the dilution factor varied at the different sites. For the drilling scenario, the values are very inconsistent (i.e., almost three orders of magnitude difference). Although a recommended value for use in final waste classification analyses is not defined at this time, it is not desirable to have this large of a spread in a factor that is somewhat arbitrarily defined and can have an influence on dose estimates and inventory limits.

TABLE II

Comparison of Soil Dilution Factors

Site	Drilling Scenario	Excavation Scenario
1	2.0E-2	2.0E-1
2	9.3E-4	2.0E-1
3	4.6E-5	9.9E-2
4	7.9E-4	1.1E-1
5	4.8E-5	9.5E-2
NRC	N/A	1.3E-1

Parameters of interest for inhalation include breathing rate, average dust loading, and dose conversion factors. The average yearly dust loading is calculated by summing the product of time and dust loading for each situation (e.g., gardening, outdoors, and/or indoors) and dividing by the total exposure time. These factors are all relatively consistent among sites. Different assumptions have been used to estimate inhalation doses, but the factor that varies the most is the average dust loading. It should be noted, however, that the uncertain parameters affecting inhalation rates and soil dilution can also result in differences in inhalation dose estimates, which is the dominant pathway for ^{239}Pu.

The significant parameters for ingestion are the types and amounts of food eaten, dose conversion factors, and the various uptake factors in the food chains. There were a number of differences in numbers and types of food addressed by the sites. However, these differences did not significantly affect dose estimates. Assumptions regarding uptake of ^{14}C were found to significantly impact doses. Assumptions made at the sites ranged from assuming no uptake of ^{14}C (i.e., no ingestion dose) to assuming a relatively large concentration ratio for ^{14}C (i.e., relatively large ingestion dose). Carbon-14 uptake is one area where some level of standardization appears to be warranted.

The significant parameters for the external exposure pathway are exposure time, mixing depth, and dose conversion factors. Exposure times were determined assuming strictly outdoor exposure or a combination of outdoor and

TABLE III

Comparison of Dominant Pathways by Radionuclide

Site	^{14}C	^{99}Tc	^{129}I	^{137}Cs	^{239}Pu
1	*External*	Ingestion	Ingestion	External	Inhalation
2	Inhalation	Ingestion	Ingestion	External	Inhalation
3	Ingestion	Ingestion	Ingestion	External	Inhalation
4	Inhalation	Ingestion	Ingestion	External	Inhalation

indoor exposures. When indoor time is used, a shielding factor is required to account for the shielding affect of the housing structure. Differences were also noted in the modeling of ^{14}C for external exposure. These differences were a result of the approaches used in PATHRAE-EPA and GENII. Work is continuing to determine the need to standardize approaches for consideration of external exposure to ^{14}C.

Based on the comparison of assumptions, a number of differences were identified. These differences are reflected by a comparison of results obtained using the approaches at four of the sites. Table III lists the dominant pathway predicted for five radionuclides based on site models. The dominant pathways were consistent for all radionuclides except ^{14}C. The dominant pathways for ^{14}C differ depending on the site and corresponding assumptions in the computer codes or hand calculations. Further work is required to reach a consensus on a recommended solution.

CONCLUSIONS

The primary goal of the subteam activities was to identify differences in approaches and computer codes used by DOE sites to model intrusion scenarios. Two tasks were conducted to compare the approaches: a benchmark study of GENII and PATHRAE-EPA and a comparison of assumed values for selected input parameters from scenarios used for PAs at five DOE sites and by the NRC. Agreement was obtained for the results of GENII and PATHRAE-EPA within the specified criterion of $\pm 10\%$ for the ingestion and inhalation pathways. However, poor agreement was obtained for the external exposure pathway. This disagreement was due to fundamental differences in the methods used to compute external exposure. The user needs to be aware of these differences prior to application of the code.

A critical aspect of the benchmark study was to identify differences in default assumptions in the two computer codes. For example, the user must be aware that the soil dilution factor (volume of waste divided by the volume of surface in which it is mixed) is a fixed value based on the input inventory and facility dimensions in PATHRAE-EPA while GENII has the option of using similar inputs to PATHRAE-EPA (with different defaults) or simply use a soil concentration as input. Differences in this dilution factor can have a large impact on the predicted results. A second critical difference was that GENII allows plant uptake of ^{14}C but PATHRAE-EPA default assumes no uptake of ^{14}C. This default can be overridden in PATHRAE-EPA, but the user needs to be aware of the difference. A similar difference was identified in external exposure calculations for ^{14}C. PATHRAE-EPA predicts a dose of zero for external exposure while GENII predicts a non-zero dose. Differences in scenario definitions and assumed parameter values were also found among the sites. For example, soil dilution factors used at different sites varied by orders of magnitude. and assumptions regarding the number and types of food consumed were also different. Treatment of ^{14}C and selection of values for the soil dilution factors were recommended as parameters requiring some level of standardization by the subteam.

Results of this comparison demonstrate a wide variety of assumptions and inputs for scenarios that are typically considered relatively standardized across applications. The variation illustrated in this somewhat limited comparison would suggest that there is further variation in applications outside of DOE and the NRC. The users of computer codes that use a large number of default inputs need to be aware that such variations are not unusual. Typically, default values will be based site-specific conditions at the site for which the computer code was developed and (or) the developers preferences. This should be expected because one set of default assumptions cannot be expected to apply to all sites. Thus, it is critical that the users of such computer codes scrutinize the assumptions and the applicability of the default values used in such codes prior to application at a given site.

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