CONF-951209--4

WHC-SA-2964-FP

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Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

Westinghouse
Hanford Company Richland, Washington

Management and Operations Contractor for the
U.S. Department of Energy under Contract DE-AC06-87RL10930

WHC-SA-2964-FP

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Date Published
September 1995

To Be Presented at
17th Annual U.S. Department of Energy
Low-Level Radioactive Waste Management Conference
Phoenix, Arizona
December 12-14, 1995

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COMPARISON OF RESRAD WITH HAND CALCULATIONS

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ABSTRACT

This report is a continuation of an earlier comparison (*Benchmarking of Computer Codes and Approaches for Modeling Exposure Scenarios*, DOE/LLW-188) done with two other computer programs, GENII and PATHRAE. The dose calculations by the two programs were compared with each other and with hand calculations. These hand calculations have now been compared with RESRAD Version 5.41 to examine the use of standard models and parameters in this computer program. The hand calculations disclosed a significant computational error in RESRAD. The Pu-241 ingestion doses are five orders of magnitude too small. In addition, the external doses from some nuclides differ greatly from expected values. Both of these deficiencies have been corrected in later versions of RESRAD.

INTRODUCTION

The U.S. Department of Energy (DOE) has established a Performance Assessment Task Team to integrate the activities of the sites that are preparing performance assessments for disposal of new low level radioactive waste. One activity of the team is to compare the computer programs which are being used at the sites to assess potential human exposures. The first programs examined[1] were GENII[2] and PATHRAE.[3] The two computer programs were compared with each other and with hand calculations. The hand calculations were necessary to understand differences between the computed results from the two programs.

The third program examined was RESRAD Version 5.41.[4] The computed results from RESRAD were also compared with hand calculations and a few irregularities were noted. First among these is an error in the calculations of the Pu-241 ingestion dose from vegetation grown on contaminated soil. Subsequent versions of RESRAD have eliminated this error and generally improved the calculations.

The following sections describe the hand calculations are described first, along with the parameters used in these calculations. The RESRAD program is then described and the RESRAD results are compared with the hand calculations.

HAND CALCULATION MODELS AND PARAMETERS

Two exposure scenarios are frequently used to evaluate the impacts of low-level waste disposal. The first is intrusion by an unsuspecting individual who drills a water well through the waste site and later grows a garden on the exhumed material. For the purposes of comparison, a unit concentration in the surface soil was assumed. The second scenario assumes the radionuclides in the waste have migrated into the groundwater. An individual drills a water well near the disposal site and uses contaminated water for domestic needs as well as watering the grass and hay fed to a cow. For the purposes of comparison, a unit concentration in the well water was assumed. The methods used to calculate the doses are described below. Refinements for radioactive decay were not included, since the nuclides of importance have long decay half lives.

Doses from an Initial Soil Concentration

The typical waste intrusion scenario includes doses that result from gardening activities on contaminated soil. Dose pathways include external dose from the soil, inhalation of resuspended dust, and ingestion of garden produce. The computer programs were compared with hand calculations starting with each nuclide at a soil concentration of 1 $\mu Ci/m^3$. The hand calculated doses are shown in Table 1.

The external dose accumulated during the first year is the product of the soil concentration, the time of exposure, and the external dose rate factor. The exposure duration was taken to be one year. The external dose rate factors are taken from Federal Guidance Report Number 12[5] for soil with a 15 cm depth of contamination. The tabulated dose rate factors use a higher soil density than was assumed in the hand calculations. The tabulated values were adjusted upward by the factor 1.067 to compensate for this. Equation 1 summarizes this calculation. Appropriate unit conversion factors must be applied.

$$\text{External Dose} = \text{(Soil Conc)(Exposure Time)(Dose Rate Factor)} \quad (1)$$

The inhalation dose is the product of the soil concentration, the volume of soil inhaled during the year of exposure, and the inhalation dose factor.[6] The volume of soil inhaled is based on an average mass loading of 0.1 mg/m³ and a total of 8500 m³ air inhaled during the year. The volume of soil inhaled is calculated by dividing the mass of soil inhaled by the assumed soil density, 1.5 g/cc. Equations 2 and 3 summarize this calculation.

$$\text{Volume of Soil Inhaled} = (0.1\ \text{mg/m}^3)(8500\ \text{m}^3)/(1.5\ \text{g/cc}) = 0.567\ \text{cc} \quad (2)$$

$$\text{Inhalation Dose} = \text{(Soil Conc)(Soil Volume Inhaled)(Inhalation Dose Factor)} \quad (3)$$

The ingestion dose from contaminated garden vegetables is the product of the nuclide concentration in the vegetable at the time of harvest, the quantity of the vegetable consumed, and the ingestion dose factor.[6] The concentration of nuclides in vegetables is based on root uptake from the soil into the edible portions of the plants. The transfer of contamination from soil to the plants by mechanical means (rain splash) is not considered. Soil-to-plant concentration ratios[7,8] are used to estimate the plant concentration. These concentration ratios are based on the dry weight of the plants and must be adjusted downward to include the water in the plants at the time of consumption. Equations 4, 5, and 6 summarize the calculation of ingestion dose from garden produce.

$$\text{Leafy Concentration} = Cs \cdot DWv \cdot Bv \quad (4)$$

$$\text{Grain Concentration} = Cs \cdot DWr \cdot Br \quad (5)$$

$$\text{Ingestion Dose} = [\text{Leafy} \cdot Qv + \text{Grain} \cdot Qr] \cdot DF_{ing} \quad (6)$$

where,

Cs = Soil concentration, 1 μCi/m³. The hand calculations assume this remains constant during the year of exposure. There is no radioactive decay or leaching from the surface layer of soil.

DW = Ratio of dry weight of a plant to the wet weight. For leafy vegetables DWv is 0.066, while for grains DWr is 0.187. These somewhat low values are hard-coded into PATHRAE and were chosen for ease of comparison.

B = Ratio of the concentration of a nuclide in a plant to the concentration in the soil. Dry weights of the soil and plants are used. The Bv is for leafy vegetables, while the Br is for non-leafy vegetables. Values for H-3 and C-14 are taken from Reference 8. Values for the other nuclides are taken from Reference 7.

Q = Quantity of a vegetable that is eaten. For leafy vegetables, Qv is 20 kg, while for grains Qr is 172 kg.

DF_{ing} = Dose received from the ingestion of a unit amount of activity. Values are taken from Reference 6.

Table 1. Hand Calculated Doses from Contaminated Soil

Nuclide	External	Inhale	Ingest	Total
H-3	0.00E+00	5.36E-05	1.69E+00	1.69E+00
C-14	8.91E-03	1.19E-03	1.52E+01	1.52E+01
Co-60	8.97E+03	8.50E-02	1.09E+00	8.97E+03
Ni-59	0.00E+00	7.37E-04	6.70E-02	6.77E-02
Se-79	1.23E-02	5.04E-03	1.16E+00	1.18E+00
Sr-90	1.53E+01	1.35E-01	2.65E+02	2.80E+02
Tc-99	8.29E-02	4.25E-03	1.32E+01	1.33E+01
I-129	8.58E+00	1.02E-01	8.43E+01	9.30E+01
Cs-137	2.00E+03	1.81E-02	8.92E+00	2.01E+03
Pb-210	3.96E+00	1.21E+01	3.92E+02	4.08E+02
Ra-226	6.25E+03	4.48E+00	1.25E+01	6.27E+03
U-238	7.87E+01	6.80E+01	5.66E+00	1.52E+02
Np-237	6.90E+02	2.78E+02	2.95E+02	1.26E+03
Pu-239	1.88E-01	2.89E+02	1.46E+00	2.91E+02
Pu-241	1.23E-02	5.67E+00	2.93E-02	5.71E+00
Am-241	2.90E+01	2.95E+02	1.15E+01	3.35E+02

NOTE: Units are rem/y per $\mu Ci/m^3$ in the surface soil.

<u>Doses from Contaminated Irrigation Water</u>

Contaminated irrigation water could come from groundwater or surface water. The typical irrigation scenario includes ingestion doses from drinking water, garden produce, beef, and milk. The soil becomes contaminated from application of the irrigation water. Plants become contaminated through root uptake and direct deposition on the foliage by the overhead irrigation system. The animal products become contaminated when the cows eat contaminated produce and drink contaminated water. Inhalation and external doses were not computed because the calculation would differ little from what was computed previously for contaminated soil. The hand calculated doses are shown in Table 2.

The ingestion dose from drinking untreated water during the first year is the product of the water concentration, the volume of water consumed, and the ingestion dose factor. The annual volume of water consumed is taken to be 730 L. Equation 7 summarizes this calculation. Appropriate unit conversion factors must be applied.

$$\text{Drinking Water Dose} = (\text{Water Conc})(\text{Water Consumed})(\text{Dose Factor}) \tag{7}$$

The ingestion dose from vegetables irrigated with contaminated irrigation water is the product of the nuclide concentration in the vegetable at the time of harvest, the quantity of the vegetable consumed, and the ingestion dose factor. The radioactivity accumulating in the soil contributes to the contamination of vegetables by root uptake. Transfer of contamination from soil to the plants by mechanical means (rain splash) is not considered. Most of the contamination in the plants comes from direct deposition of the radioactivity on the plants by the overhead irrigation system. Equations 8 and 9 summarize this calculation.

$$\text{Plant Conc} = \frac{Cw \cdot I \cdot DW \cdot B}{\text{Density} \cdot \text{Thick}} + \frac{Cw \cdot I \cdot F_{dep} \cdot \text{Trans} \cdot [1\text{-}\mathrm{Exp}(\text{-}Lw \cdot T_{gro})]}{T_{irr} \cdot \text{Yield} \cdot Lw} \tag{8}$$

$$\text{Ingestion Dose} = [\text{Leafy} \cdot Qv + \text{Grain} \cdot Qr] \cdot DF_{ing} \tag{9}$$

where,

Cw = Water concentration, 1 μCi/L. The hand calculations assume this remains constant during the year of exposure. There is no radioactive decay or ingrowth of progeny nuclides.

I = Irrigation applied during the year, 36 inches (91.4 cm). This is converted to liters per square meter with the factor 25.4 L/m^2 per inch of water.

DW = Ratio of dry weight of a plant to the wet weight. For leafy vegetables DWv is 0.066, while for grains DWr is 0.187. These somewhat low values are hard-coded into PATHRAE and were chosen for ease of comparison.

B = Ratio of the concentration of a nuclide in a plant to the concentration in the soil. Dry weights of the soil and plants are used. The Bv is for leafy vegetables, while the Br is for non-leafy vegetables. Values for H-3 and C-14 are taken from Reference 8. Values for the other nuclides are taken from Reference 7.

Density = Soil density of the surface layer, 1500 kg/m³.

Thick = Thickness of soil that the deposited activity contaminates, 0.15 meters. This is a customary tilling depth for gardening and farming activities.

F_{dep} = Interception fraction, i.e., the fraction of the activity in the applied irrigation water which remains on the plant surfaces. It is assumed that F_{dep}=0.25 for both leafy vegetables and grains.

Trans = Translocation factor, i.e., the fraction of the activity deposited on plant surfaces that ends up in the edible portions of the plant. For leafy vegetables this is 1.0, while for grains this is 0.1.

Lw = Weathering removal constant, Ln(2)/(14 days) = 18.084 per year. If radioactive decay were included, the decay constant of the nuclide would be added to the weathering constant.

T_{gro} = Growing period of the crop. This is assumed to be 60 days for both leafy vegetables and grains.

T_{irr} = Irrigation period is assumed to be 0.5 year. The activity from direct deposition depends on the rate at which the contaminated irrigation water is applied.

Yield = Crop yield, kg/m². The greater the mass of foliage, the lower the average concentration in the foliage. This is assumed to be 2.0 kg/m² for both leafy vegetables and grains.

Leafy = The concentration of a nuclide in leafy vegetables. This is computed by substituting the leafy vegetable parameters into the "Plant Conc" formula.

Grain = The concentration of a nuclide in grains. This is computed by substituting the grain parameters into the "Plant Conc" formula.

Q = Quantity of a vegetable that is eaten. For leafy vegetables, Qv is 20 kg, while for grains Qr is 172 kg.

DF_{ing} = Dose received from the ingestion of a unit amount of activity.

Table 2. Hand Calculated Ingestion Doses from Contaminated Irrigation Water

Nuclide	Water	Vegetable	Beef	Milk
H-3	4.60E-02	1.73E-02	8.31E-02	8.01E-02
C-14	1.53E+00	3.27E-01	5.60E+00	2.51E+00
Co-60	1.90E+01	2.91E+00	4.02E+01	4.66E+00
Ni-59	1.46E-01	2.27E-02	9.32E-02	1.80E-02
Se-79	6.06E+00	9.33E-01	9.64E+00	2.98E+00
Sr-90	1.02E+02	1.72E+01	3.65E+00	2.11E+01
Tc-99	9.49E-01	2.25E-01	1.28E+00	1.74E+00
I-129	2.04E+02	3.17E+01	1.53E+02	2.53E+02
Cs-137	3.65E+01	5.63E+00	7.76E+01	3.14E+01
Pb-210	4.92E+03	7.54E+02	1.56E+02	1.51E+02
Ra-226	8.04E+02	1.23E+02	2.13E+01	4.43E+01
U-238	1.77E+02	2.71E+01	3.76E+00	1.30E+01
Np-237	2.85E+03	4.37E+02	1.67E+01	1.75E+00
Pu-239	3.14E+03	4.80E+02	1.66E-01	3.84E-02
Pu-241	6.28E+01	9.59E+00	3.32E-03	7.69E-04
Am-241	3.28E+03	5.02E+02	1.22E+00	1.61E-01

NOTE: Units are rem/y per μCi/L in the irrigation water.

Ingestion doses from consumption of beef or milk are the product of the beef or milk concentration, the quantity consumed, and the ingestion dose factor. The irrigator is assumed to consume 95 kg of contaminated beef and 110 L of contaminated milk each year. The nuclide concentration in the beef or milk is proportional to the daily intake of radioactivity. Equilibrium transfer factors[7,8] are used to relate the rate of intake of a nuclide to the steady-state concentration in beef or milk. The rate of intake of the nuclide depends on the cow's diet.

Both types of cattle are assumed to have the same diet for simplicity. They both drink 55 L of untreated water each day and consume 50 kg of fodder each day. The fodder is assumed to be 75 percent fresh grass and 25 percent stored grain. The concentration of a nuclide in grass is calculated using the "Plant Conc" formula (equation 8) with the leafy vegetable parameters and the following changes: the dry-to-wet ratio is 0.243, the growing period is 30 days, and the grass yield is 1.0 kg/m². The concentration of a nuclide in stored grain is calculated using the "Plant Conc" formula (equation 8) with grain parameters and the following changes: the dry-to-wet ratio is 0.68, the growing period is 30 days, and the grass yield is 1.0 kg/m². Equations 10, 11, and 12 summarize this calculation.

$$\text{Daily Intake} = Cw \cdot Qw + \text{Fresh} \cdot (37.5\ \text{kg/d}) + \text{Stored} \cdot (12.5\ \text{kg/d}) \qquad (10)$$

$$\text{Dose from Beef} = F_{beef} \cdot (\text{Daily Intake}) \cdot Q_{beef} \cdot DF_{ing} \qquad (11)$$

$$\text{Dose from Milk} = F_{milk} \cdot (\text{Daily Intake}) \cdot Q_{milk} \cdot DF_{ing} \qquad (12)$$

where,

Cw = Water concentration, 1 μCi/L.

Qw = Quantity of untreated water (50 L) that is consumed by the cow each day.

Fresh = The concentration of a nuclide in grass consumed by the cow. This is computed using the leafy vegetable parameters. The dry-to-wet ratio, the growing period, and the crop yield are different.

Stored = The concentration of a nuclide in stored grain consumed by the cow. This is computed using the grain parameters. The dry-to-wet ratio, the growing period, and the crop yield are different.

F_{milk} = Equilibrium transfer factor to relate the rate of intake of a radionuclide to the eventual steady-state concentration in milk. It is the ratio of the equilibrium concentration of a nuclide in the milk to the daily intake of the nuclide by the animal. For milk the units are Ci/L(milk) per Ci/day. In practice, the values are tabulated using units of day/L. Values for H-3 and C-14 are taken from Reference 8. Values for the other nuclides are taken from Reference 7.

F_{beef} = Equilibrium transfer factor to relate the rate of intake of a radionuclide to the eventual steady-state concentration in beef. It is the ratio of the equilibrium concentration of a nuclide in the beef to the daily intake by the animal. For beef the units are Ci/kg(beef) per Ci/day. In practice, the values are tabulated using units of day/kg.

DF_{ing} = Dose received from the ingestion of a unit amount of activity.

RESRAD INPUT AND COMPARISON WITH HAND CALCULATIONS

Version 5.41 of the RESRAD program has internal dose factors from Reference 6. Two inhalation solubility classes were changed for these comparisons. Sr-90 was changed from Class Y to Class D, and Ni-59 was changed from elemental vapor to Class D. The ingestion dose factors were left unchanged. The soil-to-plant concentration ratios and the animal transfer factors were changed to be consistent with the hand calculations. For most nuclides, these default RESRAD parameters were reduced.

Doses from an Initial Soil Concentration

For input to RESRAD, the initial soil concentration of each nuclide was entered as 666.7 pCi/g. For a soil density of 1.5 g/cc this is the same as 0.001 Ci/m^3. The soil concentration was reduced by a factor of 1000 because RESRAD reports dose equivalent in units of mrem rather than rem. Reducing the soil concentration by a factor of 1000 gives numeric results that are equivalent to the hand calculations. Two nuclides were not included in the RESRAD calculations. Se-79 is not available in RESRAD, and Pb-210 was not one of the original nuclides selected for comparison.

The soil distribution coefficients used by RESRAD were set to 100 cm^3/g to minimize the migration of contaminants from the surface layer. The emanation constants for carbon were set to zero to keep the C-14 in the surface layer. To eliminate particulate resuspension from soil to foliage, the "Mass loading for foliar deposition" term was set to zero.

The dose results from Version 5.41 of RESRAD were divided by the hand calculation results and are shown in Table 3. The external dose column shows significant departures from the hand calculations. RESRAD overestimates the external dose from the strong gamma-emitting nuclides (Co-60, Cs-137, Ra-226, and Np-237) by about 40 percent. The total dose is affected by the increase also. The RESRAD estimates for weak photon sources range from very close (Pu-241) to zero (Sr-90). The total dose is not affected by these differences because the external dose contributes little to the total dose for weak photon-emitting nuclides. Version 5.60 of RESRAD now uses the external dose rate factors in Reference 5. The hand calculations agree very well with the current version of RESRAD.

The inhalation doses are very close. The small difference is due to the area adjustment factor used in RESRAD. With the garden area set to 20,000 m^2 and the dilution length for airborne dust set to 1.0 m, the area adjustment factor is 0.993, which explains the consistent 0.7 percent difference.

Table 3. RESRAD Doses Divided by Hand Calculations for Contaminated Soil

Nuclide	External	Inhale	Ingest	Total
H-3	Both=0	0.993	0.009	0.009
C-14	RESRAD=0	0.993	1.081	1.080
Co-60	1.381	0.993	0.981	1.381
Ni-59	HandCalc=0	0.993	1.003	1.058
Sr-90	RESRAD=0	0.992	0.997	0.942
Tc-99	0.014	0.993	1.001	0.995
I-129	2.558	0.993	1.000	1.144
Cs-137	1.451	0.993	0.997	1.449
Ra-226	1.314	0.991	0.998	1.313
U-238	0.935	0.993	1.001	0.963
Np-237	1.431	0.993	0.998	1.234
Pu-239	2.590	0.993	0.997	0.994
Pu-241	1.008	0.993	2.4E-05	0.988
Am-241	1.098	0.993	0.999	1.002

The ingestion doses are very close for most nuclides. RESRAD uses special models for H-3 and C-14, which leads to the large differences. The RESRAD Version 5.41 result for Pu-241 is clearly in error. This was corrected in subsequent versions.

Doses from Contaminated Irrigation Water

For input to RESRAD, the soil concentrations were chosen to give a well water concentration of 1000 pCi/L for each nuclide. The soil distribution coefficients for each nuclide were set to zero to maximize the migration of contaminants from the surface layer.

The emanation constants for carbon were set to zero to keep the C-14 in the surface layer. To eliminate particulate resuspension from soil to foliage, the "Mass loading for foliar deposition" was set to zero.

It was necessary to use two sets of soil-to-plant concentration ratios for the benchmark comparisons. The first set was the weighted combination used for vegetables while the second set was constructed based on the different weightings for the cow diet. Since both milk and beef cows consume the same relative amounts of fresh and stored feed, the one table was sufficient for both milk and beef cows. The dose results from RESRAD were divided by the hand calculation results and are shown in Table 4.

Table 4. RESRAD Doses Divided by Hand Calculations for Contaminated Water

Nuclide	Water	Vegetable	Beef	Milk
H-3	1.001	0.121	0.038	0.066
C-14	1.001	0.018	0.029	0.049
Co-60	1.000	0.933	0.557	0.561
Ni-59	1.001	0.932	0.575	0.575
Sr-90	1.000	0.861	0.516	0.517
Tc-99	1.001	0.625	0.403	0.403
I-129	1.000	0.934	0.573	0.573
Cs-137	0.999	0.936	0.571	0.572
Ra-226	1.185	1.122	0.705	0.636
U-238	1.001	0.947	0.578	0.578
Np-237	1.000	0.944	0.575	0.575
Pu-239	1.000	0.948	0.578	0.578
Pu-241	0.086	0.081	0.347	0.198
Am-241	0.999	0.946	0.577	0.577

The doses for water ingestion are in very good agreement with the hand calculations with two exceptions. RESRAD does not allow the activity of parent nuclides in the well water to decay during the year of pumping, but it does allow the daughter nuclides to accumulate. Thus, the dose for Co-60 does not change, while the dose for Ra-226 increases due to the ingrowth of Pb-210. The Pu-241 dose increases from a value five orders of magnitude too small to a value which is a factor of 8 too small by the ingrowth of Am-241. In the current version of RESRAD, this ratio turns out to be 1.086 rather than 0.086.

The doses for the other ingestion pathways show rather consistent differences. The first two nuclides, H-3 and C-14 use special models and should differ. The differences for other nuclides were traced to parameters in RESRAD that cannot be changed by the user. In RESRAD, the plant concentration from direct deposition on foliage is computed using the following unalterable parameters: the length of the growing period, the weathering constant, the interception fraction, the translocation factors, and the crop yield. Different parameters are used for the vegetable garden and the cow fodder. The calculated ratio between the RESRAD method and the hand calculations is 0.948, which is close to the ratios found in the Vegetable column. For the cow fodder, the ratio turns out to be 0.578. The ratios for beef and milk are very similar.

The ratios for Co-60, Sr-90, Tc-99, Ra-226, and Pu-241 differ from the expected ratios. Co-60 is decreased by radioactive decay. Ra-226 is increased by the ingrowth of Pb-210. Both Sr-90 and Tc-99 have significant root uptake contributions in the hand calculations. The hand calculations assume no leaching and the root uptake is calculated at the end of the irrigation season. In the RESRAD calculations, there was leaching, and RESRAD computes root uptake at the end of the growing season. Hence, the root uptake contribution is very small in RESRAD, and the dose ratios are less than expected. The Pu-241 dose is nearly zero, but the ingrowth of Am-241 gives the observed contributions. The current version of RESRAD gives Vegetable, Beef and Milk ratios for Pu-241 of 1.025, 0.923, and 0.776. Thus, the values shown for Pu-241 are based on the amount of Am-241 which has accumulated in the well water.

SUMMARY

Version 5.41 of RESRAD had an error in the calculation of ingestion dose from Pu-241. Since this pathway is typically not the main contributor to the total dose, the total doses should not be significantly affected. Calculations done with Pu-241 and earlier versions of RESRAD do not need to be redone. Since this error has been corrected, one can easily check for changes by using the current version of RESRAD on older input data.

Version 5.41 of RESRAD tended to overestimate external doses from strong gamma emitters by about 40 percent. Version 5.60 of RESRAD adopted an improved model for external dose calculations. Details of the comparisons of all three computer programs with the hand calculations are available in draft form.[9]

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